



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:28 AM UTC

PDB ID : 4J9U / pdb_00004j9u
Title : Crystal Structure of the TrkH/TrkA potassium transport complex
Authors : Cao, Y.; Jin, X.; Huang, H.; Levin, E.J.; Zhou, M.; New York Consortium on Membrane Protein Structure (NYCOMPS)
Deposited on : 2013-02-17
Resolution : 3.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

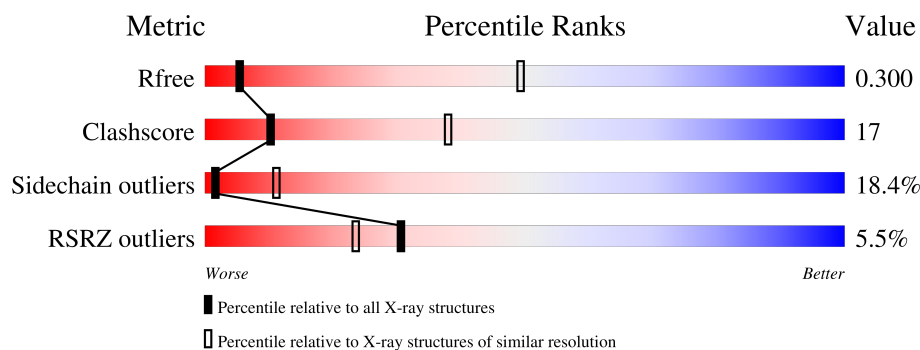
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1065 (3.96-3.64)
Clashscore	190562	1012 (3.94-3.66)
Sidechain outliers	187428	1043 (3.96-3.64)
RSRZ outliers	180081	1064 (3.96-3.64)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	485	
1	B	485	
1	C	485	
1	D	485	
2	E	458	
2	F	458	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	G	458	
2	H	458	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	TBR	A	501	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 28567 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

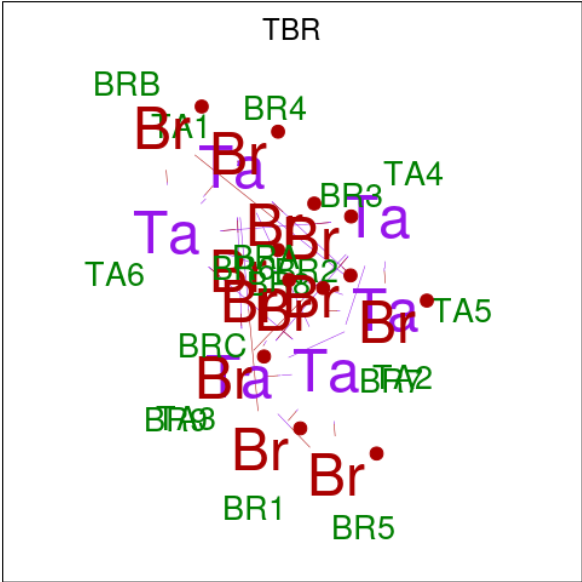
- Molecule 1 is a protein called Trk system potassium uptake protein TrkH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	462	Total	C	N	O	S	0	0	0
			3569	2389	564	598	18			
1	B	462	Total	C	N	O	S	0	0	0
			3569	2389	564	598	18			
1	C	462	Total	C	N	O	S	0	0	0
			3569	2389	564	598	18			
1	D	462	Total	C	N	O	S	0	0	0
			3569	2389	564	598	18			

- Molecule 2 is a protein called Potassium uptake protein TrkA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	451	Total	C	N	O	S	0	0	0
			3454	2162	611	669	12			
2	F	444	Total	C	N	O	S	0	0	0
			3410	2138	600	660	12			
2	G	452	Total	C	N	O	S	0	0	0
			3468	2174	612	670	12			
2	H	450	Total	C	N	O	S	0	0	0
			3455	2165	610	668	12			

- Molecule 3 is HEXATANTALUM DODECABROMIDE (CCD ID: TBR) (formula: Br₁₂Ta₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Br	Ta	0	0
			18	12	6		
3	A	1	Total	Br	Ta	0	0
			18	12	6		
3	A	1	Total	Br	Ta	0	0
			18	12	6		
3	B	1	Total	Br	Ta	0	0
			18	12	6		
3	B	1	Total	Br	Ta	0	0
			18	12	6		
3	C	1	Total	Br	Ta	0	0
			18	12	6		
3	C	1	Total	Br	Ta	0	0
			18	12	6		
3	D	1	Total	Br	Ta	0	0
			18	12	6		
3	D	1	Total	Br	Ta	0	0
			18	12	6		
3	D	1	Total	Br	Ta	0	0
			18	12	6		
3	E	1	Total	Br	Ta	0	0
			18	12	6		
3	E	1	Total	Br	Ta	0	0
			18	12	6		
3	F	1	Total	Br	Ta	0	0
			18	12	6		
3	F	1	Total	Br	Ta	0	0
			18	12	6		

Continued on next page...

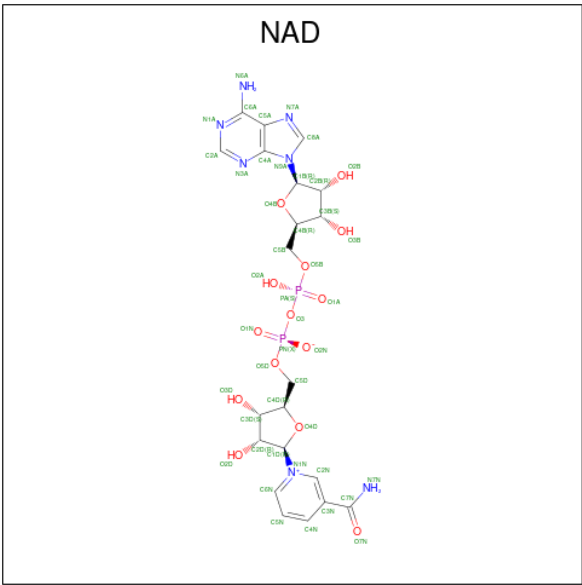
Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	G	1	Total	Br	Ta	0	0
			18	12	6		
3	G	1	Total	Br	Ta	0	0
			18	12	6		
3	H	1	Total	Br	Ta	0	0
			18	12	6		
3	H	1	Total	Br	Ta	0	0
			18	12	6		

- Molecule 4 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	K	0	0
			1	1		
4	B	1	Total	K	0	0
			1	1		
4	C	1	Total	K	0	0
			1	1		
4	D	1	Total	K	0	0
			1	1		

- Molecule 5 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	E	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

Continued on next page...

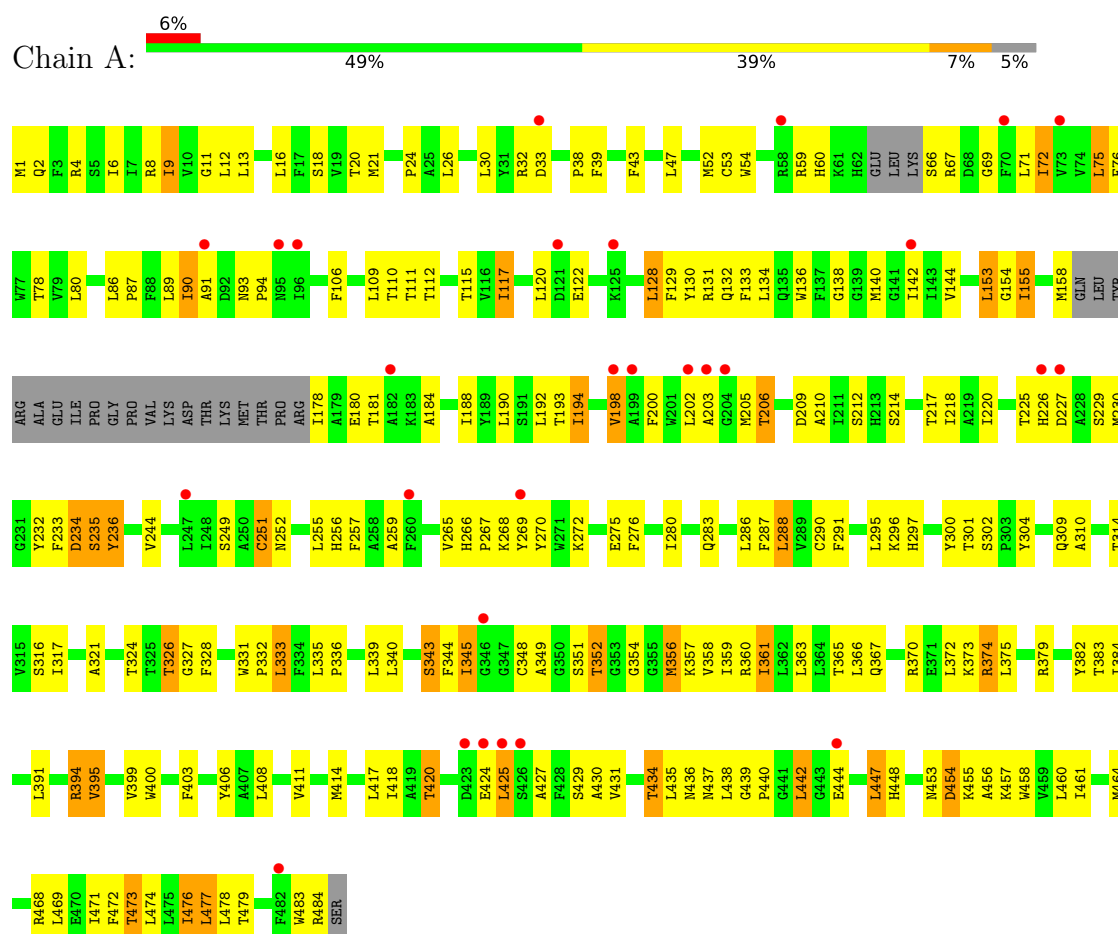
Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	F	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
5	G	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
5	H	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

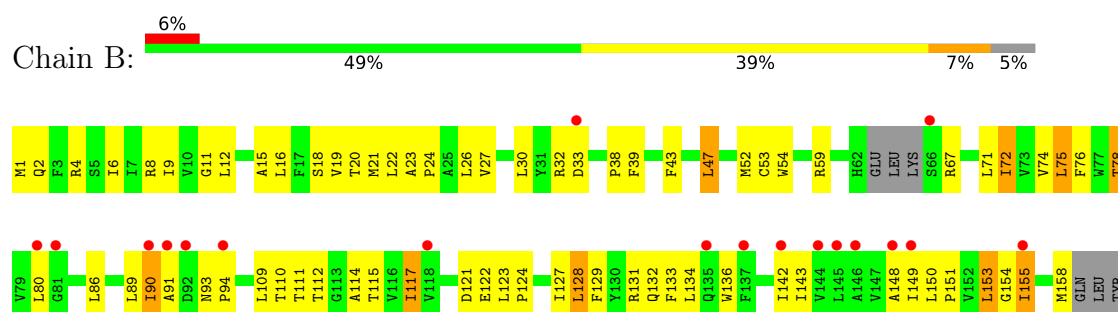
3 Residue-property plots [i](#)

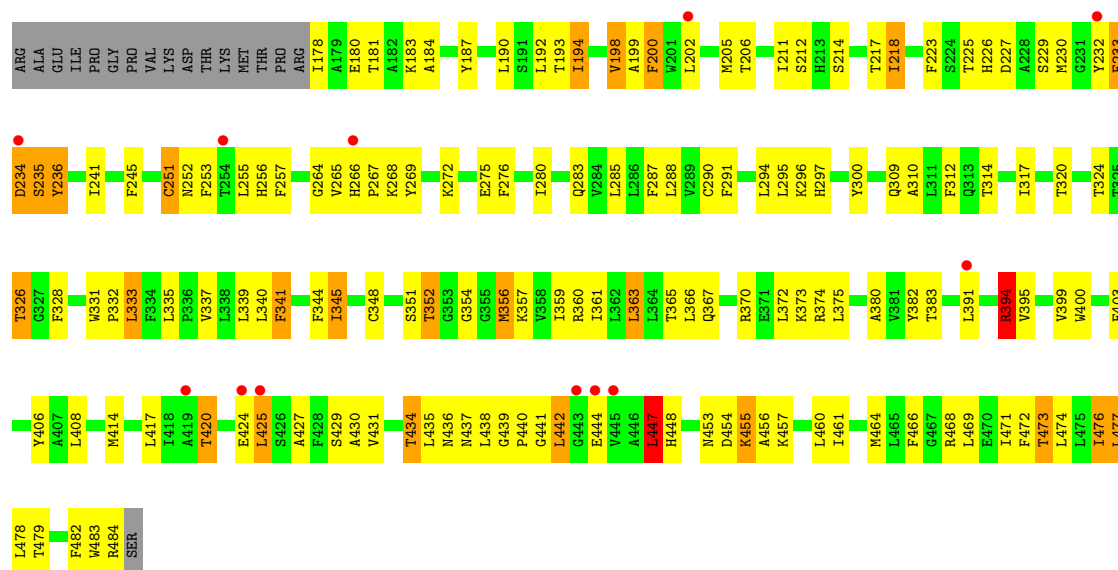
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Trk system potassium uptake protein TrkH

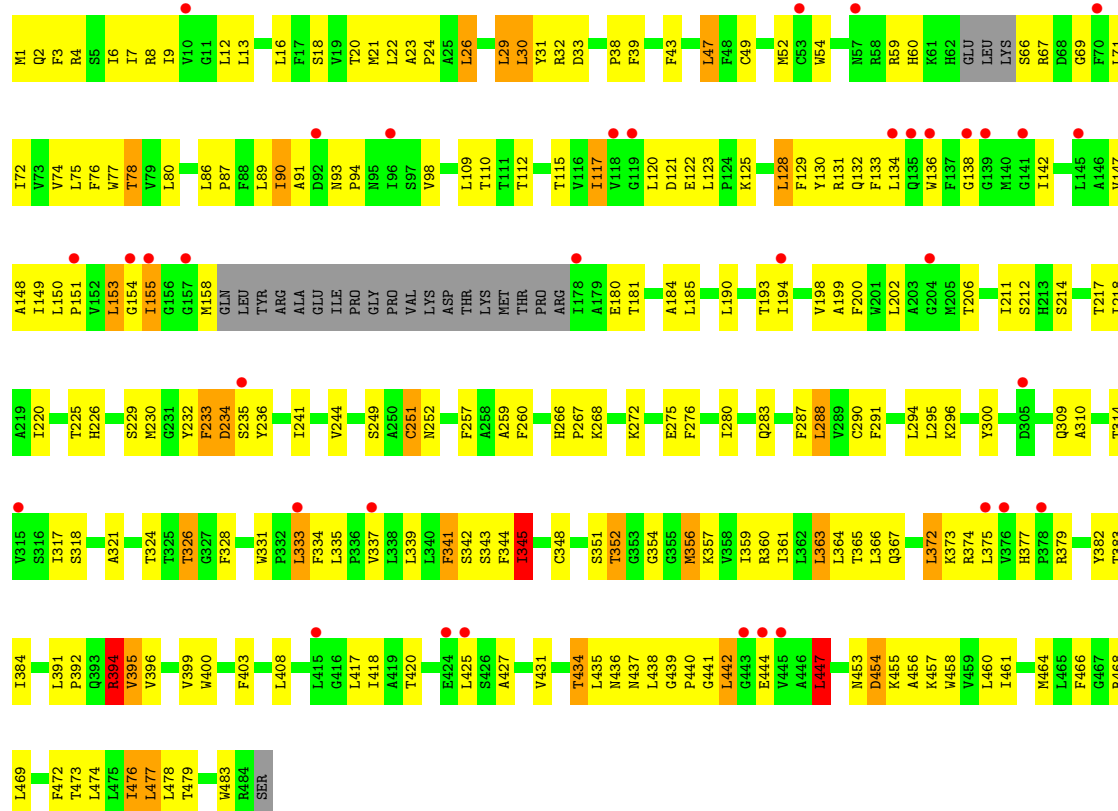


- Molecule 1: Trk system potassium uptake protein TrkH



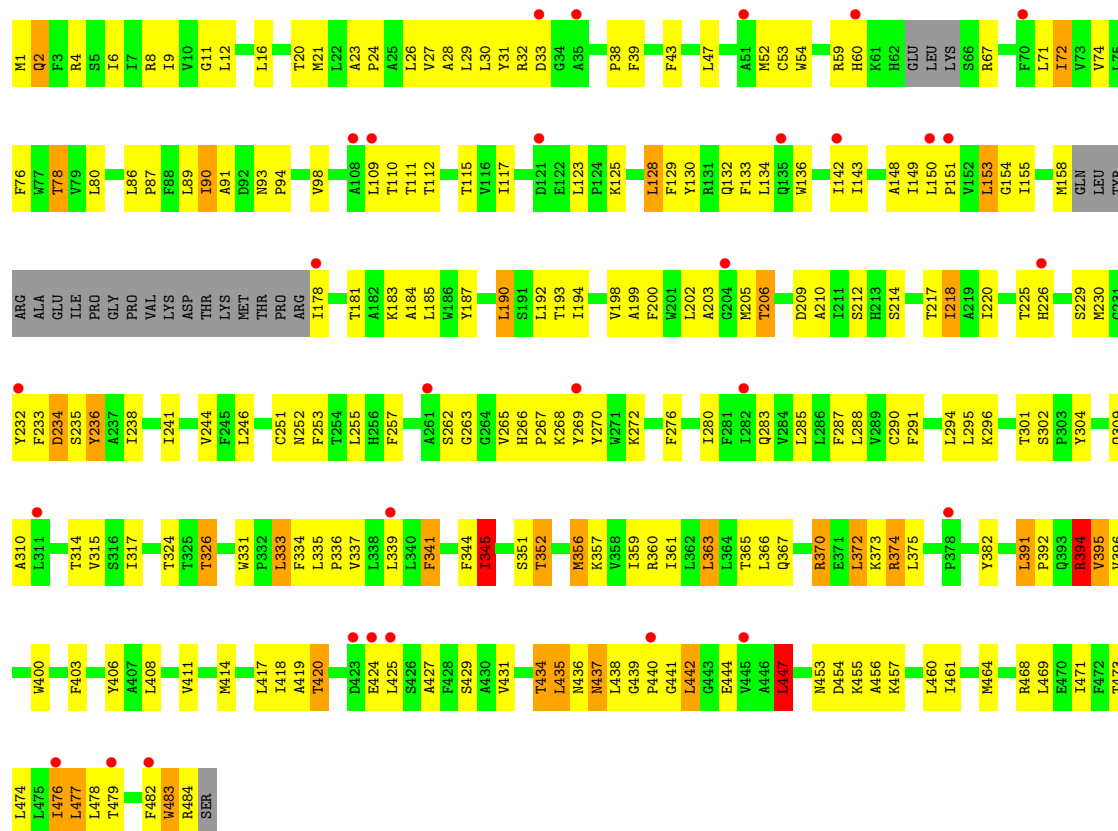


• Molecule 1: Trk system potassium uptake protein TrkH

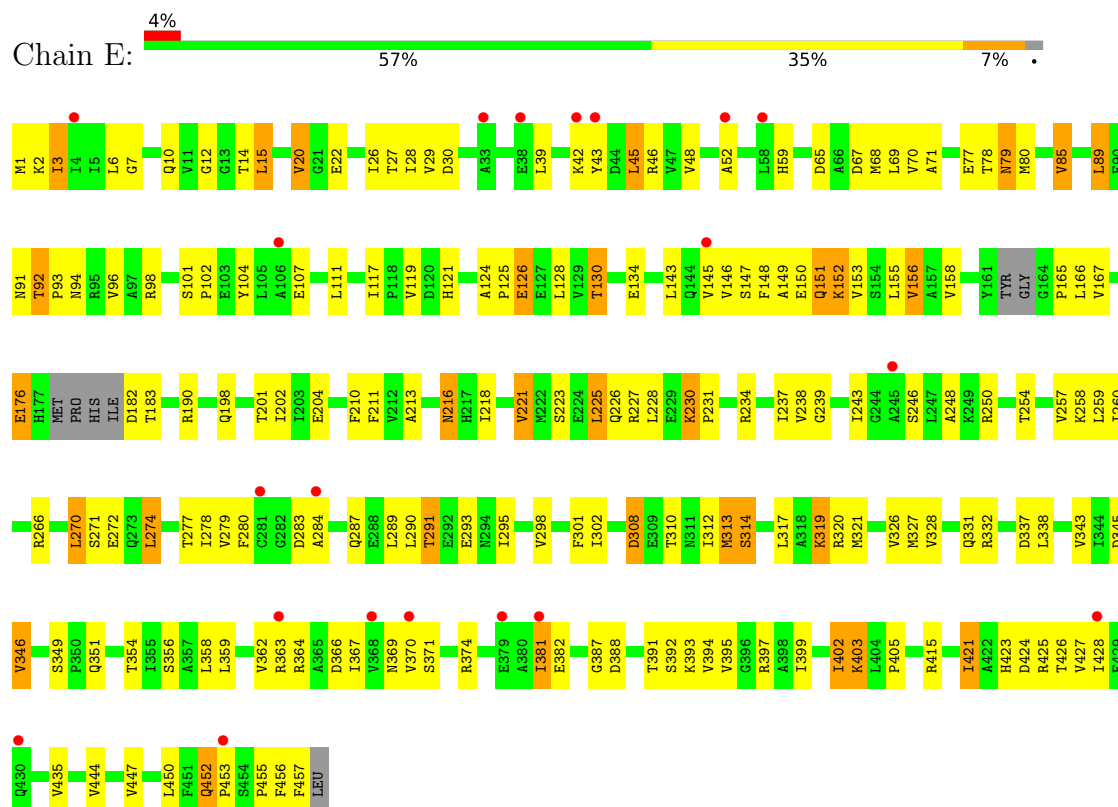


• Molecule 1: Trk system potassium uptake protein TrkH

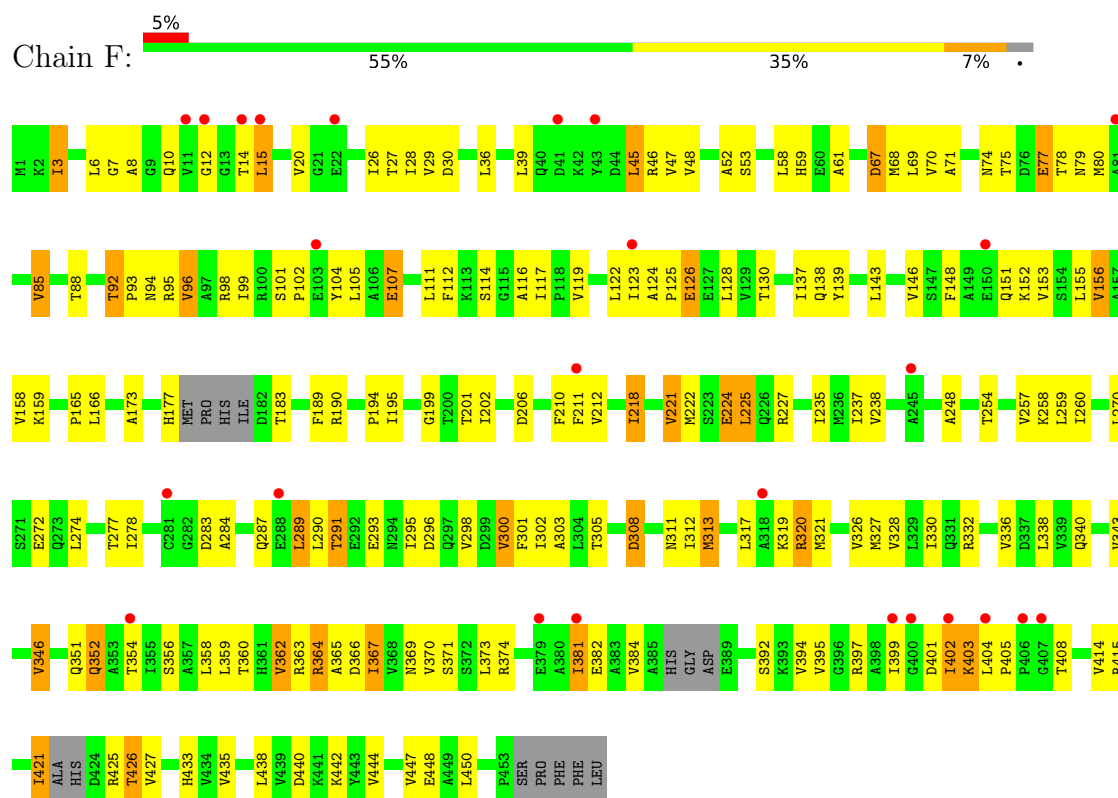




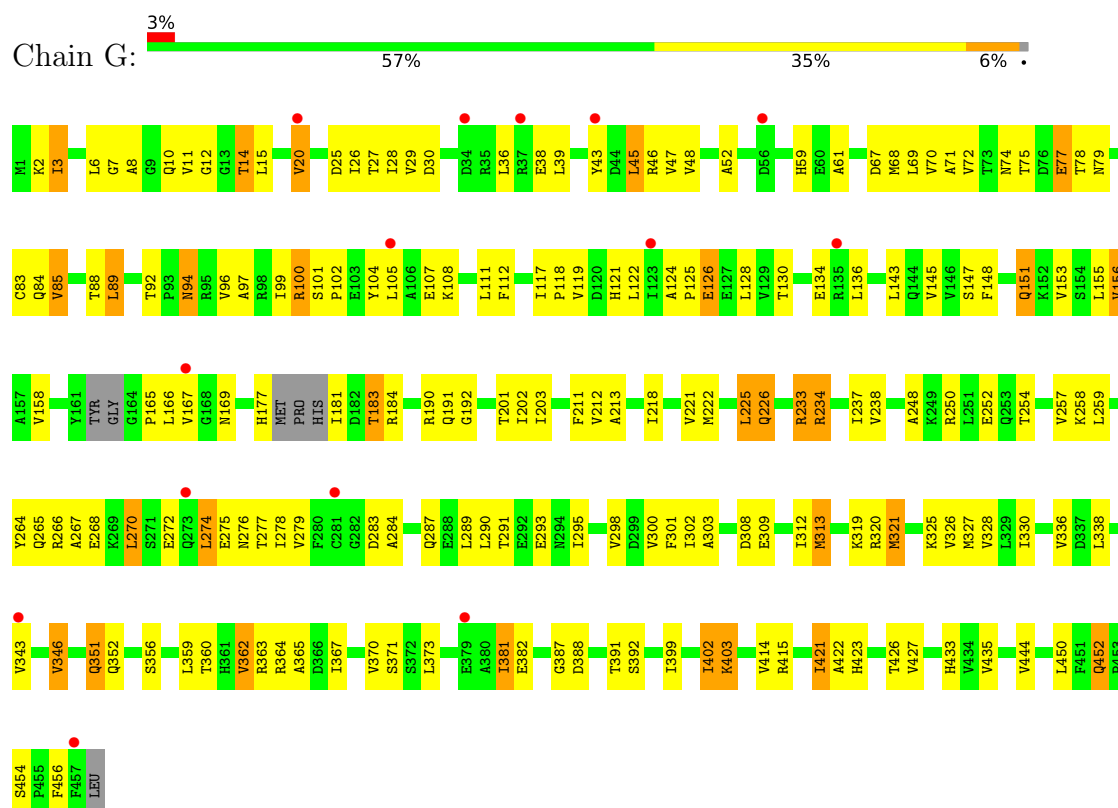
• Molecule 2: Potassium uptake protein TrkA



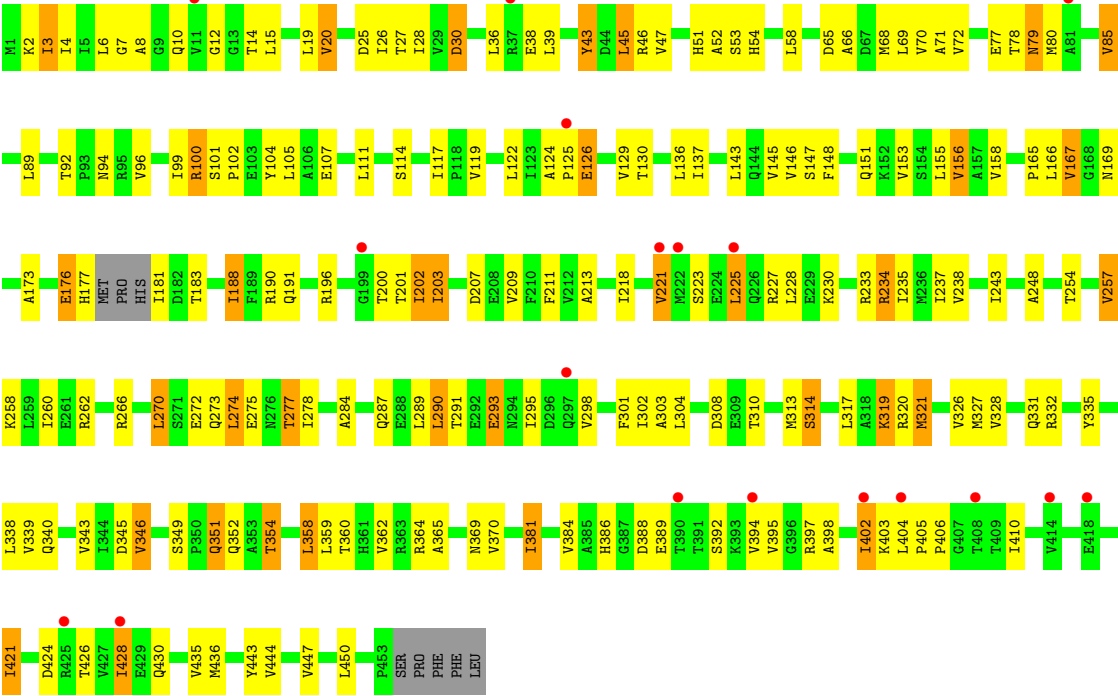
• Molecule 2: Potassium uptake protein TrkA



• Molecule 2: Potassium uptake protein TrkA



• Molecule 2: Potassium uptake protein TrkA



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	133.72Å 146.63Å 163.67Å 90.00° 99.32° 90.00°	Depositor
Resolution (Å)	49.79 – 3.80 49.79 – 3.80	Depositor EDS
% Data completeness (in resolution range)	99.5 (49.79-3.80) 99.5 (49.79-3.80)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.52 (at 3.77Å)	Xtrriage
Refinement program	PHENIX 1.8.1_1168	Depositor
R, R_{free}	0.232 , 0.280 0.258 , 0.300	Depositor DCC
R_{free} test set	3130 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	118.3	Xtrriage
Anisotropy	0.337	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 85.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	28567	wwPDB-VP
Average B, all atoms (Å ²)	89.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 20.89 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.8858e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NAD, TBR, K

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.40	0/3670	0.90	6/5000 (0.1%)
1	B	0.39	0/3670	0.94	12/5000 (0.2%)
1	C	0.39	0/3670	0.91	9/5000 (0.2%)
1	D	0.38	0/3670	0.90	8/5000 (0.2%)
2	E	0.36	0/3498	0.91	8/4743 (0.2%)
2	F	0.36	0/3451	0.91	5/4676 (0.1%)
2	G	0.36	0/3513	0.89	5/4763 (0.1%)
2	H	0.38	0/3500	0.94	14/4746 (0.3%)
All	All	0.38	0/28642	0.91	67/38928 (0.2%)

There are no bond length outliers.

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	27	VAL	N-CA-C	-9.37	104.20	113.20
1	A	447	LEU	N-CA-C	8.19	121.32	111.82
1	D	394	ARG	N-CA-C	-7.65	104.85	114.56
1	A	155	ILE	N-CA-C	-7.64	105.24	111.81
1	D	27	VAL	N-CA-C	-7.58	105.93	113.20
1	B	394	ARG	N-CA-C	-7.46	105.08	114.56
2	H	230	LYS	CA-C-N	7.41	127.46	119.90
2	H	230	LYS	C-N-CA	7.41	127.46	119.90
1	B	155	ILE	N-CA-C	-7.05	104.97	111.67
1	B	264	GLY	N-CA-C	-6.94	102.96	114.48
2	H	203	ILE	N-CA-C	6.93	118.55	107.73
1	C	211	ILE	N-CA-C	-6.93	105.00	111.45
2	E	230	LYS	CA-C-N	6.85	126.89	119.90
2	E	230	LYS	C-N-CA	6.85	126.89	119.90
2	F	394	VAL	N-CA-C	6.75	118.08	111.67
1	C	394	ARG	N-CA-C	-6.73	106.01	114.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	447	LEU	N-CA-C	6.62	119.50	111.82
1	D	447	LEU	N-CA-C	6.46	119.14	111.71
2	E	452	GLN	CA-C-N	6.44	127.89	119.84
2	E	452	GLN	C-N-CA	6.44	127.89	119.84
1	C	345	ILE	CB-CA-C	-6.41	104.16	111.59
1	D	345	ILE	CB-CA-C	-6.39	103.59	111.32
1	B	345	ILE	CB-CA-C	-6.31	104.27	111.59
1	A	394	ARG	N-CA-C	-6.23	106.28	114.31
2	E	30	ASP	N-CA-C	6.19	118.71	108.99
1	C	23	ALA	CA-C-N	-6.10	113.66	121.04
1	C	23	ALA	C-N-CA	-6.10	113.66	121.04
1	B	251	CYS	N-CA-C	6.05	118.67	107.60
1	C	251	CYS	N-CA-C	6.02	118.62	107.60
1	A	251	CYS	N-CA-C	5.88	118.35	107.60
1	B	211	ILE	N-CA-C	-5.86	106.00	111.45
2	H	227	ARG	N-CA-C	5.86	118.91	109.83
2	G	351	GLN	N-CA-C	-5.85	105.81	113.12
1	A	203	ALA	N-CA-C	-5.81	105.78	112.92
2	H	43	TYR	N-CA-C	5.78	120.03	112.92
2	G	183	THR	N-CA-C	5.73	118.54	110.23
2	F	30	ASP	N-CA-C	5.70	117.94	108.99
1	D	203	ALA	N-CA-C	-5.68	105.94	112.92
1	D	23	ALA	CA-C-N	-5.68	114.17	121.04
1	D	23	ALA	C-N-CA	-5.68	114.17	121.04
2	E	92	THR	CA-C-N	5.64	126.89	119.84
2	E	92	THR	C-N-CA	5.64	126.89	119.84
2	H	200	THR	N-CA-C	5.59	118.03	110.88
1	C	260	PHE	N-CA-C	5.58	117.44	111.36
1	C	447	LEU	N-CA-C	5.49	118.19	111.82
2	F	92	THR	CA-C-N	5.48	126.69	119.84
2	F	92	THR	C-N-CA	5.48	126.69	119.84
2	G	399	ILE	N-CA-C	5.47	115.67	110.42
2	G	226	GLN	N-CA-C	5.43	119.39	112.12
2	H	196	ARG	CA-C-N	5.37	126.55	119.84
2	H	196	ARG	C-N-CA	5.37	126.55	119.84
1	B	23	ALA	CA-C-N	-5.33	114.59	121.04
1	B	23	ALA	C-N-CA	-5.33	114.59	121.04
2	H	257	VAL	N-CA-C	5.29	115.73	108.12
1	D	2	GLN	N-CA-C	5.27	117.61	111.02
2	H	351	GLN	N-CA-C	-5.27	106.53	113.12
2	H	92	THR	CA-C-N	5.25	126.40	119.84
2	H	92	THR	C-N-CA	5.25	126.40	119.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	30	ASP	N-CA-C	5.22	117.18	108.99
1	A	448	HIS	N-CA-C	5.22	117.25	108.96
1	B	448	HIS	N-CA-C	5.17	116.74	108.41
2	F	199	GLY	N-CA-C	5.10	120.52	113.99
1	B	455	LYS	N-CA-C	-5.08	105.64	111.07
2	H	202	ILE	N-CA-C	5.08	115.59	108.89
2	E	456	PHE	N-CA-C	5.03	121.52	110.80
1	C	29	LEU	N-CA-C	-5.00	107.83	114.04
2	G	30	ASP	N-CA-C	5.00	116.84	108.99

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3569	0	3638	149	0
1	B	3569	0	3638	136	0
1	C	3569	0	3638	136	0
1	D	3569	0	3638	135	0
2	E	3454	0	3489	110	0
2	F	3410	0	3458	118	0
2	G	3468	0	3507	119	0
2	H	3455	0	3497	112	0
3	A	54	0	0	0	0
3	B	36	0	0	0	0
3	C	36	0	0	1	0
3	D	54	0	0	2	0
3	E	36	0	0	3	0
3	F	36	0	0	2	0
3	G	36	0	0	3	0
3	H	36	0	0	3	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	44	0	26	6	0
5	F	44	0	26	3	0
5	G	44	0	26	5	0
5	H	44	0	26	5	0
All	All	28567	0	28607	980	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 17.

All (980) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:420:THR:HG21	1:B:456:ALA:HB2	1.50	0.94
2:F:3:ILE:HG22	2:F:68:MET:HB3	1.59	0.85
1:A:420:THR:HG21	1:A:456:ALA:HB2	1.58	0.85
1:B:132:GLN:HG3	1:B:212:SER:HB2	1.57	0.84
1:D:420:THR:HG21	1:D:456:ALA:HB2	1.60	0.83
2:E:96:VAL:HG12	2:E:121:HIS:HB2	1.63	0.81
2:E:3:ILE:HG22	2:E:68:MET:HB3	1.62	0.80
1:C:132:GLN:HG3	1:C:212:SER:HB2	1.64	0.80
2:E:77:GLU:HG3	2:H:78:THR:HG22	1.62	0.80
1:A:132:GLN:HG3	1:A:212:SER:HB2	1.62	0.79
1:D:132:GLN:HG3	1:D:212:SER:HB2	1.64	0.79
1:C:181:THR:HA	1:C:184:ALA:HB3	1.63	0.79
1:B:136:TRP:HE1	1:B:193:THR:HG21	1.48	0.79
1:A:136:TRP:HE1	1:A:193:THR:HG21	1.47	0.79
2:E:190:ARG:NH2	2:E:202:ILE:O	2.16	0.78
2:E:455:PRO:O	2:E:457:PHE:N	2.16	0.78
2:G:20:VAL:HG23	2:G:26:ILE:HD12	1.64	0.78
2:G:364:ARG:HG3	2:G:365:ALA:H	1.49	0.78
1:A:112:THR:HA	1:A:437:ASN:HB3	1.65	0.77
2:F:77:GLU:HG3	2:G:78:THR:HG22	1.64	0.77
2:E:78:THR:HG22	2:H:77:GLU:HG3	1.67	0.77
1:D:136:TRP:HE1	1:D:193:THR:HG21	1.49	0.76
2:F:78:THR:HG22	2:G:77:GLU:HG3	1.66	0.76
2:H:169:ASN:HB2	2:H:203:ILE:HG12	1.68	0.76
2:H:237:ILE:HG22	2:H:302:ILE:HB	1.68	0.75
2:F:190:ARG:NH2	2:F:202:ILE:O	2.19	0.75
1:C:268:LYS:HE3	1:C:272:LYS:HE3	1.68	0.74
2:E:363:ARG:HB2	2:E:367:ILE:HD11	1.68	0.74
2:H:20:VAL:HG23	2:H:26:ILE:HD12	1.69	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:LYS:HE3	1:A:272:LYS:HE3	1.68	0.74
1:D:181:THR:HA	1:D:184:ALA:HB3	1.69	0.74
1:C:356:MET:HE1	1:C:403:PHE:HD1	1.52	0.74
2:E:176:GLU:OE2	2:E:182:ASP:N	2.21	0.73
2:G:3:ILE:HG22	2:G:68:MET:HB3	1.69	0.73
1:B:268:LYS:HE3	1:B:272:LYS:HE3	1.71	0.73
1:D:24:PRO:HB3	1:D:129:PHE:HD2	1.54	0.72
2:G:96:VAL:HG12	2:G:121:HIS:HB2	1.69	0.72
2:E:6:LEU:HB2	2:E:71:ALA:HA	1.69	0.72
2:F:6:LEU:HD22	2:F:52:ALA:HB1	1.72	0.71
2:H:3:ILE:HG22	2:H:68:MET:HB3	1.70	0.71
2:E:20:VAL:HG23	2:E:26:ILE:HD12	1.73	0.71
1:D:356:MET:HE1	1:D:403:PHE:HD1	1.55	0.70
2:G:156:VAL:HG12	2:G:211:PHE:HB2	1.71	0.70
2:H:156:VAL:HG12	2:H:211:PHE:HB2	1.71	0.70
2:F:237:ILE:HG22	2:F:302:ILE:HB	1.72	0.70
1:B:441:GLY:HA3	1:B:447:LEU:HA	1.74	0.70
2:H:284:ALA:H	5:H:501:NAD:H61A	1.37	0.70
2:G:10:GLN:NE2	2:G:74:ASN:OD1	2.23	0.70
2:E:301:PHE:HB3	2:E:326:VAL:HG12	1.72	0.69
1:C:440:PRO:HB2	1:C:442:LEU:HD23	1.74	0.69
2:E:284:ALA:H	5:E:501:NAD:H61A	1.39	0.69
2:G:370:VAL:HG23	2:G:381:ILE:HG22	1.74	0.69
2:G:177:HIS:HA	2:G:181:ILE:HB	1.73	0.69
2:H:143:LEU:HD13	2:H:158:VAL:HA	1.72	0.69
1:C:24:PRO:HB3	1:C:129:PHE:HD2	1.58	0.69
1:C:93:ASN:HB2	1:C:94:PRO:HD3	1.75	0.69
2:E:15:LEU:HD11	2:E:358:LEU:HG	1.72	0.69
2:G:100:ARG:NH2	5:G:501:NAD:O7N	2.26	0.69
2:G:388:ASP:HB2	2:G:391:THR:HG22	1.74	0.69
1:A:214:SER:HA	1:A:217:THR:HG22	1.75	0.69
2:H:20:VAL:HG11	2:H:43:TYR:HB3	1.74	0.69
1:B:214:SER:HA	1:B:217:THR:HG22	1.75	0.68
1:D:214:SER:HA	1:D:217:THR:HG22	1.72	0.68
1:B:265:VAL:HG13	1:B:269:TYR:HE2	1.57	0.68
2:F:352:GLN:NE2	2:F:373:LEU:O	2.26	0.68
1:A:290:CYS:HA	1:A:335:LEU:HD11	1.76	0.68
1:C:214:SER:HA	1:C:217:THR:HG22	1.76	0.68
1:A:136:TRP:NE1	1:A:193:THR:HG21	2.08	0.68
1:D:93:ASN:HB2	1:D:94:PRO:HD3	1.75	0.67
1:A:128:LEU:HD11	1:A:225:THR:HA	1.77	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:128:LEU:HD11	1:B:225:THR:HA	1.75	0.67
2:E:22:GLU:OE2	2:E:363:ARG:NH1	2.28	0.67
1:B:356:MET:HE1	1:B:403:PHE:HD1	1.60	0.67
1:C:420:THR:HG21	1:C:456:ALA:HB2	1.75	0.67
2:H:100:ARG:NH2	5:H:501:NAD:O7N	2.28	0.67
1:B:93:ASN:HB2	1:B:94:PRO:HD3	1.77	0.67
1:A:24:PRO:HB3	1:A:129:PHE:HD2	1.60	0.67
2:G:415:ARG:NH2	2:G:427:VAL:O	2.27	0.67
2:H:6:LEU:HB2	2:H:71:ALA:HA	1.78	0.66
1:B:114:ALA:HB2	1:B:439:GLY:HA2	1.78	0.66
1:D:110:THR:O	1:D:468:ARG:NH1	2.28	0.66
1:D:438:LEU:HB2	1:D:439:GLY:HA2	1.77	0.66
1:B:136:TRP:NE1	1:B:193:THR:HG21	2.11	0.66
1:D:205:MET:HB2	1:D:210:ALA:HB2	1.78	0.66
2:E:6:LEU:HD22	2:E:52:ALA:HB1	1.78	0.66
2:E:387:GLY:HA3	2:E:392:SER:HB2	1.78	0.65
2:F:27:THR:HG22	2:F:46:ARG:HB3	1.79	0.65
2:H:233:ARG:HH22	2:H:234:ARG:HH21	1.44	0.65
2:H:332:ARG:HG3	3:H:503:TBR:BR2	2.51	0.65
1:A:379:ARG:HD3	2:G:289:LEU:HD13	1.79	0.65
1:C:230:MET:SD	1:C:232:TYR:OH	2.53	0.65
1:C:112:THR:HA	1:C:437:ASN:HB3	1.79	0.65
1:C:391:LEU:HD12	1:C:395:VAL:HG11	1.79	0.65
2:G:6:LEU:HD22	2:G:52:ALA:HB1	1.79	0.65
2:H:183:THR:HB	2:H:213:ALA:HB2	1.79	0.65
1:B:24:PRO:HB3	1:B:129:PHE:HD2	1.62	0.64
2:F:258:LYS:HG2	2:F:278:ILE:HD11	1.79	0.64
2:G:8:ALA:HA	2:G:28:ILE:HD11	1.78	0.64
2:H:238:VAL:HG12	2:H:260:ILE:HB	1.79	0.64
1:D:440:PRO:HB2	1:D:442:LEU:HD23	1.78	0.64
2:H:27:THR:HG22	2:H:46:ARG:HB3	1.80	0.64
1:C:112:THR:HG23	1:C:437:ASN:HA	1.79	0.64
1:D:136:TRP:NE1	1:D:193:THR:HG21	2.11	0.64
2:E:370:VAL:HG23	2:E:381:ILE:HG22	1.79	0.64
2:G:6:LEU:HB2	2:G:71:ALA:HA	1.78	0.64
1:D:206:THR:HG23	1:D:209:ASP:HB2	1.80	0.64
1:A:93:ASN:HB2	1:A:94:PRO:HD3	1.80	0.64
2:G:295:ILE:HD12	2:G:298:VAL:HG11	1.80	0.64
2:H:145:VAL:HG22	2:H:156:VAL:HG23	1.80	0.64
2:F:284:ALA:H	5:F:501:NAD:H61A	1.45	0.64
2:E:327:MET:HG2	2:E:346:VAL:HG13	1.79	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:ASN:H	1:A:351:SER:HB3	1.63	0.63
2:H:129:VAL:HG11	2:H:243:ILE:HD13	1.81	0.63
2:E:156:VAL:HG12	2:E:211:PHE:HB2	1.80	0.63
2:H:370:VAL:HG23	2:H:381:ILE:HG22	1.81	0.63
1:A:234:ASP:OD2	1:A:234:ASP:N	2.31	0.63
1:A:354:GLY:HA2	1:A:357:LYS:HE3	1.81	0.63
2:F:364:ARG:HG3	2:F:365:ALA:H	1.64	0.63
1:A:440:PRO:HB2	1:A:442:LEU:HD23	1.81	0.63
1:A:38:PRO:HB3	1:A:90:ILE:HG23	1.81	0.62
1:C:287:PHE:HA	1:C:314:THR:HG21	1.81	0.62
2:F:107:GLU:HG3	2:G:89:LEU:HD11	1.81	0.62
2:H:99:ILE:HG13	2:H:122:LEU:HD23	1.80	0.62
2:H:15:LEU:HD11	2:H:358:LEU:HG	1.82	0.62
2:G:237:ILE:HG22	2:G:302:ILE:HB	1.81	0.62
2:H:68:MET:HG3	2:H:94:ASN:HB3	1.81	0.62
1:A:180:GLU:HG3	1:A:181:THR:HG23	1.80	0.62
2:G:258:LYS:HG2	2:G:278:ILE:HD11	1.82	0.62
2:F:221:VAL:HG13	2:F:225:LEU:HD23	1.81	0.62
1:A:38:PRO:HG2	1:A:91:ALA:HB2	1.81	0.62
1:A:206:THR:HG23	1:A:209:ASP:HB2	1.82	0.62
2:F:235:ILE:HB	2:F:257:VAL:HG22	1.82	0.62
2:G:20:VAL:HG11	2:G:43:TYR:HB3	1.81	0.62
1:B:420:THR:O	1:B:453:ASN:ND2	2.33	0.62
1:C:417:LEU:O	1:C:420:THR:HG22	1.99	0.62
2:G:14:THR:HG23	3:G:503:TBR:BRB	2.55	0.61
3:D:501:TBR:BRB	2:E:42:LYS:HA	2.55	0.61
1:D:453:ASN:OD1	1:D:454:ASP:N	2.34	0.61
2:H:77:GLU:HA	2:H:80:MET:HE2	1.82	0.61
1:D:2:GLN:HA	1:D:4:ARG:HH11	1.63	0.61
2:F:397:ARG:HB3	2:F:401:ASP:HB3	1.83	0.61
2:H:221:VAL:HG13	2:H:225:LEU:HD23	1.82	0.61
1:D:24:PRO:HB2	1:D:39:PHE:HE1	1.66	0.61
2:E:134:GLU:OE2	2:E:250:ARG:NH1	2.34	0.61
2:E:182:ASP:HB2	2:E:421:ILE:HD11	1.83	0.61
1:A:344:PHE:HA	1:A:436:ASN:OD1	2.00	0.61
1:B:38:PRO:HB3	1:B:90:ILE:HG23	1.83	0.61
1:B:234:ASP:OD2	1:B:234:ASP:N	2.34	0.61
2:F:70:VAL:HA	2:F:96:VAL:HG23	1.81	0.61
2:E:237:ILE:HG22	2:E:302:ILE:HB	1.81	0.61
2:H:364:ARG:HG3	2:H:365:ALA:H	1.66	0.61
1:D:287:PHE:HA	1:D:314:THR:HG21	1.83	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:ILE:HG13	1:A:120:LEU:HD23	1.83	0.60
1:A:438:LEU:HB2	1:A:439:GLY:HA2	1.83	0.60
1:B:484:ARG:HG3	2:G:234:ARG:HH12	1.65	0.60
2:G:27:THR:HG22	2:G:46:ARG:HB3	1.83	0.60
1:C:136:TRP:NE1	1:C:193:THR:HG21	2.16	0.60
1:C:252:ASN:H	1:C:351:SER:HB3	1.67	0.60
2:F:392:SER:HB3	2:F:395:VAL:HG22	1.83	0.60
1:B:180:GLU:HG3	1:B:181:THR:HG23	1.83	0.60
1:C:110:THR:O	1:C:468:ARG:NH1	2.34	0.60
1:D:252:ASN:H	1:D:351:SER:HB3	1.66	0.59
2:F:301:PHE:HB3	2:F:326:VAL:HG12	1.83	0.59
1:B:109:LEU:HD13	1:B:134:LEU:HD22	1.85	0.59
2:F:238:VAL:HG12	2:F:260:ILE:HB	1.85	0.59
1:B:420:THR:OG1	1:B:455:LYS:HB2	2.03	0.59
1:D:265:VAL:HG13	1:D:269:TYR:HE2	1.67	0.59
1:D:344:PHE:HA	1:D:436:ASN:OD1	2.03	0.59
2:E:146:VAL:HG13	2:E:155:LEU:HB3	1.85	0.59
1:C:150:LEU:HD11	3:C:502:TBR:BR5	2.58	0.59
1:D:469:LEU:HD12	1:D:474:LEU:HD12	1.85	0.59
2:G:287:GLN:HB3	2:G:321:MET:HE1	1.85	0.59
2:F:153:VAL:HG11	2:F:435:VAL:HG21	1.85	0.59
2:H:188:ILE:HG23	2:H:209:VAL:HG22	1.84	0.59
1:B:153:LEU:HD13	1:B:154:GLY:H	1.68	0.58
2:H:258:LYS:HG2	2:H:278:ILE:HD11	1.85	0.58
2:F:6:LEU:HB2	2:F:71:ALA:HA	1.85	0.58
2:F:415:ARG:NH2	2:F:427:VAL:O	2.34	0.58
1:C:290:CYS:HA	1:C:335:LEU:HD11	1.85	0.58
1:C:372:LEU:HG	1:D:476:ILE:HG22	1.84	0.58
2:G:301:PHE:HB3	2:G:326:VAL:HG12	1.84	0.58
2:H:310:THR:O	2:H:314:SER:HB3	2.02	0.58
1:D:112:THR:HA	1:D:437:ASN:HB3	1.84	0.58
1:A:453:ASN:OD1	1:A:454:ASP:N	2.36	0.58
1:D:290:CYS:HA	1:D:335:LEU:HD11	1.84	0.58
2:E:148:PHE:HB2	2:E:153:VAL:HG13	1.86	0.58
1:C:469:LEU:HD12	1:C:474:LEU:HD12	1.86	0.58
2:F:68:MET:HG3	2:F:94:ASN:HB3	1.86	0.58
2:F:126:GLU:O	2:F:130:THR:HG23	2.04	0.58
1:B:290:CYS:HA	1:B:335:LEU:HD11	1.85	0.58
1:C:8:ARG:HD3	1:C:59:ARG:H	1.69	0.58
1:C:377:HIS:ND1	2:F:293:GLU:OE2	2.27	0.58
1:B:344:PHE:HA	1:B:436:ASN:OD1	2.04	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:136:TRP:HE1	1:C:193:THR:HG21	1.69	0.57
1:C:234:ASP:N	1:C:234:ASP:OD2	2.37	0.57
1:D:236:TYR:H	1:D:236:TYR:HD2	1.51	0.57
2:G:364:ARG:HG3	2:G:365:ALA:N	2.18	0.57
1:B:112:THR:HA	1:B:437:ASN:HB3	1.86	0.57
2:F:183:THR:HA	2:F:421:ILE:HG21	1.85	0.57
2:G:274:LEU:HD13	2:G:277:THR:OG1	2.04	0.57
2:G:275:GLU:O	2:G:275:GLU:HG3	2.03	0.57
2:G:184:ARG:HH21	2:G:422:ALA:HB3	1.69	0.57
1:A:420:THR:OG1	1:A:455:LYS:HB2	2.04	0.57
2:E:310:THR:O	2:E:314:SER:HB3	2.04	0.57
1:A:374:ARG:HD2	1:B:394:ARG:HH21	1.70	0.57
1:D:38:PRO:HB3	1:D:90:ILE:HG23	1.86	0.57
2:E:295:ILE:HD12	2:E:298:VAL:HG11	1.85	0.57
2:F:370:VAL:HG23	2:F:381:ILE:HG22	1.86	0.57
2:F:99:ILE:HG13	2:F:122:LEU:HD23	1.86	0.57
1:A:142:ILE:HG23	1:A:352:THR:HG22	1.86	0.57
1:B:287:PHE:HA	1:B:314:THR:HG21	1.85	0.57
1:C:343:SER:HB2	1:C:438:LEU:HD21	1.85	0.57
2:F:237:ILE:HG13	2:F:259:LEU:HG	1.86	0.57
2:F:116:ALA:HB2	2:G:88:THR:HG21	1.85	0.57
2:F:117:ILE:HG22	2:F:119:VAL:HG23	1.87	0.57
2:G:125:PRO:HB2	5:G:501:NAD:N7N	2.20	0.57
1:B:38:PRO:HG3	1:B:90:ILE:HG12	1.86	0.56
1:A:71:LEU:HD13	1:A:477:LEU:HD11	1.87	0.56
2:G:20:VAL:HG21	2:G:45:LEU:HD12	1.87	0.56
1:B:469:LEU:HD12	1:B:474:LEU:HD12	1.88	0.56
1:C:420:THR:OG1	1:C:455:LYS:HB2	2.06	0.56
1:D:262:SER:OG	1:D:263:GLY:N	2.37	0.56
2:H:395:VAL:HA	2:H:428:ILE:HB	1.87	0.56
1:C:379:ARG:HD3	2:F:289:LEU:HD22	1.87	0.56
1:A:226:HIS:CE1	1:A:232:TYR:HB3	2.41	0.56
2:F:237:ILE:HD11	2:F:248:ALA:HB2	1.88	0.56
1:C:117:ILE:HD11	1:C:131:ARG:HD2	1.86	0.56
2:E:20:VAL:HG21	2:E:45:LEU:HD12	1.86	0.56
2:E:388:ASP:HB2	2:E:391:THR:HG22	1.86	0.56
2:G:68:MET:HG3	2:G:94:ASN:HB3	1.88	0.56
1:A:427:ALA:O	1:A:431:VAL:HG22	2.06	0.56
2:E:274:LEU:HD13	2:E:277:THR:OG1	2.05	0.56
2:E:415:ARG:NH2	2:E:427:VAL:O	2.33	0.56
2:G:143:LEU:HD13	2:G:158:VAL:HA	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:359:LEU:HA	2:H:362:VAL:HG22	1.87	0.56
1:C:24:PRO:HB2	1:C:39:PHE:HE1	1.70	0.56
1:C:453:ASN:OD1	1:C:454:ASP:N	2.39	0.56
1:D:441:GLY:HA3	1:D:447:LEU:HA	1.87	0.56
2:H:398:ALA:O	2:H:402:ILE:HG12	2.06	0.55
1:B:20:THR:HB	1:B:133:PHE:HE1	1.71	0.55
2:E:70:VAL:HA	2:E:96:VAL:HG23	1.88	0.55
2:E:111:LEU:HD21	2:H:85:VAL:HG22	1.89	0.55
2:F:287:GLN:O	2:F:291:THR:OG1	2.24	0.55
2:F:305:THR:OG1	2:F:311:ASN:OD1	2.12	0.55
1:B:453:ASN:OD1	1:B:454:ASP:N	2.39	0.55
1:C:2:GLN:HA	1:C:4:ARG:NH1	2.22	0.55
2:F:363:ARG:HB3	2:F:367:ILE:HD13	1.88	0.55
2:H:176:GLU:HG3	2:H:225:LEU:HD22	1.89	0.55
1:D:11:GLY:HA3	1:D:53:CYS:HB2	1.88	0.55
1:D:439:GLY:N	1:D:440:PRO:HD3	2.22	0.55
2:G:117:ILE:HG22	2:G:119:VAL:HG23	1.89	0.55
1:B:117:ILE:HD11	1:B:131:ARG:HD2	1.88	0.55
1:C:38:PRO:HB3	1:C:90:ILE:HG23	1.89	0.55
2:E:221:VAL:HG13	2:E:225:LEU:HD23	1.89	0.55
1:B:440:PRO:HB2	1:B:442:LEU:HD23	1.87	0.54
1:C:309:GLN:NE2	1:C:326:THR:HG22	2.21	0.54
1:A:110:THR:O	1:A:468:ARG:NH1	2.37	0.54
2:H:397:ARG:HB2	2:H:402:ILE:HG23	1.88	0.54
1:C:266:HIS:CG	1:C:267:PRO:HD3	2.43	0.54
2:E:27:THR:HG22	2:E:46:ARG:HE	1.72	0.54
2:G:421:ILE:HD13	2:G:421:ILE:H	1.73	0.54
2:E:237:ILE:HD11	2:E:248:ALA:HB2	1.90	0.54
2:F:189:PHE:CD1	2:F:194:PRO:HB3	2.42	0.54
2:G:257:VAL:HB	2:G:277:THR:HG22	1.90	0.54
1:B:86:LEU:HD12	1:B:89:LEU:HD12	1.90	0.54
2:F:295:ILE:HD12	2:F:298:VAL:HG11	1.89	0.54
2:G:284:ALA:H	5:G:501:NAD:H61A	1.55	0.54
1:C:344:PHE:HA	1:C:436:ASN:OD1	2.08	0.54
2:G:387:GLY:HA3	2:G:392:SER:HB2	1.89	0.54
2:H:146:VAL:HG13	2:H:155:LEU:HB3	1.89	0.54
1:A:205:MET:HB2	1:A:210:ALA:HB2	1.90	0.54
2:H:70:VAL:HA	2:H:96:VAL:HG23	1.90	0.54
2:H:167:VAL:O	2:H:203:ILE:HB	2.08	0.54
1:A:420:THR:O	1:A:453:ASN:ND2	2.41	0.54
2:E:42:LYS:HE3	3:E:503:TBR:BRA	2.63	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:68:MET:HG3	2:E:94:ASN:HB3	1.88	0.54
2:E:319:LYS:NZ	2:E:345:ASP:OD2	2.41	0.54
2:H:137:ILE:HD11	2:H:302:ILE:HD11	1.89	0.54
2:E:287:GLN:HB3	2:E:321:MET:HE1	1.90	0.53
1:B:457:LYS:O	1:B:461:ILE:HG13	2.08	0.53
1:D:226:HIS:CE1	1:D:232:TYR:HB3	2.43	0.53
1:D:234:ASP:OD2	1:D:234:ASP:N	2.41	0.53
1:A:20:THR:HB	1:A:133:PHE:HE1	1.73	0.53
1:D:420:THR:HG23	1:D:453:ASN:HD22	1.71	0.53
2:G:38:GLU:HB3	3:G:503:TBR:BR9	2.63	0.53
1:A:117:ILE:HD11	1:A:131:ARG:HD2	1.90	0.53
1:A:349:ALA:HB2	1:A:359:ILE:HG12	1.90	0.53
1:A:356:MET:HE1	1:A:403:PHE:HD1	1.72	0.53
1:D:142:ILE:HG23	1:D:352:THR:HG22	1.89	0.53
2:E:223:SER:HA	2:E:228:LEU:HB2	1.90	0.53
2:F:308:ASP:O	2:F:312:ILE:HD12	2.08	0.53
2:H:233:ARG:NH2	2:H:234:ARG:HH21	2.07	0.53
1:B:38:PRO:HG2	1:B:91:ALA:HB2	1.89	0.53
1:C:427:ALA:O	1:C:431:VAL:HG22	2.09	0.53
1:C:109:LEU:HD13	1:C:134:LEU:HD22	1.91	0.53
2:E:143:LEU:HD13	2:E:158:VAL:HA	1.89	0.53
1:A:24:PRO:HB2	1:A:39:PHE:HE1	1.72	0.53
1:A:354:GLY:HA3	1:A:468:ARG:NH2	2.23	0.53
1:B:252:ASN:H	1:B:351:SER:HB3	1.74	0.53
1:C:220:ILE:HG22	1:C:321:ALA:HA	1.91	0.53
2:G:252:GLU:O	2:G:276:ASN:ND2	2.42	0.53
1:A:468:ARG:HA	1:A:468:ARG:NE	2.24	0.53
2:F:327:MET:HG2	2:F:346:VAL:HG13	1.91	0.53
1:A:425:LEU:HD11	1:B:424:GLU:HB3	1.90	0.53
1:B:149:ILE:O	1:B:153:LEU:N	2.39	0.53
1:D:20:THR:HB	1:D:133:PHE:HE1	1.73	0.53
2:E:153:VAL:HG11	2:E:435:VAL:HG21	1.91	0.53
2:E:67:ASP:HA	2:E:93:PRO:HG2	1.91	0.53
2:G:352:GLN:NE2	2:G:373:LEU:O	2.41	0.52
1:A:233:PHE:C	1:A:235:SER:H	2.17	0.52
1:A:317:ILE:HD13	1:A:442:LEU:HD11	1.92	0.52
1:D:268:LYS:HE3	1:D:272:LYS:HE3	1.90	0.52
1:D:301:THR:OG1	1:D:302:SER:N	2.43	0.52
1:D:420:THR:O	1:D:453:ASN:ND2	2.42	0.52
2:F:15:LEU:HD11	2:F:358:LEU:HG	1.89	0.52
2:F:68:MET:HE1	2:F:362:VAL:HG22	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:139:TYR:HE1	2:F:218:ILE:HG23	1.74	0.52
2:G:183:THR:HB	2:G:213:ALA:HB2	1.91	0.52
1:B:363:LEU:HD12	1:B:399:VAL:HG21	1.91	0.52
1:C:181:THR:HG22	1:C:257:PHE:HE2	1.74	0.52
1:D:109:LEU:HD13	1:D:134:LEU:HD22	1.91	0.52
1:D:345:ILE:HG12	1:D:361:ILE:HG13	1.91	0.52
2:H:38:GLU:HB3	3:H:503:TBR:BR9	2.65	0.52
2:H:301:PHE:HB3	2:H:326:VAL:HG12	1.91	0.52
2:F:146:VAL:HG13	2:F:155:LEU:HB3	1.91	0.52
2:H:125:PRO:HB2	5:H:501:NAD:N7N	2.24	0.52
1:A:373:LYS:HD2	1:A:382:TYR:CE1	2.45	0.52
1:D:441:GLY:H	1:D:447:LEU:HB3	1.74	0.52
2:F:126:GLU:N	5:F:501:NAD:H72N	2.07	0.52
1:A:2:GLN:HA	1:A:4:ARG:HH11	1.74	0.52
1:B:354:GLY:HA2	1:B:357:LYS:HE3	1.92	0.52
1:D:21:MET:HE1	1:D:130:TYR:HE1	1.75	0.52
2:F:137:ILE:HD11	2:F:302:ILE:HD11	1.91	0.52
2:H:3:ILE:HD11	2:H:26:ILE:HG12	1.91	0.52
1:B:71:LEU:HD13	1:B:477:LEU:HD11	1.91	0.52
1:A:357:LYS:H	1:A:357:LYS:HD2	1.74	0.52
1:A:430:ALA:HB1	1:A:460:LEU:HD21	1.90	0.52
1:A:439:GLY:N	1:A:440:PRO:HD3	2.25	0.52
1:C:233:PHE:C	1:C:235:SER:H	2.18	0.52
1:C:310:ALA:O	1:C:314:THR:HG23	2.10	0.52
1:D:153:LEU:HD22	1:D:154:GLY:H	1.73	0.52
2:E:126:GLU:N	5:E:501:NAD:H72N	2.07	0.52
1:B:15:ALA:O	1:B:19:VAL:HG23	2.09	0.52
1:C:21:MET:HE1	1:C:130:TYR:HE1	1.75	0.52
2:E:68:MET:HE2	2:E:70:VAL:HG22	1.92	0.52
2:H:100:ARG:NE	2:H:126:GLU:HG3	2.24	0.52
2:F:367:ILE:HD11	2:F:448:GLU:HG3	1.91	0.51
2:E:190:ARG:NH2	2:E:201:THR:HG22	2.25	0.51
1:C:441:GLY:H	1:C:447:LEU:HB3	1.74	0.51
1:D:184:ALA:HB1	1:D:257:PHE:HE1	1.76	0.51
1:A:265:VAL:HG13	1:A:269:TYR:HE2	1.76	0.51
1:A:266:HIS:N	1:A:267:PRO:HD2	2.26	0.51
1:C:24:PRO:HB2	1:C:39:PHE:CE1	2.46	0.51
1:C:420:THR:O	1:C:453:ASN:ND2	2.43	0.51
1:C:457:LYS:O	1:C:461:ILE:HG13	2.10	0.51
1:D:2:GLN:HA	1:D:4:ARG:NH1	2.24	0.51
2:E:152:LYS:HE3	2:E:216:ASN:HD21	1.76	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:370:ARG:HD3	1:D:374:ARG:CZ	2.41	0.51
2:G:70:VAL:HA	2:G:96:VAL:HG23	1.93	0.51
1:B:427:ALA:O	1:B:431:VAL:HG22	2.10	0.51
2:F:414:VAL:HB	2:F:433:HIS:HB2	1.92	0.51
1:B:233:PHE:C	1:B:235:SER:H	2.19	0.51
1:D:233:PHE:C	1:D:235:SER:H	2.18	0.51
1:A:8:ARG:HD3	1:A:59:ARG:H	1.76	0.51
1:A:106:PHE:O	1:A:110:THR:OG1	2.23	0.51
1:B:357:LYS:O	1:B:360:ARG:HB2	2.10	0.51
1:C:142:ILE:HG23	1:C:352:THR:HG22	1.93	0.51
1:D:94:PRO:HG3	1:D:123:LEU:HD13	1.93	0.51
2:E:20:VAL:HG11	2:E:43:TYR:HB3	1.92	0.51
2:F:440:ASP:OD2	2:F:442:LYS:HB2	2.11	0.51
1:B:74:VAL:HG12	1:B:469:LEU:HD13	1.93	0.50
1:D:309:GLN:NE2	1:D:326:THR:HG22	2.25	0.50
1:A:434:THR:HG22	1:A:464:MET:HB3	1.93	0.50
1:A:438:LEU:CB	1:A:439:GLY:HA2	2.41	0.50
1:B:110:THR:O	1:B:468:ARG:NH1	2.44	0.50
2:E:27:THR:HG22	2:E:46:ARG:HB3	1.94	0.50
2:H:8:ALA:HA	2:H:28:ILE:HD11	1.93	0.50
2:H:404:LEU:HD21	2:H:410:ILE:HG12	1.93	0.50
1:C:117:ILE:HG13	1:C:120:LEU:HD23	1.93	0.50
1:C:476:ILE:HG22	1:D:372:LEU:HG	1.94	0.50
2:F:111:LEU:HD21	2:G:85:VAL:HG22	1.92	0.50
2:F:143:LEU:HD21	2:F:159:LYS:HG2	1.93	0.50
1:C:74:VAL:HG12	1:C:469:LEU:HD13	1.93	0.50
1:D:8:ARG:HD3	1:D:59:ARG:H	1.76	0.50
2:H:287:GLN:HB3	2:H:321:MET:HE1	1.93	0.50
1:C:472:PHE:O	1:C:476:ILE:HG23	2.12	0.50
1:D:89:LEU:HD21	1:D:98:VAL:HA	1.93	0.50
1:D:438:LEU:CB	1:D:439:GLY:HA2	2.38	0.50
2:E:104:TYR:HH	2:H:53:SER:HG	1.60	0.50
2:E:290:LEU:HD12	2:E:295:ILE:HD13	1.94	0.50
1:D:24:PRO:HB2	1:D:39:PHE:CE1	2.46	0.50
1:C:354:GLY:HA2	1:C:357:LYS:HE3	1.93	0.50
1:D:71:LEU:HD13	1:D:477:LEU:HD11	1.94	0.50
2:E:89:LEU:HD12	2:H:111:LEU:HD13	1.92	0.50
2:H:85:VAL:O	2:H:89:LEU:HB2	2.11	0.50
1:A:309:GLN:NE2	1:A:326:THR:HG22	2.27	0.50
1:B:373:LYS:HD2	1:B:382:TYR:CE1	2.47	0.50
1:C:334:PHE:HD2	1:C:335:LEU:HD22	1.77	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:117:ILE:HG22	2:E:119:VAL:HG23	1.94	0.50
2:H:8:ALA:N	2:H:30:ASP:OD2	2.35	0.50
2:E:183:THR:HB	2:E:213:ALA:HB2	1.92	0.50
2:E:221:VAL:O	2:E:225:LEU:HB2	2.12	0.50
2:F:155:LEU:HD11	2:F:210:PHE:HD2	1.76	0.50
2:F:369:ASN:HB2	2:F:382:GLU:HB3	1.94	0.50
2:H:136:LEU:HD13	2:H:346:VAL:HG21	1.92	0.50
2:H:221:VAL:O	2:H:225:LEU:HB2	2.12	0.50
1:A:476:ILE:HA	1:A:479:THR:HG23	1.92	0.49
1:C:86:LEU:HD12	1:C:89:LEU:HD12	1.93	0.49
2:E:145:VAL:HG22	2:E:156:VAL:HG23	1.93	0.49
2:E:364:ARG:HB3	2:E:366:ASP:OD1	2.12	0.49
2:H:100:ARG:HE	2:H:126:GLU:HG3	1.77	0.49
1:A:142:ILE:HD12	1:A:468:ARG:CZ	2.41	0.49
1:B:441:GLY:H	1:B:447:LEU:HB3	1.76	0.49
2:E:313:MET:HE3	2:E:313:MET:HA	1.95	0.49
2:E:359:LEU:HA	2:E:362:VAL:HG22	1.93	0.49
2:F:124:ALA:O	2:F:128:LEU:HG	2.13	0.49
1:A:24:PRO:HB2	1:A:39:PHE:CE1	2.47	0.49
1:A:112:THR:HG23	1:A:437:ASN:HA	1.95	0.49
1:B:438:LEU:HB3	1:B:440:PRO:HD2	1.94	0.49
1:D:434:THR:HG22	1:D:464:MET:HB3	1.93	0.49
2:E:77:GLU:HA	2:E:80:MET:HE2	1.94	0.49
2:E:266:ARG:O	2:E:270:LEU:HB2	2.13	0.49
2:E:287:GLN:O	2:E:291:THR:OG1	2.31	0.49
1:B:468:ARG:NE	1:B:468:ARG:HA	2.27	0.49
2:F:101:SER:HB3	2:F:104:TYR:HD2	1.76	0.49
2:G:300:VAL:HG12	2:G:325:LYS:HB2	1.94	0.49
1:A:39:PHE:CE2	1:A:87:PRO:HB3	2.48	0.49
1:A:430:ALA:O	1:A:434:THR:OG1	2.31	0.49
1:C:226:HIS:CE1	1:C:232:TYR:HB3	2.47	0.49
1:D:373:LYS:HD2	1:D:382:TYR:CE1	2.46	0.49
1:B:11:GLY:HA3	1:B:53:CYS:HB2	1.94	0.49
1:B:94:PRO:HG3	1:B:123:LEU:HD13	1.93	0.49
1:B:472:PHE:O	1:B:476:ILE:HG23	2.12	0.49
1:D:74:VAL:HG12	1:D:469:LEU:HD13	1.94	0.49
2:E:258:LYS:HG2	2:E:278:ILE:HD11	1.94	0.49
2:G:126:GLU:O	2:G:130:THR:HG23	2.12	0.49
2:G:327:MET:HG2	2:G:346:VAL:HG13	1.94	0.49
1:C:294:LEU:HD12	1:C:310:ALA:HB2	1.94	0.49
1:D:149:ILE:O	1:D:153:LEU:N	2.41	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:391:LEU:HD12	1:D:395:VAL:HG11	1.95	0.49
1:D:427:ALA:O	1:D:431:VAL:HG22	2.12	0.49
2:G:153:VAL:HG11	2:G:435:VAL:HG21	1.94	0.49
1:A:406:TYR:HA	1:A:471:ILE:HD13	1.94	0.49
1:D:220:ILE:HD12	1:D:352:THR:C	2.38	0.49
2:E:7:GLY:O	2:E:12:GLY:HA3	2.13	0.49
2:G:29:VAL:HG22	2:G:48:VAL:HB	1.95	0.49
1:B:112:THR:HG23	1:B:437:ASN:HA	1.94	0.49
1:B:476:ILE:HA	1:B:479:THR:HG23	1.95	0.49
2:F:27:THR:HG22	2:F:46:ARG:HE	1.77	0.49
2:F:258:LYS:HD3	2:F:293:GLU:HG3	1.94	0.49
2:H:237:ILE:HD11	2:H:248:ALA:HB2	1.93	0.49
1:A:236:TYR:H	1:A:236:TYR:HD2	1.59	0.48
2:G:169:ASN:ND2	2:G:203:ILE:HD11	2.28	0.48
2:H:388:ASP:HA	2:H:430:GLN:HG2	1.95	0.48
1:C:417:LEU:HD11	1:C:460:LEU:HD21	1.95	0.48
2:E:308:ASP:O	2:E:312:ILE:HD12	2.13	0.48
2:F:330:ILE:HB	2:F:336:VAL:HG22	1.95	0.48
1:B:434:THR:HG22	1:B:464:MET:HB3	1.95	0.48
2:F:85:VAL:HG22	2:G:111:LEU:HD21	1.95	0.48
2:F:313:MET:HE3	2:F:313:MET:HA	1.94	0.48
2:H:2:LYS:HB3	2:H:25:ASP:HB3	1.96	0.48
2:H:2:LYS:HD2	2:H:65:ASP:O	2.13	0.48
2:E:399:ILE:HB	2:E:424:ASP:HA	1.95	0.48
2:G:147:SER:HB2	2:G:151:GLN:HA	1.95	0.48
2:G:283:ASP:OD2	5:G:501:NAD:N6A	2.46	0.48
1:B:143:ILE:HG21	1:B:253:PHE:CD2	2.49	0.48
1:B:294:LEU:HD12	1:B:310:ALA:HB2	1.94	0.48
1:C:142:ILE:HD12	1:C:468:ARG:CZ	2.43	0.48
1:C:149:ILE:O	1:C:153:LEU:N	2.44	0.48
1:D:112:THR:HG23	1:D:437:ASN:HA	1.96	0.48
2:E:190:ARG:HD3	2:E:204:GLU:CD	2.38	0.48
2:H:6:LEU:HD22	2:H:52:ALA:HB1	1.94	0.48
1:A:361:ILE:O	1:A:365:THR:HG23	2.13	0.48
1:A:460:LEU:O	1:A:464:MET:HG2	2.13	0.48
1:B:178:ILE:C	1:B:180:GLU:H	2.20	0.48
1:B:251:CYS:SG	1:B:276:PHE:HD1	2.36	0.48
2:F:36:LEU:HD22	2:F:47:VAL:HG13	1.96	0.48
2:H:36:LEU:HD22	2:H:47:VAL:HG13	1.96	0.48
1:B:2:GLN:HA	1:B:4:ARG:HH11	1.79	0.48
1:C:20:THR:HB	1:C:133:PHE:HE1	1.78	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:153:LEU:HD22	1:C:154:GLY:H	1.79	0.48
2:G:238:VAL:HG23	2:G:303:ALA:HA	1.96	0.48
2:H:2:LYS:HG3	2:H:66:ALA:HA	1.96	0.48
1:B:181:THR:HA	1:B:184:ALA:HB3	1.96	0.48
2:E:257:VAL:HB	2:E:277:THR:HG22	1.95	0.48
2:F:8:ALA:HA	2:F:28:ILE:HD11	1.95	0.48
2:G:134:GLU:OE2	2:G:250:ARG:NH1	2.46	0.48
2:G:258:LYS:HE2	2:G:278:ILE:HD11	1.96	0.48
1:A:181:THR:HA	1:A:184:ALA:HB3	1.96	0.48
1:A:301:THR:OG1	1:A:302:SER:N	2.47	0.48
1:B:142:ILE:HD12	1:B:468:ARG:CZ	2.44	0.48
1:D:183:LYS:HE3	1:D:187:TYR:HE2	1.78	0.48
1:D:406:TYR:HA	1:D:471:ILE:HD13	1.95	0.48
1:A:11:GLY:HA3	1:A:53:CYS:HB2	1.94	0.47
1:C:38:PRO:HG2	1:C:91:ALA:HB2	1.94	0.47
1:C:300:TYR:CZ	1:C:309:GLN:HG3	2.48	0.47
1:D:468:ARG:HA	1:D:468:ARG:NE	2.29	0.47
2:G:99:ILE:HG13	2:G:122:LEU:HD23	1.95	0.47
2:G:290:LEU:HD12	2:G:295:ILE:HD13	1.96	0.47
1:A:109:LEU:HD13	1:A:134:LEU:HD22	1.95	0.47
2:H:26:ILE:O	2:H:45:LEU:HB2	2.14	0.47
2:H:126:GLU:O	2:H:130:THR:HG23	2.14	0.47
2:H:148:PHE:HB2	2:H:153:VAL:HG13	1.95	0.47
1:A:86:LEU:HD12	1:A:89:LEU:HD12	1.96	0.47
1:C:76:PHE:O	1:C:80:LEU:HB2	2.13	0.47
2:E:237:ILE:HG13	2:E:259:LEU:HG	1.96	0.47
2:F:332:ARG:HA	3:F:503:TBR:BR2	2.69	0.47
1:C:468:ARG:HA	1:C:468:ARG:NE	2.29	0.47
2:G:237:ILE:HD11	2:G:248:ALA:HB2	1.96	0.47
2:G:283:ASP:OD2	2:G:284:ALA:N	2.47	0.47
2:H:266:ARG:O	2:H:270:LEU:HB2	2.14	0.47
1:B:158:MET:HE3	1:B:158:MET:HB2	1.74	0.47
1:B:184:ALA:HB1	1:B:257:PHE:HE1	1.79	0.47
2:E:258:LYS:HE2	2:E:278:ILE:HD11	1.97	0.47
2:F:111:LEU:HD11	2:G:85:VAL:HG22	1.97	0.47
1:A:194:ILE:O	1:A:198:VAL:HG12	2.15	0.47
1:A:384:ILE:HG22	1:A:391:LEU:HD23	1.97	0.47
1:B:226:HIS:CE1	1:B:232:TYR:HB3	2.50	0.47
1:B:300:TYR:CZ	1:B:309:GLN:HG3	2.50	0.47
1:B:420:THR:HG23	1:B:453:ASN:HD22	1.80	0.47
1:C:77:TRP:CD1	1:C:469:LEU:HD21	2.50	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:153:LEU:HD13	1:C:154:GLY:H	1.79	0.47
1:D:158:MET:HE3	1:D:158:MET:HB2	1.81	0.47
2:G:7:GLY:O	2:G:12:GLY:HA3	2.15	0.47
1:A:220:ILE:HG22	1:A:321:ALA:HA	1.96	0.47
1:A:357:LYS:O	1:A:360:ARG:HB2	2.14	0.47
1:B:24:PRO:HB2	1:B:39:PHE:CE1	2.49	0.47
1:C:251:CYS:SG	1:C:276:PHE:HD1	2.37	0.47
2:F:10:GLN:HE21	2:F:98:ARG:HH12	1.63	0.47
2:F:138:GLN:HG3	2:F:139:TYR:CD2	2.50	0.47
1:A:153:LEU:HD22	1:A:154:GLY:H	1.78	0.47
1:A:438:LEU:HB3	1:A:440:PRO:HD2	1.95	0.47
1:C:21:MET:HE1	1:C:130:TYR:CE1	2.50	0.47
1:C:439:GLY:N	1:C:440:PRO:HD3	2.29	0.47
1:D:205:MET:HE2	1:D:238:ILE:HD13	1.97	0.47
1:D:457:LYS:O	1:D:461:ILE:HG13	2.14	0.47
2:F:235:ILE:HG12	2:F:300:VAL:HG23	1.97	0.47
2:F:360:THR:CG2	2:F:370:VAL:HG12	2.45	0.47
2:G:126:GLU:N	5:G:501:NAD:H72N	2.13	0.47
2:H:153:VAL:HG11	2:H:435:VAL:HG21	1.97	0.47
1:A:472:PHE:O	1:A:476:ILE:HG23	2.14	0.47
1:B:357:LYS:H	1:B:357:LYS:HD2	1.79	0.47
1:D:361:ILE:O	1:D:365:THR:HG23	2.15	0.47
2:E:271:SER:HA	2:E:279:VAL:HG21	1.97	0.47
2:E:392:SER:HB3	2:E:395:VAL:HG22	1.97	0.47
2:F:125:PRO:HB3	2:F:354:THR:CG2	2.44	0.47
2:F:143:LEU:HD13	2:F:158:VAL:HA	1.97	0.47
1:A:417:LEU:O	1:A:420:THR:HG22	2.15	0.46
1:B:8:ARG:HD3	1:B:59:ARG:H	1.79	0.46
1:C:128:LEU:HD11	1:C:225:THR:HA	1.97	0.46
2:H:238:VAL:HG23	2:H:303:ALA:HA	1.98	0.46
2:H:258:LYS:HD3	2:H:293:GLU:HG3	1.98	0.46
1:B:76:PHE:O	1:B:80:LEU:HB2	2.15	0.46
1:C:2:GLN:HA	1:C:4:ARG:HH11	1.80	0.46
1:D:38:PRO:HG2	1:D:91:ALA:HB2	1.96	0.46
2:F:364:ARG:HG3	2:F:365:ALA:N	2.30	0.46
2:G:48:VAL:HG21	2:G:61:ALA:HA	1.97	0.46
2:G:117:ILE:O	2:G:119:VAL:N	2.45	0.46
1:B:74:VAL:O	1:B:78:THR:HB	2.15	0.46
1:B:333:LEU:HD22	1:B:337:VAL:HG23	1.96	0.46
1:B:430:ALA:O	1:B:434:THR:OG1	2.34	0.46
1:D:148:ALA:O	1:D:151:PRO:HD2	2.14	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:294:LEU:HD11	1:D:331:TRP:CZ2	2.49	0.46
2:G:36:LEU:HD22	2:G:47:VAL:HG13	1.98	0.46
1:C:31:TYR:HD1	1:C:125:LYS:HG3	1.80	0.46
1:D:229:SER:OG	1:D:230:MET:N	2.48	0.46
1:D:291:PHE:CZ	1:D:295:LEU:HD11	2.51	0.46
2:F:80:MET:HE1	2:F:104:TYR:CD1	2.51	0.46
1:B:24:PRO:HB2	1:B:39:PHE:HE1	1.80	0.46
1:B:124:PRO:HG2	1:B:127:ILE:HD12	1.98	0.46
1:C:384:ILE:HG22	1:C:391:LEU:HD23	1.97	0.46
1:D:142:ILE:HD12	1:D:468:ARG:CZ	2.45	0.46
1:D:236:TYR:N	1:D:236:TYR:CD2	2.83	0.46
2:H:4:ILE:HG12	2:H:27:THR:OG1	2.15	0.46
2:H:243:ILE:HG22	2:H:304:LEU:HD13	1.97	0.46
1:A:80:LEU:HB3	1:A:109:LEU:HD21	1.97	0.46
1:A:286:LEU:HD22	1:A:314:THR:HB	1.98	0.46
1:C:148:ALA:O	1:C:151:PRO:HD2	2.14	0.46
1:A:153:LEU:HD13	1:A:154:GLY:H	1.80	0.46
1:A:343:SER:HB2	1:A:438:LEU:HD11	1.97	0.46
1:B:142:ILE:HD13	1:B:352:THR:HA	1.96	0.46
1:C:89:LEU:HD21	1:C:98:VAL:HA	1.96	0.46
1:C:259:ALA:HA	1:C:266:HIS:HB3	1.98	0.46
1:D:442:LEU:H	1:D:447:LEU:HD22	1.81	0.46
1:D:476:ILE:HA	1:D:479:THR:HG23	1.97	0.46
2:E:67:ASP:O	2:E:93:PRO:HB2	2.15	0.46
2:E:402:ILE:H	2:E:402:ILE:HG13	1.42	0.46
2:G:258:LYS:HD3	2:G:293:GLU:HG3	1.97	0.46
2:H:421:ILE:H	2:H:421:ILE:HG12	1.47	0.46
1:B:236:TYR:N	1:B:236:TYR:CD2	2.84	0.46
1:D:302:SER:C	1:D:304:TYR:H	2.23	0.46
2:E:403:LYS:H	2:E:403:LYS:HG3	1.58	0.46
2:G:359:LEU:HD13	2:G:363:ARG:HH21	1.80	0.46
1:A:326:THR:OG1	1:A:327:GLY:N	2.47	0.46
1:A:345:ILE:HG21	1:A:361:ILE:HD12	1.99	0.46
2:E:356:SER:HB3	2:E:371:SER:HA	1.98	0.46
2:G:29:VAL:HA	2:G:48:VAL:O	2.16	0.46
2:G:308:ASP:O	2:G:312:ILE:HD12	2.16	0.46
1:A:192:LEU:HD23	1:A:192:LEU:HA	1.74	0.45
1:C:158:MET:HE3	1:C:158:MET:HB2	1.70	0.45
2:E:238:VAL:HG12	2:E:260:ILE:HB	1.97	0.45
2:G:148:PHE:HB3	2:G:382:GLU:OE2	2.16	0.45
1:A:72:ILE:HD13	1:A:72:ILE:HA	1.82	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:72:ILE:HD13	1:D:72:ILE:HA	1.80	0.45
1:D:420:THR:OG1	1:D:455:LYS:HB2	2.17	0.45
2:F:238:VAL:HG23	2:F:303:ALA:HA	1.98	0.45
1:A:229:SER:OG	1:A:230:MET:N	2.48	0.45
1:A:310:ALA:O	1:A:314:THR:HG23	2.17	0.45
2:H:274:LEU:HD13	2:H:277:THR:OG1	2.16	0.45
1:A:287:PHE:HA	1:A:314:THR:HG21	1.99	0.45
1:A:418:ILE:HD12	1:B:337:VAL:HG11	1.98	0.45
2:F:222:MET:HE2	2:F:227:ARG:HG3	1.99	0.45
2:G:136:LEU:HD13	2:G:346:VAL:HG21	1.97	0.45
2:G:222:MET:HE3	2:G:222:MET:HA	1.98	0.45
2:H:321:MET:HE2	2:H:321:MET:HB3	1.91	0.45
2:H:335:TYR:O	2:H:339:VAL:HG22	2.16	0.45
1:A:257:PHE:C	1:A:259:ALA:H	2.23	0.45
1:C:476:ILE:HA	1:C:479:THR:HG23	1.97	0.45
2:G:360:THR:HG22	2:G:370:VAL:H	1.80	0.45
2:H:188:ILE:HG22	2:H:207:ASP:HB3	1.98	0.45
1:A:76:PHE:O	1:A:80:LEU:HB2	2.16	0.45
1:A:297:HIS:CG	1:A:332:PRO:HG3	2.52	0.45
1:A:317:ILE:HG21	1:A:339:LEU:HB3	1.98	0.45
1:A:328:PHE:HA	1:A:331:TRP:CD1	2.51	0.45
1:A:477:LEU:HD13	1:A:477:LEU:HA	1.75	0.45
1:C:226:HIS:ND1	1:C:232:TYR:HB3	2.32	0.45
1:D:21:MET:HE1	1:D:130:TYR:CE1	2.52	0.45
1:D:178:ILE:HB	3:D:502:TBR:BRA	2.72	0.45
2:F:384:VAL:HG22	2:F:433:HIS:ND1	2.32	0.45
2:H:410:ILE:HD13	2:H:436:MET:HB3	1.98	0.45
1:A:406:TYR:HA	1:A:471:ILE:CD1	2.47	0.45
1:B:21:MET:HB2	1:B:43:PHE:HB2	1.99	0.45
1:B:230:MET:HG3	1:B:312:PHE:HZ	1.80	0.45
1:D:86:LEU:HA	1:D:86:LEU:HD12	1.82	0.45
2:E:283:ASP:OD2	5:E:501:NAD:N6A	2.49	0.45
2:G:233:ARG:NH2	2:G:234:ARG:HH21	2.15	0.45
2:G:330:ILE:HB	2:G:336:VAL:HG22	1.98	0.45
2:H:79:ASN:HD22	2:H:79:ASN:HA	1.59	0.45
1:A:140:MET:HE3	1:A:144:VAL:CG1	2.46	0.45
1:A:473:THR:HA	1:A:476:ILE:HD12	1.99	0.45
1:C:71:LEU:HD13	1:C:477:LEU:HD11	1.98	0.45
2:G:26:ILE:O	2:G:45:LEU:HB2	2.16	0.45
2:H:173:ALA:HB1	2:H:177:HIS:NE2	2.32	0.45
1:A:302:SER:C	1:A:304:TYR:H	2.25	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:418:ILE:HD13	1:B:337:VAL:HG21	1.98	0.44
1:B:94:PRO:HG2	1:B:127:ILE:HG21	1.99	0.44
1:D:39:PHE:N	1:D:39:PHE:CD2	2.85	0.44
1:D:417:LEU:O	1:D:420:THR:HG22	2.17	0.44
2:F:27:THR:HA	2:F:46:ARG:O	2.17	0.44
2:F:222:MET:HE3	2:F:222:MET:HA	1.98	0.44
2:F:359:LEU:HA	2:F:362:VAL:HG23	1.99	0.44
1:A:66:SER:O	1:A:69:GLY:N	2.49	0.44
1:C:425:LEU:HD11	1:D:424:GLU:HB3	1.98	0.44
2:E:2:LYS:HD2	2:E:65:ASP:O	2.17	0.44
1:A:469:LEU:HD12	1:A:474:LEU:HD12	1.99	0.44
1:C:94:PRO:HG3	1:C:123:LEU:HD13	1.99	0.44
2:F:10:GLN:NE2	2:F:74:ASN:OD1	2.43	0.44
2:G:145:VAL:HG22	2:G:156:VAL:HG23	1.99	0.44
2:H:190:ARG:NH2	2:H:202:ILE:O	2.51	0.44
2:H:223:SER:HA	2:H:228:LEU:HB2	1.99	0.44
2:E:190:ARG:HH22	2:E:201:THR:HG22	1.82	0.44
2:G:112:PHE:CD1	2:G:122:LEU:HD21	2.52	0.44
2:G:321:MET:HE2	2:G:321:MET:HB3	1.82	0.44
2:H:360:THR:HG23	2:H:370:VAL:HG12	2.00	0.44
2:H:364:ARG:HD2	2:H:364:ARG:HA	1.80	0.44
1:A:252:ASN:HB2	1:A:348:CYS:HB3	2.00	0.44
1:A:358:VAL:O	1:A:361:ILE:HG22	2.17	0.44
1:B:266:HIS:N	1:B:267:PRO:HD2	2.32	0.44
1:C:199:ALA:HB1	1:C:241:ILE:HD13	1.99	0.44
1:D:246:LEU:HD23	1:D:246:LEU:HA	1.87	0.44
2:F:408:THR:HG23	2:F:438:LEU:HD13	2.00	0.44
2:G:309:GLU:HG2	2:H:310:THR:HA	2.00	0.44
2:H:117:ILE:HG22	2:H:119:VAL:HG23	1.99	0.44
2:H:319:LYS:NZ	2:H:345:ASP:OD2	2.51	0.44
1:A:345:ILE:HG21	1:A:361:ILE:HB	1.99	0.44
1:C:418:ILE:HD13	1:D:337:VAL:HG21	1.99	0.44
2:G:11:VAL:HG11	2:G:72:VAL:HG21	2.00	0.44
2:H:360:THR:CG2	2:H:370:VAL:HG12	2.47	0.44
1:A:39:PHE:N	1:A:39:PHE:CD2	2.84	0.44
1:C:39:PHE:N	1:C:39:PHE:CD2	2.86	0.44
1:C:236:TYR:H	1:C:236:TYR:HD2	1.65	0.44
1:D:392:PRO:C	1:D:394:ARG:H	2.26	0.44
2:E:125:PRO:HB2	5:E:501:NAD:N7N	2.33	0.44
2:E:369:ASN:HB2	2:E:382:GLU:HB3	2.00	0.44
2:F:125:PRO:HB2	5:F:501:NAD:N7N	2.32	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:108:LYS:HG3	2:G:122:LEU:HD13	1.99	0.44
2:H:136:LEU:HD23	2:H:136:LEU:HA	1.82	0.44
2:H:327:MET:HG2	2:H:346:VAL:HG13	1.99	0.44
1:B:22:LEU:HD21	1:B:43:PHE:CD2	2.53	0.44
1:D:310:ALA:O	1:D:314:THR:HG23	2.18	0.44
2:E:59:HIS:CE1	3:H:502:TBR:BRC	3.26	0.44
2:E:149:ALA:O	2:E:152:LYS:HB2	2.18	0.44
2:G:233:ARG:HB3	2:G:234:ARG:HG2	2.00	0.44
2:G:237:ILE:HG13	2:G:259:LEU:HG	2.00	0.44
2:G:359:LEU:HA	2:G:362:VAL:HG23	2.00	0.44
2:H:406:PRO:HB2	2:H:443:TYR:CE2	2.53	0.44
1:C:185:LEU:HD23	1:C:185:LEU:HA	1.87	0.44
1:C:477:LEU:HD13	1:C:477:LEU:HA	1.87	0.44
2:F:48:VAL:HG21	2:F:61:ALA:HA	2.00	0.44
2:G:155:LEU:HD13	2:G:212:VAL:HG22	1.99	0.44
2:G:391:THR:HA	2:G:456:PHE:CD2	2.53	0.44
1:A:357:LYS:H	1:A:357:LYS:CD	2.31	0.43
1:A:458:TRP:CE3	1:A:461:ILE:HD12	2.53	0.43
1:C:149:ILE:HD11	1:C:155:ILE:HD12	2.00	0.43
1:C:150:LEU:HB2	1:C:151:PRO:HD3	1.98	0.43
1:C:356:MET:HE2	1:C:361:ILE:HD11	2.00	0.43
2:G:124:ALA:O	2:G:128:LEU:HG	2.18	0.43
2:G:266:ARG:O	2:G:270:LEU:HB2	2.18	0.43
1:B:148:ALA:O	1:B:151:PRO:HD2	2.18	0.43
1:B:236:TYR:N	1:B:236:TYR:HD2	2.16	0.43
1:B:476:ILE:HG12	1:B:482:PHE:CD1	2.53	0.43
1:C:334:PHE:CD1	1:D:419:ALA:HB2	2.54	0.43
2:E:92:THR:HA	2:E:93:PRO:HD3	1.86	0.43
1:B:192:LEU:HD23	1:B:192:LEU:HA	1.87	0.43
2:E:283:ASP:OD2	2:E:284:ALA:N	2.51	0.43
1:A:468:ARG:HA	1:A:468:ARG:HE	1.83	0.43
1:C:49:CYS:O	1:C:52:MET:HG2	2.18	0.43
1:C:74:VAL:O	1:C:78:THR:HB	2.19	0.43
1:D:341:PHE:HD1	1:D:341:PHE:HA	1.74	0.43
1:D:435:LEU:HD21	1:D:471:ILE:HD11	1.99	0.43
2:F:10:GLN:H	2:F:10:GLN:CD	2.26	0.43
2:F:165:PRO:HB2	2:F:166:LEU:H	1.47	0.43
2:F:399:ILE:HG12	2:F:426:THR:O	2.18	0.43
1:B:472:PHE:C	1:B:474:LEU:H	2.26	0.43
1:C:438:LEU:HB3	1:C:440:PRO:HD2	2.00	0.43
1:D:80:LEU:HB3	1:D:109:LEU:HD21	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:75:THR:HG22	2:F:77:GLU:HG2	1.98	0.43
2:F:283:ASP:OD2	2:F:284:ALA:N	2.51	0.43
2:F:356:SER:HB3	2:F:371:SER:HA	2.00	0.43
2:G:165:PRO:HB2	2:G:166:LEU:H	1.57	0.43
1:A:333:LEU:O	1:A:336:PRO:HD2	2.19	0.43
1:B:253:PHE:CD1	1:B:256:HIS:HD2	2.36	0.43
1:C:466:PHE:HE1	1:C:474:LEU:HD22	1.83	0.43
1:D:4:ARG:H	1:D:4:ARG:HG2	1.53	0.43
1:D:74:VAL:O	1:D:78:THR:HB	2.19	0.43
1:D:192:LEU:HD23	1:D:192:LEU:HA	1.74	0.43
1:D:317:ILE:HG21	1:D:339:LEU:HB3	2.01	0.43
2:F:112:PHE:C	2:F:114:SER:H	2.27	0.43
1:A:13:LEU:HD23	1:A:13:LEU:HA	1.76	0.43
1:A:39:PHE:N	1:A:39:PHE:HD2	2.17	0.43
1:A:411:VAL:HG13	1:B:341:PHE:CE2	2.53	0.43
1:B:406:TYR:HA	1:B:471:ILE:HD13	2.00	0.43
1:C:43:PHE:O	1:C:47:LEU:HB2	2.19	0.43
1:C:229:SER:OG	1:C:230:MET:N	2.49	0.43
2:E:29:VAL:HA	2:E:48:VAL:O	2.19	0.43
2:F:92:THR:O	2:F:95:ARG:NH1	2.52	0.43
2:F:173:ALA:O	2:F:177:HIS:ND1	2.52	0.43
2:F:405:PRO:HG2	2:F:447:VAL:HG23	2.01	0.43
2:H:176:GLU:O	2:H:176:GLU:HG2	2.19	0.43
2:H:290:LEU:HD12	2:H:295:ILE:HD13	2.00	0.43
1:B:297:HIS:CD2	1:B:332:PRO:HG3	2.54	0.43
1:C:288:LEU:HD22	1:C:288:LEU:HA	1.83	0.43
2:F:189:PHE:HD2	2:F:374:ARG:HE	1.66	0.43
2:F:403:LYS:H	2:F:403:LYS:HG3	1.59	0.43
2:G:264:TYR:C	2:G:264:TYR:CD2	2.97	0.43
1:B:75:LEU:HD12	1:B:75:LEU:HA	1.78	0.43
1:B:473:THR:HA	1:B:476:ILE:HD12	2.01	0.43
1:C:328:PHE:HA	1:C:331:TRP:CD1	2.54	0.43
1:C:333:LEU:HD22	1:C:337:VAL:HG23	1.99	0.43
1:D:255:LEU:HD22	1:D:270:TYR:CD1	2.54	0.43
3:F:502:TBR:BRC	2:G:59:HIS:CG	3.27	0.43
2:H:10:GLN:H	2:H:10:GLN:CD	2.26	0.43
1:A:9:ILE:H	1:A:9:ILE:HG12	1.56	0.43
1:A:457:LYS:O	1:A:461:ILE:HG13	2.18	0.43
1:B:4:ARG:H	1:B:4:ARG:HG2	1.42	0.43
1:D:128:LEU:HD11	1:D:225:THR:HA	2.00	0.43
2:E:125:PRO:C	5:E:501:NAD:H72N	2.27	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:29:VAL:HA	2:F:48:VAL:O	2.18	0.43
2:H:101:SER:HB3	2:H:104:TYR:HD2	1.83	0.43
2:H:165:PRO:HB2	2:H:166:LEU:H	1.51	0.43
2:H:295:ILE:HD12	2:H:298:VAL:HG11	2.01	0.43
2:H:428:ILE:H	2:H:428:ILE:HG12	1.57	0.43
1:C:13:LEU:HD23	1:C:13:LEU:HA	1.79	0.42
1:C:134:LEU:HD23	1:C:134:LEU:HA	1.81	0.42
1:C:138:GLY:O	1:C:142:ILE:HG22	2.18	0.42
1:C:361:ILE:O	1:C:365:THR:HG23	2.19	0.42
1:D:76:PHE:O	1:D:80:LEU:HB2	2.18	0.42
1:D:476:ILE:HG12	1:D:482:PHE:CD1	2.53	0.42
2:H:406:PRO:HB2	2:H:443:TYR:HE2	1.83	0.42
1:A:21:MET:HE1	1:A:130:TYR:CE1	2.54	0.42
1:D:31:TYR:HD1	1:D:125:LYS:HG3	1.84	0.42
1:D:438:LEU:HB3	1:D:440:PRO:HD2	2.01	0.42
2:E:43:TYR:HE2	3:E:503:TBR:BR7	2.56	0.42
2:G:452:GLN:O	2:G:454:SER:N	2.52	0.42
1:B:194:ILE:O	1:B:198:VAL:HG12	2.18	0.42
2:E:393:LYS:O	2:E:397:ARG:HD2	2.19	0.42
2:F:235:ILE:O	2:F:257:VAL:HA	2.19	0.42
2:H:124:ALA:HA	2:H:125:PRO:HD3	1.86	0.42
2:H:262:ARG:HB2	5:H:501:NAD:N7A	2.33	0.42
1:A:21:MET:HB2	1:A:43:PHE:HB2	2.00	0.42
1:A:291:PHE:CZ	1:A:295:LEU:HD11	2.54	0.42
1:B:142:ILE:HG23	1:B:352:THR:HG22	2.00	0.42
1:B:150:LEU:HB2	1:B:151:PRO:HD3	2.01	0.42
1:B:406:TYR:HA	1:B:471:ILE:CD1	2.49	0.42
1:C:39:PHE:CE2	1:C:87:PRO:HB3	2.55	0.42
1:C:252:ASN:N	1:C:348:CYS:HB2	2.34	0.42
1:C:341:PHE:CE2	1:D:411:VAL:HG13	2.54	0.42
1:A:251:CYS:SG	1:A:276:PHE:HD1	2.43	0.42
1:B:18:SER:HB2	1:B:47:LEU:HD23	2.00	0.42
1:C:357:LYS:O	1:C:360:ARG:HB2	2.20	0.42
1:D:190:LEU:C	1:D:192:LEU:H	2.28	0.42
2:E:452:GLN:HA	2:E:453:PRO:HD2	1.74	0.42
2:F:152:LYS:HD2	2:F:152:LYS:HA	1.79	0.42
2:H:2:LYS:CB	2:H:25:ASP:HB3	2.49	0.42
2:H:405:PRO:HG2	2:H:447:VAL:HG23	2.00	0.42
1:B:72:ILE:HD13	1:B:72:ILE:HA	1.84	0.42
1:B:309:GLN:NE2	1:B:326:THR:HG22	2.33	0.42
1:B:361:ILE:O	1:B:365:THR:HG23	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:230:MET:SD	1:D:232:TYR:OH	2.67	0.42
1:D:317:ILE:HD13	1:D:442:LEU:HD11	2.01	0.42
2:G:403:LYS:H	2:G:403:LYS:HG3	1.59	0.42
1:A:316:SER:O	1:A:321:ALA:HB3	2.19	0.42
1:B:218:ILE:HD11	1:B:245:PHE:HD1	1.85	0.42
1:B:340:LEU:HD13	1:B:442:LEU:HB3	2.00	0.42
2:F:295:ILE:O	2:F:298:VAL:HG12	2.19	0.42
2:H:235:ILE:HB	2:H:257:VAL:HG22	2.01	0.42
1:B:178:ILE:C	1:B:180:GLU:N	2.78	0.42
1:D:28:ALA:O	1:D:29:LEU:HD23	2.20	0.42
2:E:85:VAL:O	2:E:89:LEU:HB2	2.19	0.42
2:E:130:THR:HG21	2:E:246:SER:OG	2.19	0.42
2:E:332:ARG:HG3	3:E:503:TBR:BR2	2.75	0.42
2:F:101:SER:HA	2:F:102:PRO:HD3	1.76	0.42
2:F:360:THR:HG23	2:F:370:VAL:HG12	2.01	0.42
1:B:39:PHE:N	1:B:39:PHE:CD2	2.87	0.42
1:B:354:GLY:HA3	1:B:468:ARG:NH2	2.35	0.42
1:B:466:PHE:HE1	1:B:474:LEU:HD22	1.85	0.42
1:D:150:LEU:HB2	1:D:151:PRO:HD3	2.02	0.42
1:D:333:LEU:O	1:D:336:PRO:HD2	2.19	0.42
1:D:460:LEU:O	1:D:464:MET:HG2	2.20	0.42
2:E:85:VAL:HG22	2:H:111:LEU:HD21	2.02	0.42
2:E:405:PRO:HG2	2:E:447:VAL:HG23	2.00	0.42
2:F:155:LEU:HD13	2:F:212:VAL:HG22	2.00	0.42
2:H:125:PRO:HB3	2:H:354:THR:HG21	2.01	0.42
1:A:300:TYR:CZ	1:A:309:GLN:HG3	2.55	0.42
1:B:252:ASN:HB2	1:B:348:CYS:CB	2.50	0.42
1:C:18:SER:HB2	1:C:47:LEU:HD23	2.02	0.42
1:C:342:SER:HA	1:C:345:ILE:HD12	2.01	0.42
2:H:101:SER:HA	2:H:102:PRO:HD3	1.78	0.42
1:A:200:PHE:HD1	1:A:200:PHE:HA	1.76	0.41
1:B:232:TYR:HD2	1:B:233:PHE:HB2	1.84	0.41
1:D:134:LEU:HA	1:D:134:LEU:HD23	1.78	0.41
2:E:147:SER:HB2	2:E:151:GLN:HA	2.02	0.41
2:G:101:SER:HA	2:G:102:PRO:HD3	1.81	0.41
1:A:75:LEU:HD12	1:A:75:LEU:HA	1.80	0.41
1:A:142:ILE:CG2	1:A:352:THR:HG22	2.49	0.41
1:B:380:ALA:HB2	2:E:280:PHE:CE1	2.56	0.41
1:C:392:PRO:C	1:C:394:ARG:H	2.27	0.41
1:D:217:THR:HG23	1:D:218:ILE:HD13	2.01	0.41
1:D:266:HIS:N	1:D:267:PRO:HD2	2.35	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:158:VAL:HG21	2:F:227:ARG:HD3	2.02	0.41
2:G:356:SER:HB3	2:G:371:SER:HA	2.01	0.41
1:C:363:LEU:HD12	1:C:399:VAL:HG21	2.01	0.41
2:F:59:HIS:CE1	3:G:502:TBR:BRC	3.28	0.41
2:F:195:ILE:HD12	2:F:195:ILE:HA	1.91	0.41
2:G:83:CYS:SG	2:G:97:ALA:HB2	2.60	0.41
2:G:225:LEU:HB3	2:G:226:GLN:H	1.61	0.41
2:G:295:ILE:O	2:G:298:VAL:HG12	2.20	0.41
2:H:36:LEU:HB3	2:H:47:VAL:HG11	2.02	0.41
2:H:126:GLU:N	5:H:501:NAD:H72N	2.17	0.41
1:A:86:LEU:HD12	1:A:86:LEU:HA	1.86	0.41
1:A:184:ALA:O	1:A:188:ILE:HG13	2.20	0.41
1:A:424:GLU:CD	1:B:425:LEU:HD11	2.46	0.41
1:B:328:PHE:HB3	1:B:331:TRP:HB2	2.00	0.41
1:C:26:LEU:O	1:C:30:LEU:HB2	2.21	0.41
1:C:317:ILE:HG21	1:C:339:LEU:HB3	2.02	0.41
1:D:334:PHE:HD2	1:D:335:LEU:HD22	1.84	0.41
2:G:10:GLN:HG2	2:G:11:VAL:H	1.85	0.41
1:B:199:ALA:HB1	1:B:241:ILE:HD13	2.02	0.41
1:D:251:CYS:SG	1:D:276:PHE:HD1	2.43	0.41
2:E:98:ARG:HG3	2:E:125:PRO:HD3	2.02	0.41
2:E:155:LEU:HD11	2:E:210:PHE:HB3	2.03	0.41
2:F:148:PHE:HB2	2:F:153:VAL:HG13	2.02	0.41
2:F:156:VAL:HG12	2:F:211:PHE:HB2	2.03	0.41
1:A:317:ILE:HD12	1:A:339:LEU:HD23	2.03	0.41
2:E:394:VAL:HG12	2:E:428:ILE:HG21	2.02	0.41
2:G:112:PHE:CE1	2:G:122:LEU:HD21	2.56	0.41
2:G:313:MET:HE3	2:G:313:MET:HA	2.01	0.41
1:A:134:LEU:HD23	1:A:134:LEU:HA	1.84	0.41
1:A:184:ALA:HB1	1:A:257:PHE:HE1	1.84	0.41
1:B:183:LYS:HE3	1:B:187:TYR:HE2	1.85	0.41
1:B:317:ILE:HG21	1:B:339:LEU:HB3	2.03	0.41
1:C:66:SER:O	1:C:69:GLY:N	2.54	0.41
1:C:142:ILE:HD13	1:C:352:THR:HA	2.03	0.41
1:C:367:GLN:OE1	1:C:396:VAL:HG13	2.19	0.41
1:C:373:LYS:HD2	1:C:382:TYR:CE1	2.56	0.41
1:D:21:MET:HB2	1:D:43:PHE:HB2	2.02	0.41
1:D:39:PHE:CE2	1:D:87:PRO:HB3	2.56	0.41
1:D:143:ILE:HG21	1:D:253:PHE:CD2	2.55	0.41
1:B:310:ALA:O	1:B:314:THR:HG23	2.20	0.41
1:C:86:LEU:HD12	1:C:86:LEU:HA	1.81	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:147:VAL:HG11	1:C:181:THR:OG1	2.20	0.41
1:C:460:LEU:O	1:C:464:MET:HG2	2.20	0.41
1:D:483:TRP:HA	1:D:484:ARG:HA	1.85	0.41
2:E:239:GLY:HA2	5:E:501:NAD:C8A	2.50	0.41
2:F:320:ARG:NE	2:F:320:ARG:HA	2.35	0.41
2:G:36:LEU:HB3	2:G:47:VAL:HG11	2.02	0.41
2:G:414:VAL:HB	2:G:433:HIS:HB2	2.03	0.41
2:H:7:GLY:O	2:H:12:GLY:HA3	2.20	0.41
1:A:252:ASN:HB2	1:A:348:CYS:CB	2.51	0.41
1:A:259:ALA:HA	1:A:266:HIS:NE2	2.35	0.41
1:A:297:HIS:CD2	1:A:332:PRO:HG3	2.55	0.41
1:A:438:LEU:HB3	1:A:440:PRO:CD	2.51	0.41
1:B:134:LEU:HD23	1:B:134:LEU:HA	1.81	0.41
1:B:363:LEU:HB3	1:B:367:GLN:HE21	1.84	0.41
1:C:71:LEU:HD12	1:C:71:LEU:HA	1.91	0.41
1:C:418:ILE:HD12	1:D:337:VAL:HG11	2.01	0.41
1:D:39:PHE:N	1:D:39:PHE:HD2	2.18	0.41
1:D:199:ALA:HB1	1:D:241:ILE:HD13	2.03	0.41
2:E:79:ASN:HD22	2:E:79:ASN:HA	1.58	0.41
2:E:124:ALA:O	2:E:128:LEU:HG	2.20	0.41
2:E:295:ILE:O	2:E:298:VAL:HG12	2.21	0.41
2:F:224:GLU:H	2:F:224:GLU:HG2	1.54	0.41
2:F:360:THR:HG22	2:F:370:VAL:H	1.86	0.41
2:G:10:GLN:HG2	2:G:11:VAL:N	2.36	0.41
2:G:148:PHE:HB2	2:G:153:VAL:HG13	2.02	0.41
2:G:191:GLN:HB3	2:G:192:GLY:H	1.79	0.41
1:A:178:ILE:C	1:A:180:GLU:H	2.28	0.41
1:A:230:MET:SD	1:A:232:TYR:OH	2.73	0.41
1:A:354:GLY:HA3	1:A:468:ARG:HH22	1.86	0.41
1:B:229:SER:OG	1:B:230:MET:N	2.53	0.41
1:B:291:PHE:CZ	1:B:295:LEU:HD11	2.56	0.41
1:D:357:LYS:O	1:D:360:ARG:HB2	2.21	0.41
2:E:101:SER:HA	2:E:102:PRO:HD3	1.77	0.41
2:F:107:GLU:H	2:F:107:GLU:HG2	1.71	0.41
2:F:124:ALA:HA	2:F:125:PRO:HD3	1.79	0.41
2:G:75:THR:HG21	2:G:78:THR:HG23	2.03	0.41
2:G:190:ARG:NH2	2:G:202:ILE:O	2.54	0.41
2:G:265:GLN:CD	2:G:265:GLN:H	2.28	0.41
2:G:267:ALA:O	2:G:279:VAL:HG11	2.21	0.41
2:G:402:ILE:H	2:G:402:ILE:HG13	1.50	0.41
1:A:138:GLY:O	1:A:142:ILE:HG22	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:LEU:O	1:A:367:GLN:HG3	2.22	0.40
1:A:395:VAL:O	1:A:399:VAL:HG23	2.21	0.40
1:B:200:PHE:CG	1:B:205:MET:HE3	2.55	0.40
1:C:434:THR:OG1	1:C:460:LEU:HD22	2.21	0.40
1:C:438:LEU:HB2	1:C:439:GLY:HA2	2.02	0.40
1:D:367:GLN:OE1	1:D:396:VAL:HG13	2.20	0.40
2:E:10:GLN:CG	2:E:98:ARG:HH22	2.34	0.40
2:F:364:ARG:HB3	2:F:366:ASP:OD1	2.21	0.40
1:A:38:PRO:HG3	1:A:90:ILE:HG12	2.02	0.40
1:A:256:HIS:HD2	1:A:270:TYR:OH	2.03	0.40
1:B:317:ILE:HD11	1:B:442:LEU:HD21	2.03	0.40
1:B:442:LEU:HD22	1:B:442:LEU:HA	1.87	0.40
1:B:466:PHE:CE1	1:B:474:LEU:HD22	2.56	0.40
1:C:142:ILE:CG2	1:C:352:THR:HG22	2.50	0.40
1:C:291:PHE:CZ	1:C:295:LEU:HD11	2.56	0.40
1:C:337:VAL:HG11	1:D:418:ILE:HD12	2.02	0.40
1:C:458:TRP:CE3	1:C:461:ILE:HD12	2.56	0.40
2:F:26:ILE:O	2:F:45:LEU:HB2	2.20	0.40
2:G:84:GLN:HA	2:G:118:PRO:CG	2.51	0.40
1:A:18:SER:O	1:A:43:PHE:HD1	2.05	0.40
1:A:374:ARG:HD2	1:B:394:ARG:NH2	2.35	0.40
1:B:121:ASP:OD1	1:B:226:HIS:HA	2.22	0.40
1:C:22:LEU:HD21	1:C:43:PHE:CD2	2.56	0.40
1:C:180:GLU:HG3	1:C:181:THR:HG23	2.02	0.40
2:E:165:PRO:HB2	2:E:166:LEU:H	1.57	0.40
2:E:230:LYS:HA	2:E:231:PRO:HD3	1.91	0.40
2:F:7:GLY:O	2:F:12:GLY:HA3	2.21	0.40
2:F:67:ASP:HA	2:F:93:PRO:HG2	2.01	0.40
2:H:19:LEU:HB2	2:H:26:ILE:HD11	2.02	0.40
2:H:169:ASN:HB3	2:H:201:THR:O	2.22	0.40
1:A:158:MET:HE3	1:A:158:MET:HB2	1.74	0.40
1:A:287:PHE:CD2	1:A:288:LEU:HD23	2.56	0.40
1:A:363:LEU:HD23	1:A:363:LEU:HA	1.77	0.40
1:B:142:ILE:CG2	1:B:352:THR:HG22	2.50	0.40
1:B:340:LEU:HB2	1:B:442:LEU:HD12	2.02	0.40
1:D:218:ILE:HD12	1:D:218:ILE:HA	1.88	0.40
2:F:53:SER:OG	2:G:104:TYR:OH	2.26	0.40
2:F:125:PRO:HB3	2:F:354:THR:HG22	2.03	0.40
2:G:2:LYS:CB	2:G:25:ASP:HB3	2.52	0.40
2:H:51:HIS:HD2	2:H:54:HIS:NE2	2.20	0.40
1:A:236:TYR:CD2	1:A:236:TYR:N	2.88	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:320:THR:HG22	1:B:320:THR:O	2.21	0.40
1:B:417:LEU:HD11	1:B:460:LEU:HD21	2.03	0.40
1:C:3:PHE:O	1:C:7:ILE:HG13	2.22	0.40
1:D:71:LEU:HA	1:D:71:LEU:HD12	1.86	0.40
1:D:283:GLN:HE21	1:D:315:VAL:HA	1.86	0.40
1:D:363:LEU:HB3	1:D:367:GLN:HE21	1.87	0.40
1:D:406:TYR:HA	1:D:471:ILE:CD1	2.52	0.40
2:F:397:ARG:HH11	2:F:402:ILE:HG23	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	374/395 (95%)	296 (79%)	78 (21%)	1	7
1	B	374/395 (95%)	296 (79%)	78 (21%)	1	7
1	C	374/395 (95%)	302 (81%)	72 (19%)	1	9
1	D	374/395 (95%)	302 (81%)	72 (19%)	1	9
2	E	370/378 (98%)	307 (83%)	63 (17%)	2	13
2	F	366/378 (97%)	305 (83%)	61 (17%)	2	13
2	G	372/378 (98%)	319 (86%)	53 (14%)	3	17
2	H	370/378 (98%)	299 (81%)	71 (19%)	1	9
All	All	2974/3092 (96%)	2426 (82%)	548 (18%)	1	11

All (548) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	6	ILE
1	A	9	ILE
1	A	12	LEU
1	A	16	LEU
1	A	26	LEU
1	A	30	LEU
1	A	32	ARG
1	A	33	ASP
1	A	47	LEU
1	A	52	MET
1	A	54	TRP
1	A	60	HIS
1	A	67	ARG
1	A	72	ILE
1	A	75	LEU
1	A	78	THR
1	A	90	ILE
1	A	111	THR
1	A	115	THR
1	A	117	ILE
1	A	122	GLU
1	A	128	LEU
1	A	153	LEU
1	A	155	ILE
1	A	190	LEU
1	A	194	ILE
1	A	198	VAL
1	A	202	LEU
1	A	206	THR
1	A	218	ILE
1	A	227	ASP
1	A	234	ASP
1	A	235	SER
1	A	236	TYR
1	A	244	VAL
1	A	249	SER
1	A	255	LEU
1	A	275	GLU
1	A	280	ILE
1	A	283	GLN
1	A	288	LEU
1	A	296	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	324	THR
1	A	326	THR
1	A	333	LEU
1	A	340	LEU
1	A	343	SER
1	A	345	ILE
1	A	352	THR
1	A	356	MET
1	A	361	ILE
1	A	366	LEU
1	A	370	ARG
1	A	372	LEU
1	A	374	ARG
1	A	375	LEU
1	A	383	THR
1	A	394	ARG
1	A	395	VAL
1	A	400	TRP
1	A	408	LEU
1	A	414	MET
1	A	420	THR
1	A	425	LEU
1	A	429	SER
1	A	434	THR
1	A	435	LEU
1	A	442	LEU
1	A	444	GLU
1	A	447	LEU
1	A	454	ASP
1	A	473	THR
1	A	476	ILE
1	A	477	LEU
1	A	478	LEU
1	A	483	TRP
1	A	484	ARG
1	B	1	MET
1	B	6	ILE
1	B	9	ILE
1	B	12	LEU
1	B	16	LEU
1	B	26	LEU
1	B	30	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	32	ARG
1	B	33	ASP
1	B	47	LEU
1	B	52	MET
1	B	54	TRP
1	B	67	ARG
1	B	72	ILE
1	B	75	LEU
1	B	78	THR
1	B	90	ILE
1	B	111	THR
1	B	115	THR
1	B	117	ILE
1	B	122	GLU
1	B	128	LEU
1	B	153	LEU
1	B	155	ILE
1	B	190	LEU
1	B	194	ILE
1	B	198	VAL
1	B	200	PHE
1	B	202	LEU
1	B	206	THR
1	B	218	ILE
1	B	223	PHE
1	B	227	ASP
1	B	233	PHE
1	B	234	ASP
1	B	235	SER
1	B	236	TYR
1	B	255	LEU
1	B	275	GLU
1	B	280	ILE
1	B	283	GLN
1	B	285	LEU
1	B	288	LEU
1	B	296	LYS
1	B	324	THR
1	B	326	THR
1	B	333	LEU
1	B	341	PHE
1	B	345	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	352	THR
1	B	356	MET
1	B	359	ILE
1	B	363	LEU
1	B	366	LEU
1	B	370	ARG
1	B	372	LEU
1	B	374	ARG
1	B	375	LEU
1	B	383	THR
1	B	391	LEU
1	B	394	ARG
1	B	395	VAL
1	B	400	TRP
1	B	408	LEU
1	B	414	MET
1	B	420	THR
1	B	425	LEU
1	B	429	SER
1	B	434	THR
1	B	435	LEU
1	B	442	LEU
1	B	444	GLU
1	B	447	LEU
1	B	473	THR
1	B	476	ILE
1	B	477	LEU
1	B	478	LEU
1	B	483	TRP
1	C	1	MET
1	C	6	ILE
1	C	9	ILE
1	C	12	LEU
1	C	16	LEU
1	C	26	LEU
1	C	29	LEU
1	C	30	LEU
1	C	32	ARG
1	C	33	ASP
1	C	47	LEU
1	C	54	TRP
1	C	60	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	67	ARG
1	C	72	ILE
1	C	75	LEU
1	C	78	THR
1	C	90	ILE
1	C	115	THR
1	C	117	ILE
1	C	121	ASP
1	C	122	GLU
1	C	128	LEU
1	C	153	LEU
1	C	155	ILE
1	C	190	LEU
1	C	194	ILE
1	C	198	VAL
1	C	200	PHE
1	C	202	LEU
1	C	206	THR
1	C	218	ILE
1	C	233	PHE
1	C	234	ASP
1	C	244	VAL
1	C	249	SER
1	C	275	GLU
1	C	280	ILE
1	C	283	GLN
1	C	288	LEU
1	C	296	LYS
1	C	318	SER
1	C	324	THR
1	C	326	THR
1	C	333	LEU
1	C	341	PHE
1	C	345	ILE
1	C	352	THR
1	C	356	MET
1	C	359	ILE
1	C	363	LEU
1	C	364	LEU
1	C	366	LEU
1	C	372	LEU
1	C	374	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	375	LEU
1	C	383	THR
1	C	394	ARG
1	C	395	VAL
1	C	400	TRP
1	C	408	LEU
1	C	434	THR
1	C	435	LEU
1	C	442	LEU
1	C	444	GLU
1	C	447	LEU
1	C	454	ASP
1	C	473	THR
1	C	476	ILE
1	C	477	LEU
1	C	478	LEU
1	C	483	TRP
1	D	1	MET
1	D	6	ILE
1	D	9	ILE
1	D	12	LEU
1	D	16	LEU
1	D	26	LEU
1	D	30	LEU
1	D	32	ARG
1	D	33	ASP
1	D	47	LEU
1	D	52	MET
1	D	54	TRP
1	D	60	HIS
1	D	67	ARG
1	D	72	ILE
1	D	78	THR
1	D	90	ILE
1	D	111	THR
1	D	115	THR
1	D	117	ILE
1	D	128	LEU
1	D	153	LEU
1	D	155	ILE
1	D	185	LEU
1	D	190	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	194	ILE
1	D	198	VAL
1	D	200	PHE
1	D	202	LEU
1	D	206	THR
1	D	218	ILE
1	D	234	ASP
1	D	236	TYR
1	D	244	VAL
1	D	280	ILE
1	D	285	LEU
1	D	288	LEU
1	D	296	LYS
1	D	324	THR
1	D	326	THR
1	D	333	LEU
1	D	341	PHE
1	D	345	ILE
1	D	352	THR
1	D	356	MET
1	D	359	ILE
1	D	363	LEU
1	D	366	LEU
1	D	370	ARG
1	D	372	LEU
1	D	374	ARG
1	D	375	LEU
1	D	391	LEU
1	D	394	ARG
1	D	395	VAL
1	D	400	TRP
1	D	408	LEU
1	D	414	MET
1	D	420	THR
1	D	425	LEU
1	D	429	SER
1	D	434	THR
1	D	435	LEU
1	D	437	ASN
1	D	442	LEU
1	D	444	GLU
1	D	447	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	473	THR
1	D	476	ILE
1	D	477	LEU
1	D	478	LEU
1	D	483	TRP
2	E	1	MET
2	E	3	ILE
2	E	14	THR
2	E	15	LEU
2	E	20	VAL
2	E	28	ILE
2	E	39	LEU
2	E	45	LEU
2	E	69	LEU
2	E	79	ASN
2	E	85	VAL
2	E	89	LEU
2	E	91	ASN
2	E	107	GLU
2	E	126	GLU
2	E	130	THR
2	E	150	GLU
2	E	151	GLN
2	E	152	LYS
2	E	156	VAL
2	E	167	VAL
2	E	176	GLU
2	E	198	GLN
2	E	216	ASN
2	E	218	ILE
2	E	221	VAL
2	E	225	LEU
2	E	226	GLN
2	E	227	ARG
2	E	234	ARG
2	E	243	ILE
2	E	254	THR
2	E	270	LEU
2	E	272	GLU
2	E	274	LEU
2	E	289	LEU
2	E	291	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	293	GLU
2	E	308	ASP
2	E	313	MET
2	E	314	SER
2	E	317	LEU
2	E	319	LYS
2	E	320	ARG
2	E	328	VAL
2	E	331	GLN
2	E	337	ASP
2	E	338	LEU
2	E	343	VAL
2	E	346	VAL
2	E	349	SER
2	E	351	GLN
2	E	354	THR
2	E	374	ARG
2	E	381	ILE
2	E	402	ILE
2	E	403	LYS
2	E	421	ILE
2	E	423	HIS
2	E	425	ARG
2	E	426	THR
2	E	444	VAL
2	E	450	LEU
2	F	3	ILE
2	F	14	THR
2	F	15	LEU
2	F	20	VAL
2	F	39	LEU
2	F	45	LEU
2	F	58	LEU
2	F	67	ASP
2	F	69	LEU
2	F	77	GLU
2	F	79	ASN
2	F	85	VAL
2	F	88	THR
2	F	96	VAL
2	F	105	LEU
2	F	107	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	F	123	ILE
2	F	126	GLU
2	F	151	GLN
2	F	156	VAL
2	F	201	THR
2	F	206	ASP
2	F	218	ILE
2	F	221	VAL
2	F	224	GLU
2	F	225	LEU
2	F	254	THR
2	F	270	LEU
2	F	272	GLU
2	F	274	LEU
2	F	277	THR
2	F	289	LEU
2	F	290	LEU
2	F	291	THR
2	F	296	ASP
2	F	300	VAL
2	F	308	ASP
2	F	313	MET
2	F	317	LEU
2	F	319	LYS
2	F	320	ARG
2	F	321	MET
2	F	328	VAL
2	F	338	LEU
2	F	340	GLN
2	F	343	VAL
2	F	346	VAL
2	F	351	GLN
2	F	352	GLN
2	F	362	VAL
2	F	364	ARG
2	F	367	ILE
2	F	381	ILE
2	F	402	ILE
2	F	403	LYS
2	F	404	LEU
2	F	421	ILE
2	F	425	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	F	426	THR
2	F	444	VAL
2	F	450	LEU
2	G	3	ILE
2	G	14	THR
2	G	15	LEU
2	G	20	VAL
2	G	39	LEU
2	G	45	LEU
2	G	67	ASP
2	G	69	LEU
2	G	77	GLU
2	G	79	ASN
2	G	85	VAL
2	G	89	LEU
2	G	92	THR
2	G	94	ASN
2	G	100	ARG
2	G	105	LEU
2	G	107	GLU
2	G	126	GLU
2	G	151	GLN
2	G	156	VAL
2	G	167	VAL
2	G	201	THR
2	G	218	ILE
2	G	221	VAL
2	G	225	LEU
2	G	233	ARG
2	G	234	ARG
2	G	254	THR
2	G	268	GLU
2	G	270	LEU
2	G	272	GLU
2	G	274	LEU
2	G	291	THR
2	G	313	MET
2	G	319	LYS
2	G	320	ARG
2	G	321	MET
2	G	328	VAL
2	G	338	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	G	343	VAL
2	G	346	VAL
2	G	351	GLN
2	G	362	VAL
2	G	367	ILE
2	G	381	ILE
2	G	402	ILE
2	G	403	LYS
2	G	421	ILE
2	G	423	HIS
2	G	426	THR
2	G	444	VAL
2	G	450	LEU
2	G	452	GLN
2	H	3	ILE
2	H	14	THR
2	H	20	VAL
2	H	39	LEU
2	H	45	LEU
2	H	58	LEU
2	H	69	LEU
2	H	72	VAL
2	H	79	ASN
2	H	85	VAL
2	H	100	ARG
2	H	105	LEU
2	H	107	GLU
2	H	114	SER
2	H	126	GLU
2	H	147	SER
2	H	151	GLN
2	H	156	VAL
2	H	167	VAL
2	H	176	GLU
2	H	181	ILE
2	H	188	ILE
2	H	191	GLN
2	H	218	ILE
2	H	221	VAL
2	H	225	LEU
2	H	234	ARG
2	H	254	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	270	LEU
2	H	272	GLU
2	H	273	GLN
2	H	274	LEU
2	H	275	GLU
2	H	277	THR
2	H	289	LEU
2	H	290	LEU
2	H	291	THR
2	H	293	GLU
2	H	308	ASP
2	H	313	MET
2	H	314	SER
2	H	317	LEU
2	H	319	LYS
2	H	320	ARG
2	H	321	MET
2	H	328	VAL
2	H	331	GLN
2	H	338	LEU
2	H	340	GLN
2	H	343	VAL
2	H	346	VAL
2	H	349	SER
2	H	351	GLN
2	H	352	GLN
2	H	354	THR
2	H	358	LEU
2	H	369	ASN
2	H	381	ILE
2	H	384	VAL
2	H	386	HIS
2	H	389	GLU
2	H	392	SER
2	H	394	VAL
2	H	402	ILE
2	H	403	LYS
2	H	421	ILE
2	H	424	ASP
2	H	426	THR
2	H	428	ILE
2	H	444	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	450	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	ASN
1	A	239	ASN
1	A	256	HIS
1	A	367	GLN
1	B	2	GLN
1	B	239	ASN
1	B	297	HIS
1	B	309	GLN
1	B	367	GLN
1	C	2	GLN
1	C	239	ASN
1	C	367	GLN
1	D	239	ASN
1	D	283	GLN
1	D	309	GLN
1	D	393	GLN
2	E	40	GLN
2	E	49	ASN
2	E	144	GLN
2	E	226	GLN
2	E	297	GLN
2	E	352	GLN
2	F	40	GLN
2	F	49	ASN
2	F	51	HIS
2	F	121	HIS
2	F	144	GLN
2	F	276	ASN
2	F	294	ASN
2	G	40	GLN
2	G	84	GLN
2	G	265	GLN
2	G	297	GLN
2	G	352	GLN
2	H	40	GLN
2	H	51	HIS
2	H	84	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	191	GLN
2	H	216	ASN
2	H	276	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 26 ligands modelled in this entry, 4 are monoatomic - leaving 22 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	TBR	C	502	-	0,36,36	-	-	-		
3	TBR	C	501	-	0,36,36	-	-	-		
3	TBR	H	502	-	0,36,36	-	-	-		
3	TBR	G	503	-	0,36,36	-	-	-		
5	NAD	H	501	-	46,48,48	1.23	4 (8%)	64,73,73	1.66	11 (17%)
3	TBR	E	502	-	0,36,36	-	-	-		
3	TBR	D	501	-	0,36,36	-	-	-		
3	TBR	E	503	-	0,36,36	-	-	-		
5	NAD	G	501	-	46,48,48	1.22	5 (10%)	64,73,73	1.63	11 (17%)
3	TBR	B	501	-	0,36,36	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAD	F	501	-	46,48,48	1.29	6 (13%)	64,73,73	1.64	8 (12%)
3	TBR	A	501	-	0,36,36	-	-	-		
3	TBR	F	503	-	0,36,36	-	-	-		
3	TBR	A	502	-	0,36,36	-	-	-		
3	TBR	G	502	-	0,36,36	-	-	-		
3	TBR	D	502	-	0,36,36	-	-	-		
3	TBR	A	503	-	0,36,36	-	-	-		
3	TBR	D	503	-	0,36,36	-	-	-		
3	TBR	B	502	-	0,36,36	-	-	-		
3	TBR	H	503	-	0,36,36	-	-	-		
5	NAD	E	501	-	46,48,48	1.22	4 (8%)	64,73,73	1.71	13 (20%)
3	TBR	F	502	-	0,36,36	-	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAD	H	501	-	-	8/30/62/62	0/5/5/5
5	NAD	E	501	-	-	5/30/62/62	0/5/5/5
5	NAD	G	501	-	-	8/30/62/62	0/5/5/5
5	NAD	F	501	-	-	9/30/62/62	0/5/5/5

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	501	NAD	C5A-C4A	5.11	1.48	1.39
5	E	501	NAD	C5A-C4A	5.08	1.48	1.39
5	G	501	NAD	C5A-C4A	4.96	1.47	1.39
5	H	501	NAD	C5A-C4A	4.94	1.47	1.39
5	H	501	NAD	C5A-N7A	-2.97	1.33	1.39
5	E	501	NAD	C5A-N7A	-2.86	1.33	1.39
5	F	501	NAD	C5A-N7A	-2.77	1.34	1.39
5	G	501	NAD	C5A-N7A	-2.69	1.34	1.39
5	F	501	NAD	C5A-C6A	2.46	1.47	1.41
5	G	501	NAD	C5A-C6A	2.44	1.47	1.41
5	H	501	NAD	C5A-C6A	2.32	1.47	1.41
5	F	501	NAD	PN-O3	2.27	1.61	1.59
5	E	501	NAD	C5A-C6A	2.24	1.47	1.41
5	F	501	NAD	C8A-N7A	2.19	1.35	1.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	501	NAD	O4D-C1D	2.12	1.43	1.40
5	G	501	NAD	C8A-N7A	2.09	1.35	1.31
5	E	501	NAD	O4D-C1D	2.07	1.43	1.40
5	H	501	NAD	C8A-N7A	2.01	1.35	1.31
5	G	501	NAD	O4D-C1D	2.00	1.43	1.40

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	501	NAD	C5A-C4A-N3A	-6.35	117.97	126.72
5	H	501	NAD	C5A-C4A-N3A	-6.26	118.10	126.72
5	G	501	NAD	C5A-C4A-N3A	-6.16	118.23	126.72
5	E	501	NAD	C5A-C4A-N3A	-6.10	118.32	126.72
5	H	501	NAD	N3A-C4A-N9A	5.37	136.31	127.17
5	E	501	NAD	N3A-C4A-N9A	5.25	136.10	127.17
5	G	501	NAD	N3A-C4A-N9A	5.16	135.94	127.17
5	F	501	NAD	N3A-C4A-N9A	5.03	135.71	127.17
5	E	501	NAD	O4B-C1B-N9A	4.75	117.21	108.09
5	G	501	NAD	O4B-C1B-N9A	3.95	115.67	108.09
5	F	501	NAD	O4B-C1B-N9A	3.72	115.23	108.09
5	H	501	NAD	O4B-C1B-N9A	3.63	115.06	108.09
5	F	501	NAD	C2A-N3A-C4A	3.53	120.45	111.83
5	H	501	NAD	C2A-N3A-C4A	3.47	120.31	111.83
5	G	501	NAD	C2A-N3A-C4A	3.44	120.23	111.83
5	E	501	NAD	C2A-N3A-C4A	3.33	119.96	111.83
5	F	501	NAD	C4A-C5A-N7A	-2.91	107.25	110.58
5	E	501	NAD	C1B-N9A-C8A	-2.81	120.85	127.09
5	H	501	NAD	N3A-C2A-N1A	-2.78	124.37	128.58
5	F	501	NAD	N3A-C2A-N1A	-2.77	124.39	128.58
5	H	501	NAD	C1B-N9A-C8A	-2.72	121.06	127.09
5	G	501	NAD	C4A-C5A-N7A	-2.70	107.49	110.58
5	G	501	NAD	N3A-C2A-N1A	-2.67	124.54	128.58
5	E	501	NAD	N3A-C2A-N1A	-2.62	124.62	128.58
5	H	501	NAD	C4A-C5A-N7A	-2.47	107.75	110.58
5	E	501	NAD	C4B-O4B-C1B	-2.44	104.09	109.47
5	E	501	NAD	C2B-C1B-N9A	2.33	119.09	113.30
5	G	501	NAD	C1B-N9A-C8A	-2.31	121.98	127.09
5	F	501	NAD	C1B-N9A-C8A	-2.28	122.03	127.09
5	E	501	NAD	C5N-C4N-C3N	-2.24	118.16	120.36
5	E	501	NAD	N6A-C6A-N1A	2.20	123.28	118.38
5	E	501	NAD	C4A-N9A-C1B	2.20	131.77	126.63
5	G	501	NAD	C5N-C4N-C3N	-2.15	118.25	120.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	501	NAD	C4A-C5A-N7A	-2.15	108.13	110.58
5	H	501	NAD	C5N-C4N-C3N	-2.14	118.26	120.36
5	H	501	NAD	C4B-O4B-C1B	-2.14	104.75	109.47
5	E	501	NAD	C2N-C3N-C4N	2.09	120.68	118.26
5	F	501	NAD	O4B-C1B-C2B	-2.06	102.21	106.62
5	G	501	NAD	C2N-C3N-C4N	2.05	120.64	118.26
5	G	501	NAD	C5A-N7A-C8A	2.03	106.64	103.45
5	G	501	NAD	C4A-N9A-C8A	2.01	107.85	105.74
5	H	501	NAD	C2B-C1B-N9A	2.00	118.28	113.30
5	H	501	NAD	N6A-C6A-N1A	2.00	122.83	118.38

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	G	501	NAD	C2N-C3N-C7N-O7N
5	G	501	NAD	C2N-C3N-C7N-N7N
5	E	501	NAD	O4B-C4B-C5B-O5B
5	G	501	NAD	C4N-C3N-C7N-N7N
5	G	501	NAD	C4N-C3N-C7N-O7N
5	E	501	NAD	C3B-C4B-C5B-O5B
5	G	501	NAD	O4B-C4B-C5B-O5B
5	H	501	NAD	O4B-C4B-C5B-O5B
5	F	501	NAD	O4B-C4B-C5B-O5B
5	G	501	NAD	C3B-C4B-C5B-O5B
5	H	501	NAD	C3B-C4B-C5B-O5B
5	H	501	NAD	C2N-C3N-C7N-N7N
5	F	501	NAD	C2N-C3N-C7N-N7N
5	H	501	NAD	C2N-C3N-C7N-O7N
5	F	501	NAD	C3B-C4B-C5B-O5B
5	F	501	NAD	C2B-C1B-N9A-C4A
5	F	501	NAD	C2N-C3N-C7N-O7N
5	H	501	NAD	C4N-C3N-C7N-N7N
5	G	501	NAD	C5B-O5B-PA-O3
5	F	501	NAD	C2B-C1B-N9A-C8A
5	F	501	NAD	C4N-C3N-C7N-N7N
5	H	501	NAD	C4N-C3N-C7N-O7N
5	F	501	NAD	C4N-C3N-C7N-O7N
5	E	501	NAD	O4B-C1B-N9A-C8A
5	G	501	NAD	O4B-C1B-N9A-C8A
5	H	501	NAD	O4B-C1B-N9A-C8A
5	F	501	NAD	O4B-C1B-N9A-C8A

Continued on next page...

Continued from previous page...

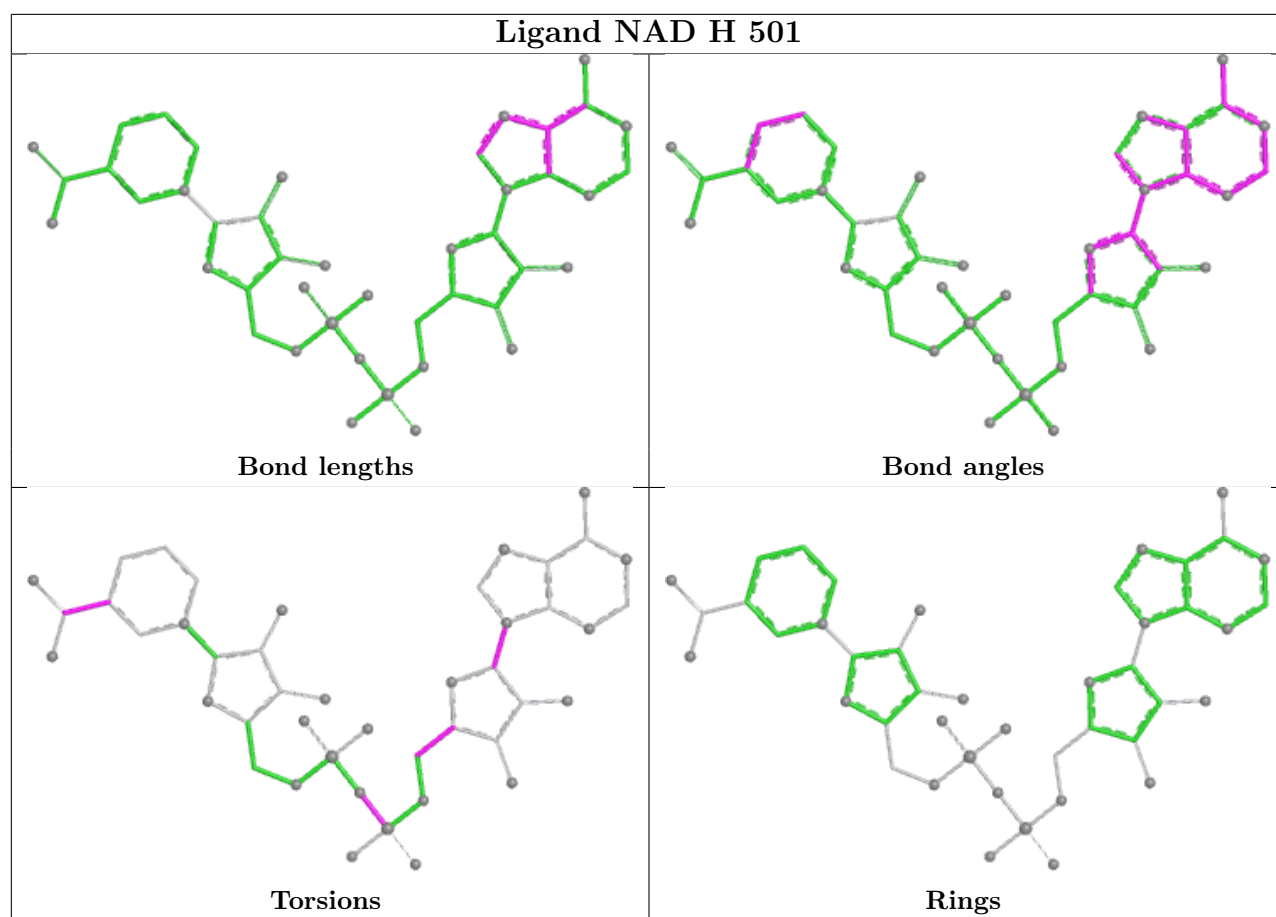
Mol	Chain	Res	Type	Atoms
5	E	501	NAD	C2N-C3N-C7N-N7N
5	E	501	NAD	PN-O3-PA-O1A
5	H	501	NAD	PN-O3-PA-O1A

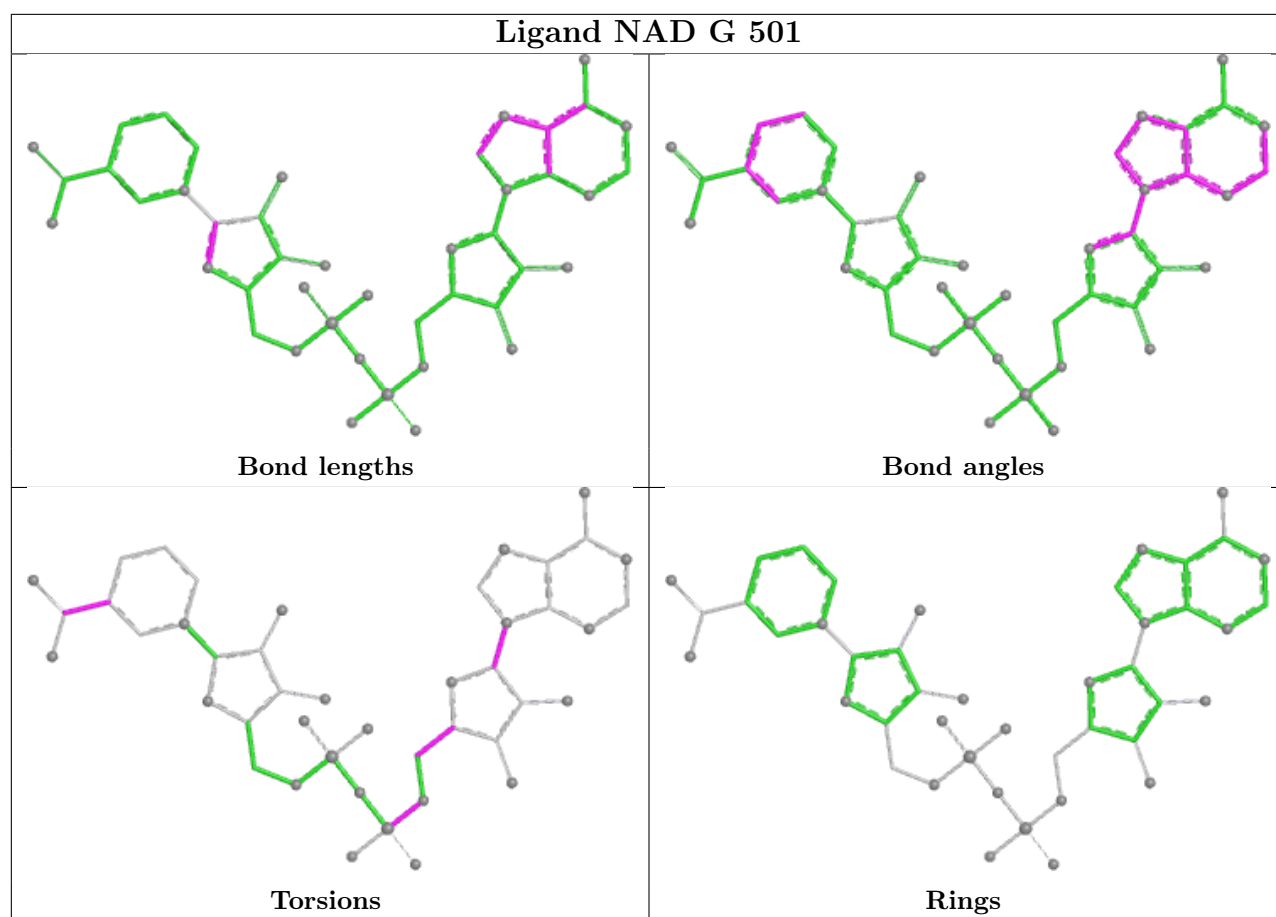
There are no ring outliers.

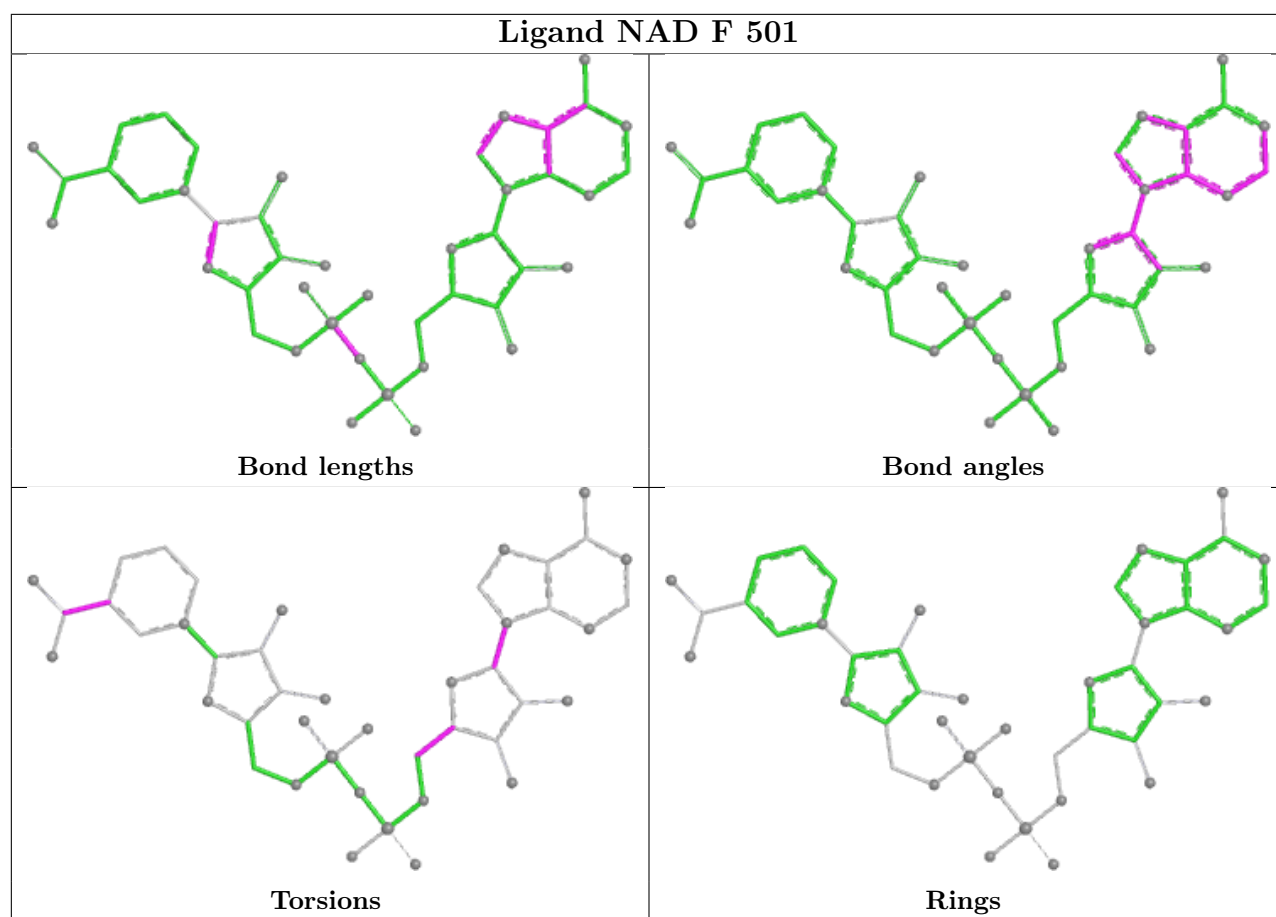
14 monomers are involved in 33 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	502	TBR	1	0
3	H	502	TBR	1	0
3	G	503	TBR	2	0
5	H	501	NAD	5	0
3	D	501	TBR	1	0
3	E	503	TBR	3	0
5	G	501	NAD	5	0
5	F	501	NAD	3	0
3	F	503	TBR	1	0
3	G	502	TBR	1	0
3	D	502	TBR	1	0
3	H	503	TBR	2	0
5	E	501	NAD	6	0
3	F	502	TBR	1	0

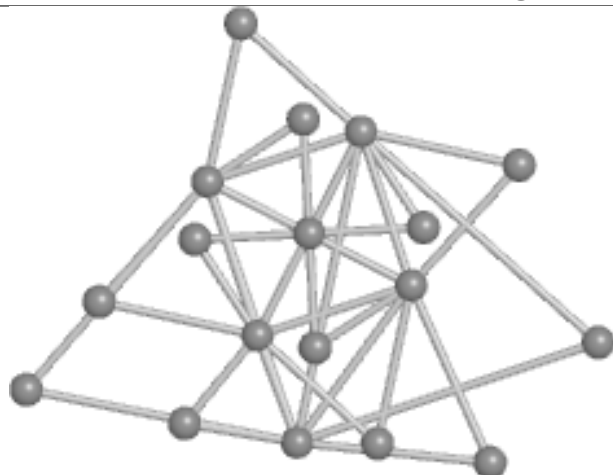
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



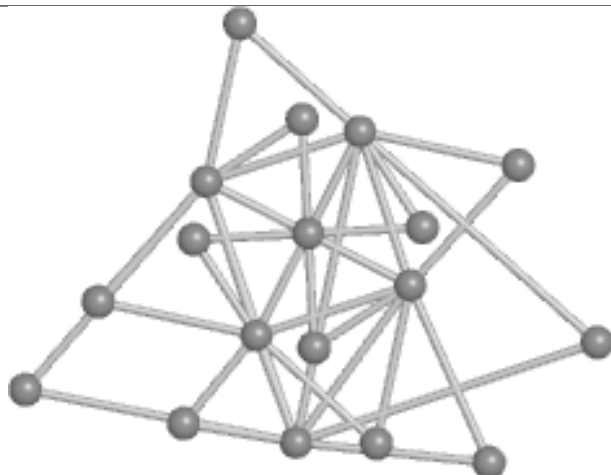




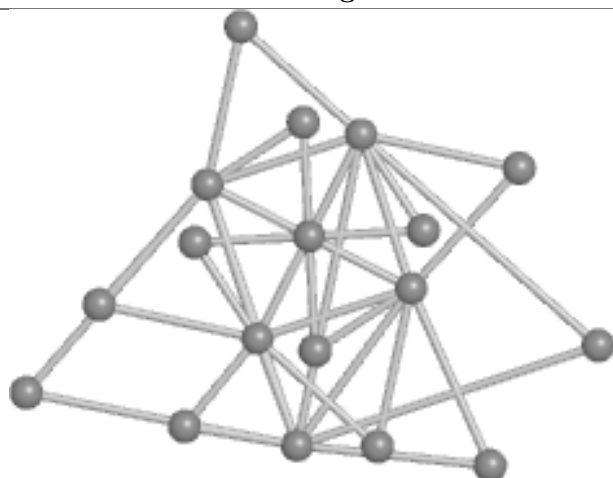
Ligand TBR A 501



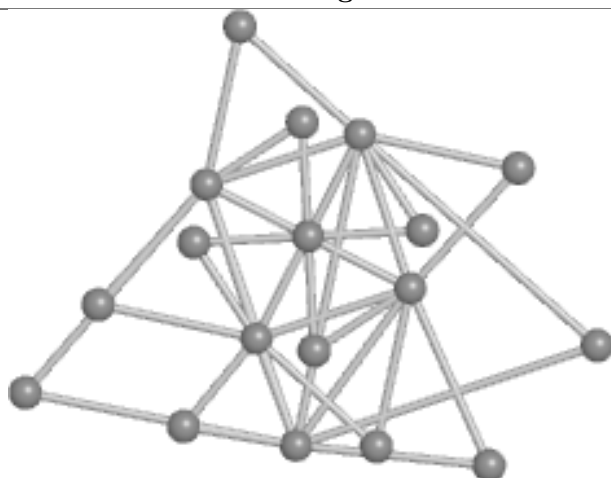
Bond lengths



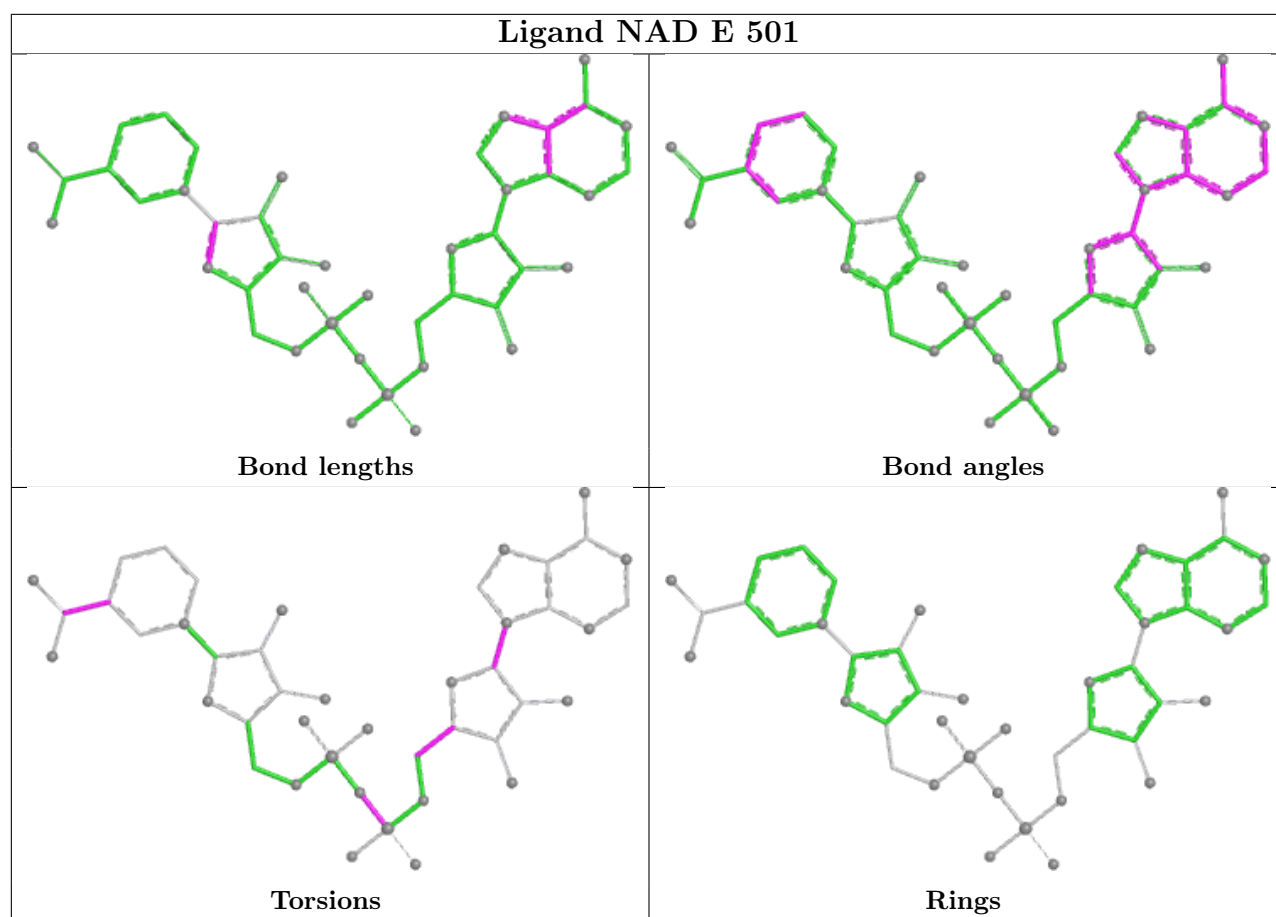
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å ²)	Q < 0.9
1	A	462/485 (95%)	0.17	28 (6%)	27	22	31, 70, 118, 155	0
1	B	462/485 (95%)	0.19	30 (6%)	25	21	29, 75, 127, 165	0
1	C	462/485 (95%)	0.43	36 (7%)	19	17	39, 94, 142, 173	0
1	D	462/485 (95%)	0.30	30 (6%)	25	21	41, 87, 139, 163	0
2	E	451/458 (98%)	0.21	20 (4%)	39	28	39, 84, 158, 186	0
2	F	444/458 (96%)	0.27	25 (5%)	30	23	43, 80, 132, 161	0
2	G	452/458 (98%)	0.16	14 (3%)	51	35	43, 89, 158, 181	0
2	H	450/458 (98%)	0.19	18 (4%)	42	30	43, 88, 158, 183	0
All	All	3645/3772 (96%)	0.24	201 (5%)	30	23	29, 83, 146, 186	0

All (201) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	443	GLY	7.4
1	B	118	VAL	7.2
2	F	11	VAL	6.1
1	D	424	GLU	5.9
1	C	118	VAL	5.8
1	C	444	GLU	5.8
1	C	155	ILE	5.7
1	A	203	ALA	5.5
1	B	145	LEU	5.3
1	A	125	LYS	5.2
2	F	14	THR	5.0
2	F	281	CYS	4.8
1	A	202	LEU	4.8
2	E	368	VAL	4.7
2	F	402	ILE	4.6
1	D	108	ALA	4.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	444	GLU	4.6
1	C	375	LEU	4.5
2	F	41	ASP	4.4
2	F	404	LEU	4.4
1	B	91	ALA	4.4
2	F	354	THR	4.4
1	C	135	GLN	4.3
1	C	378	PRO	4.3
2	F	22	GLU	4.3
1	C	154	GLY	4.3
1	C	138	GLY	4.2
2	F	103	GLU	4.2
2	F	406	PRO	4.1
1	C	337	VAL	4.1
1	D	226	HIS	4.0
1	B	424	GLU	3.9
2	F	318	ALA	3.9
2	F	399	ILE	3.9
1	D	70	PHE	3.9
2	F	400	GLY	3.9
2	F	43	TYR	3.9
2	G	37	ARG	3.9
1	D	476	ILE	3.8
1	B	149	ILE	3.8
1	A	121	ASP	3.8
2	H	125	PRO	3.7
1	A	424	GLU	3.7
1	B	234	ASP	3.7
2	H	221	VAL	3.7
2	E	145	VAL	3.6
1	B	146	ALA	3.6
2	E	43	TYR	3.6
1	C	424	GLU	3.6
1	B	266	HIS	3.6
2	E	4	ILE	3.5
1	C	333	LEU	3.5
1	C	157	GLY	3.5
1	C	194	ILE	3.4
1	C	376	VAL	3.3
1	D	482	PHE	3.3
1	B	443	GLY	3.3
1	A	33	ASP	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	33	ASP	3.2
1	C	445	VAL	3.2
1	A	91	ALA	3.2
1	D	135	GLN	3.2
1	A	204	GLY	3.2
1	C	53	CYS	3.2
2	F	211	PHE	3.2
1	D	35	ALA	3.2
2	E	428	ILE	3.1
2	G	281	CYS	3.1
1	D	121	ASP	3.1
2	H	81	ALA	3.1
1	D	269	TYR	3.1
2	G	34	ASP	3.1
1	B	135	GLN	3.0
1	B	142	ILE	3.0
1	C	10	VAL	3.0
1	C	235	SER	3.0
2	H	225	LEU	3.0
1	A	426	SER	3.0
2	H	428	ILE	3.0
1	B	66	SER	3.0
1	C	92	ASP	3.0
1	B	144	VAL	2.9
1	A	482	PHE	2.9
1	A	346	GLY	2.9
2	G	20	VAL	2.9
2	H	394	VAL	2.9
1	A	423	ASP	2.9
1	C	204	GLY	2.9
2	G	273	GLN	2.9
1	D	311	LEU	2.9
2	E	453	PRO	2.9
1	D	378	PRO	2.9
1	C	305	ASP	2.8
2	E	245	ALA	2.8
1	C	178	ILE	2.8
1	A	182	ALA	2.8
2	E	52	ALA	2.8
2	H	425	ARG	2.8
1	D	425	LEU	2.8
1	D	204	GLY	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	134	LEU	2.7
1	B	94	PRO	2.7
2	G	343	VAL	2.7
2	H	222	MET	2.7
1	A	73	VAL	2.7
1	D	440	PRO	2.7
1	B	425	LEU	2.7
1	A	142	ILE	2.7
1	A	199	ALA	2.7
2	F	12	GLY	2.7
2	E	281	CYS	2.7
1	D	282	ILE	2.6
1	A	247	LEU	2.6
1	B	202	LEU	2.6
1	A	198	VAL	2.6
1	C	145	LEU	2.6
2	F	150	GLU	2.6
2	F	245	ALA	2.5
2	H	199	GLY	2.5
2	E	379	GLU	2.5
2	E	430	GLN	2.5
1	A	226	HIS	2.5
2	E	381	ILE	2.5
2	H	404	LEU	2.5
2	F	381	ILE	2.4
2	G	105	LEU	2.4
1	B	445	VAL	2.4
2	E	38	GLU	2.4
1	A	425	LEU	2.4
2	E	284	ALA	2.4
1	D	445	VAL	2.4
2	E	42	LYS	2.4
1	C	136	TRP	2.4
1	D	151	PRO	2.4
1	C	415	LEU	2.4
2	F	15	LEU	2.4
1	D	479	THR	2.3
1	D	232	TYR	2.3
1	A	444	GLU	2.3
2	E	33	ALA	2.3
1	C	70	PHE	2.3
1	D	142	ILE	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	95	ASN	2.3
2	E	370	VAL	2.3
2	H	390	THR	2.3
1	D	51	ALA	2.3
2	H	418	GLU	2.3
2	H	402	ILE	2.3
1	C	141	GLY	2.3
2	H	408	THR	2.3
1	C	425	LEU	2.3
1	B	90	ILE	2.3
2	H	297	GLN	2.3
1	B	81	GLY	2.3
1	D	423	ASP	2.3
2	G	457	PHE	2.2
1	B	391	LEU	2.2
1	C	96	ILE	2.2
1	C	139	GLY	2.2
2	F	407	GLY	2.2
2	F	288	GLU	2.2
2	G	43	TYR	2.2
2	G	135	ARG	2.2
1	C	57	ASN	2.2
1	D	33	ASP	2.2
1	D	150	LEU	2.2
2	E	106	ALA	2.1
1	C	151	PRO	2.1
1	B	80	LEU	2.1
1	B	148	ALA	2.1
1	B	419	ALA	2.1
2	H	37	ARG	2.1
2	H	11	VAL	2.1
1	A	269	TYR	2.1
1	D	261	ALA	2.1
1	C	119	GLY	2.1
2	E	363	ARG	2.1
2	F	123	ILE	2.1
1	A	227	ASP	2.1
2	G	56	ASP	2.1
2	G	379	GLU	2.1
1	A	58	ARG	2.1
1	D	339	LEU	2.1
1	B	92	ASP	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	315	VAL	2.1
1	D	109	LEU	2.1
2	F	81	ALA	2.0
1	B	137	PHE	2.0
2	G	167	VAL	2.0
1	A	96	ILE	2.0
1	D	178	ILE	2.0
2	H	414	VAL	2.0
1	B	155	ILE	2.0
1	B	232	TYR	2.0
2	G	123	ILE	2.0
1	B	254	THR	2.0
1	D	60	HIS	2.0
1	A	70	PHE	2.0
1	A	260	PHE	2.0
2	E	58	LEU	2.0
2	F	379	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	TBR	D	503	18/18	0.53	0.24	73,128,323,367	18
3	TBR	A	503	18/18	0.64	0.13	99,160,345,346	18
3	TBR	E	502	18/18	0.69	0.12	59,128,282,314	18
3	TBR	G	502	18/18	0.69	0.12	70,139,259,285	18
3	TBR	H	502	18/18	0.70	0.12	83,180,334,361	18
3	TBR	F	502	18/18	0.75	0.15	81,118,256,309	18

Continued on next page...

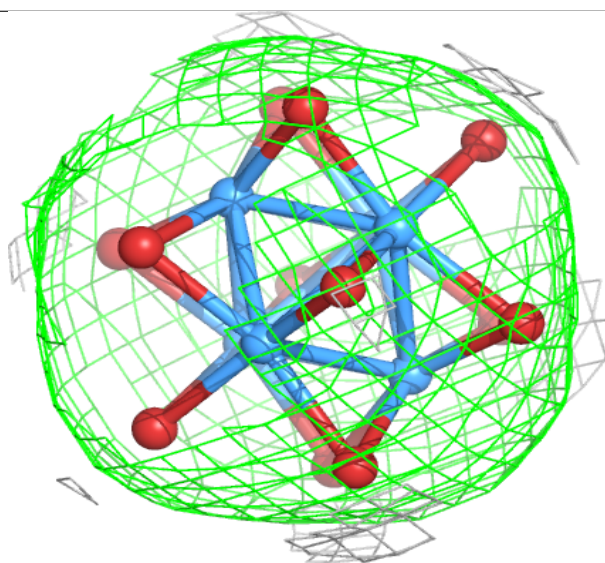
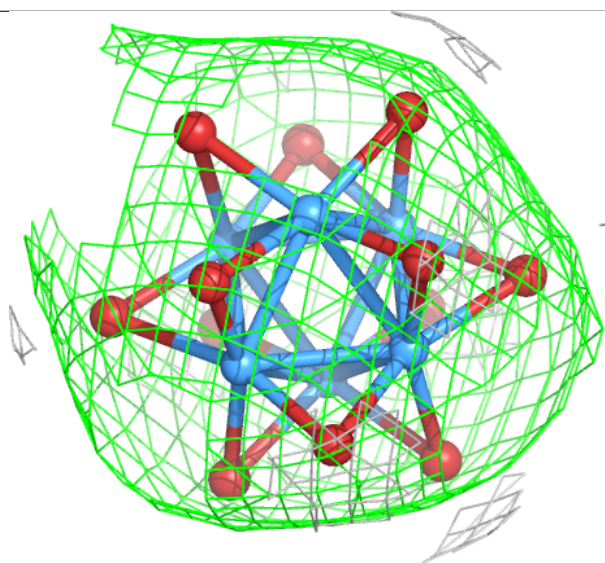
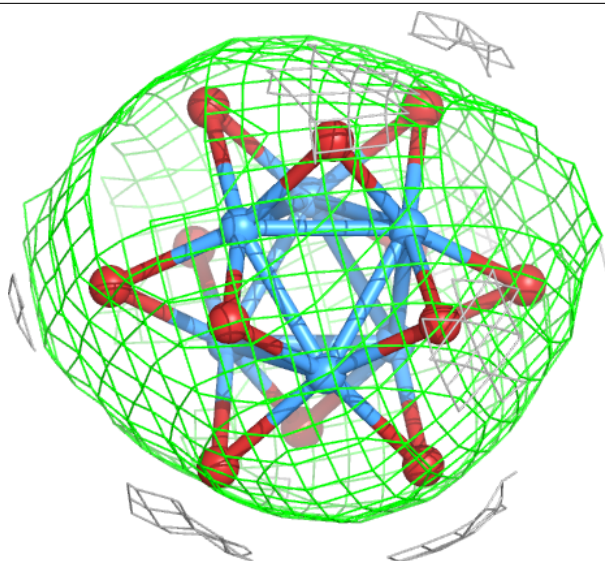
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	TBR	C	501	18/18	0.77	0.36	50,93,125,189	18
3	TBR	A	501	18/18	0.77	0.53	86,145,324,330	18
3	TBR	B	501	18/18	0.81	0.40	41,95,161,539	18
3	TBR	B	502	18/18	0.82	0.23	74,116,217,295	18
3	TBR	A	502	18/18	0.83	0.28	86,125,275,297	18
3	TBR	F	503	18/18	0.84	0.44	49,80,197,198	18
3	TBR	D	502	18/18	0.84	0.37	45,104,211,261	18
3	TBR	C	502	18/18	0.84	0.23	81,131,298,309	18
3	TBR	E	503	18/18	0.85	0.38	48,100,209,232	18
3	TBR	G	503	18/18	0.86	0.43	53,122,192,197	18
3	TBR	D	501	18/18	0.89	0.26	31,77,99,170	18
3	TBR	H	503	18/18	0.90	0.41	52,92,184,211	18
5	NAD	E	501	44/44	0.92	0.10	33,54,84,122	0
5	NAD	G	501	44/44	0.93	0.10	36,58,82,115	0
4	K	B	503	1/1	0.94	0.05	73,73,73,73	0
5	NAD	H	501	44/44	0.94	0.11	41,62,102,117	0
4	K	C	503	1/1	0.95	0.04	103,103,103,103	0
5	NAD	F	501	44/44	0.95	0.09	40,70,92,125	0
4	K	A	504	1/1	0.97	0.06	66,66,66,66	0
4	K	D	504	1/1	0.98	0.03	119,119,119,119	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

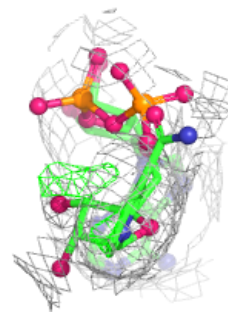
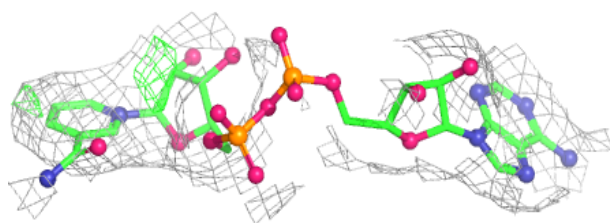
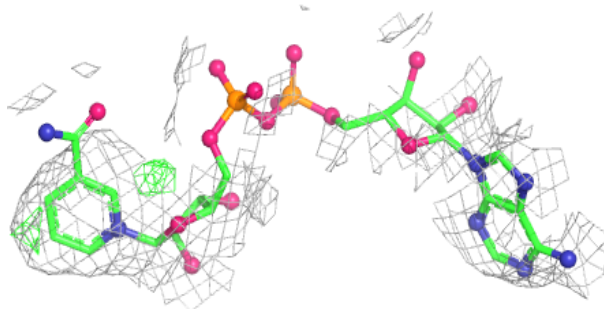
Electron density around TBR A 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

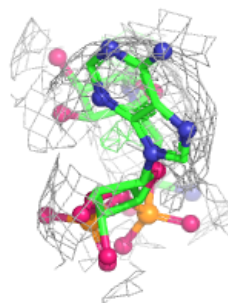
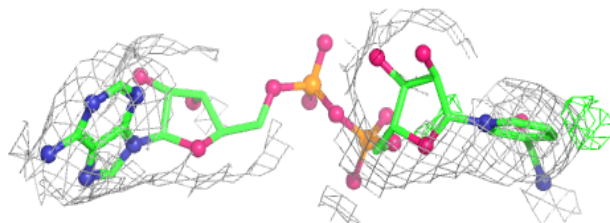
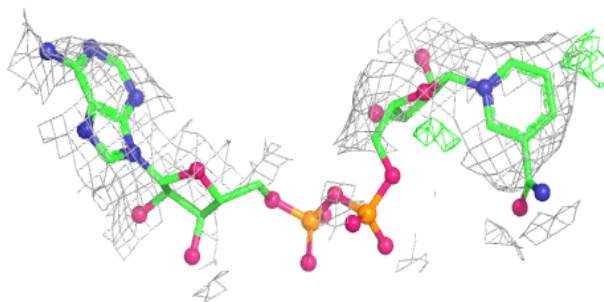


Electron density around NAD E 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

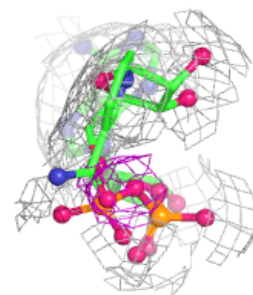
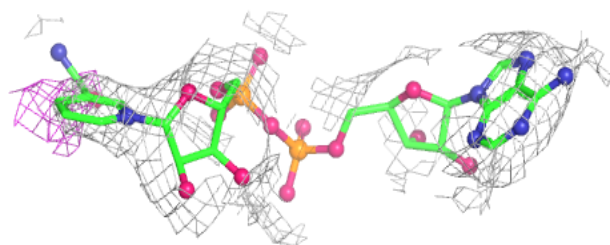
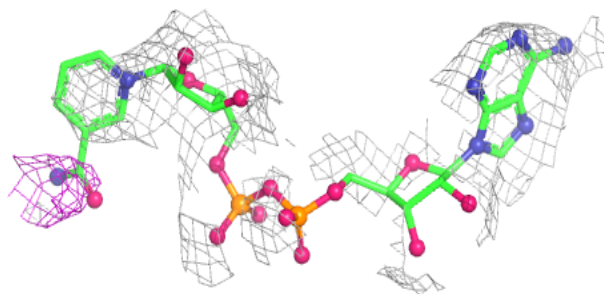
**Electron density around NAD G 501:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

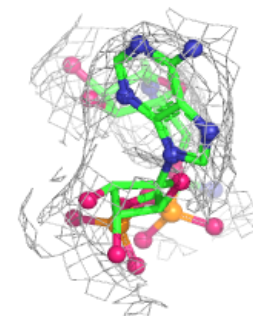
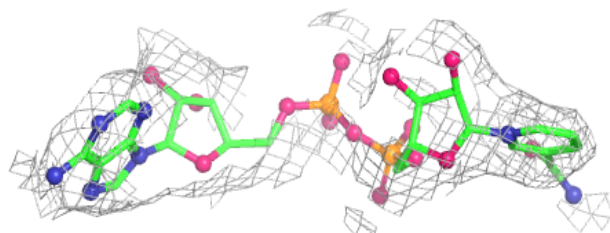
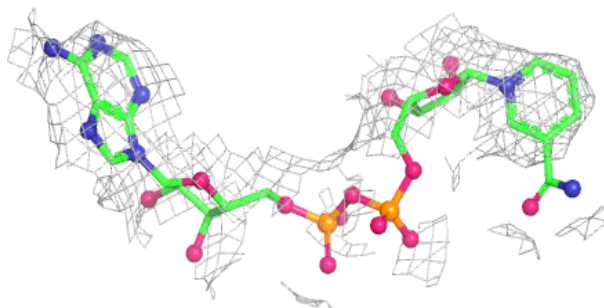


Electron density around NAD H 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around NAD F 501:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.