



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 03:30 AM UTC

PDB ID : 1E0J / pdb_00001e0j
Title : gp4d helicase from phage T7 ADPNP complex
Authors : Singleton, M.R.; Sawaya, M.R.; Ellenberger, T.; Wigley, D.B.
Deposited on : 2000-03-30
Resolution : 3.00 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

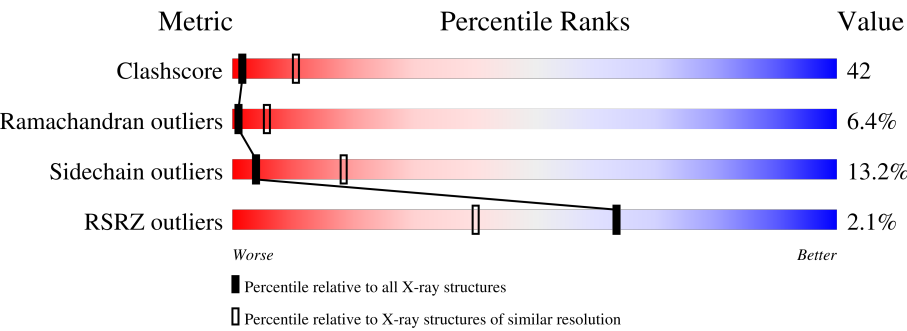
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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))
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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.

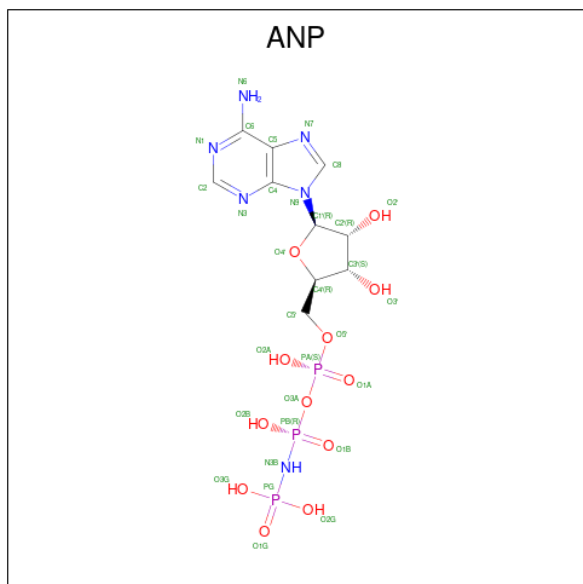
Mol	Chain	Length	Quality of chain
1	A	289	
1	B	289	
1	C	289	
1	D	289	
1	E	289	
1	F	289	

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 DNA HELICASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	287	Total 2204	C 1374	N 389	O 428	S 13	0	0	0
1	B	288	Total 2214	C 1378	N 390	O 433	S 13	0	0	0
1	C	288	Total 2214	C 1378	N 390	O 433	S 13	0	0	0
1	D	287	Total 2204	C 1374	N 389	O 428	S 13	0	0	0
1	E	288	Total 2214	C 1378	N 390	O 433	S 13	0	0	0
1	F	288	Total 2214	C 1378	N 390	O 433	S 13	0	0	0

- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: $\text{C}_{10}\text{H}_{17}\text{N}_6\text{O}_{12}\text{P}_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
2	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
2	D	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
2	E	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

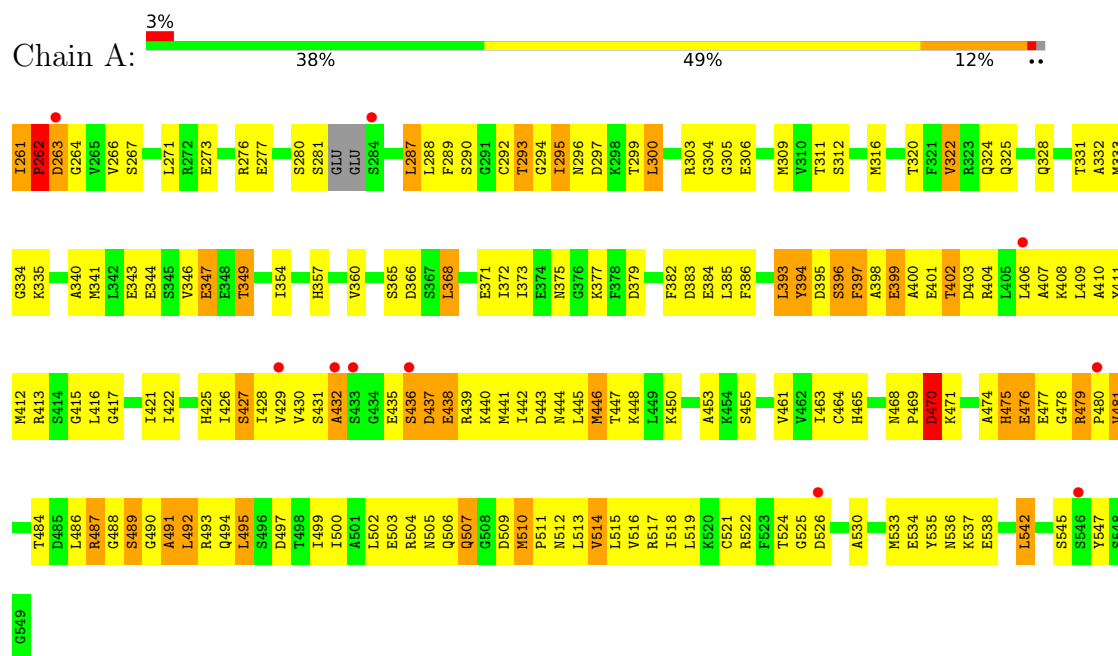
- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

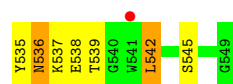
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		
3	E	1	Total	Mg	0	0
			1	1		

3 Residue-property plots

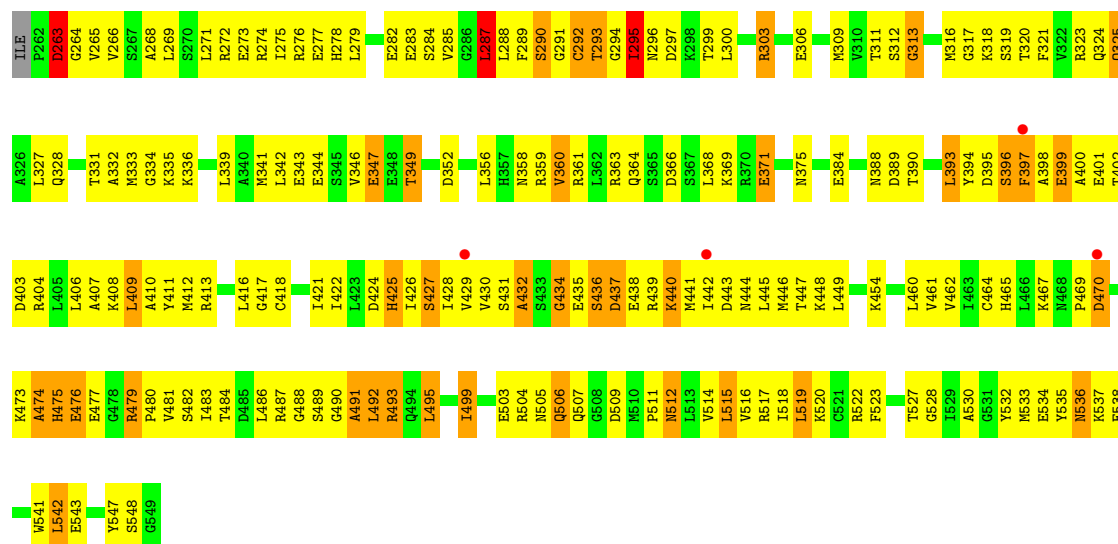
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: DNA HELICASE

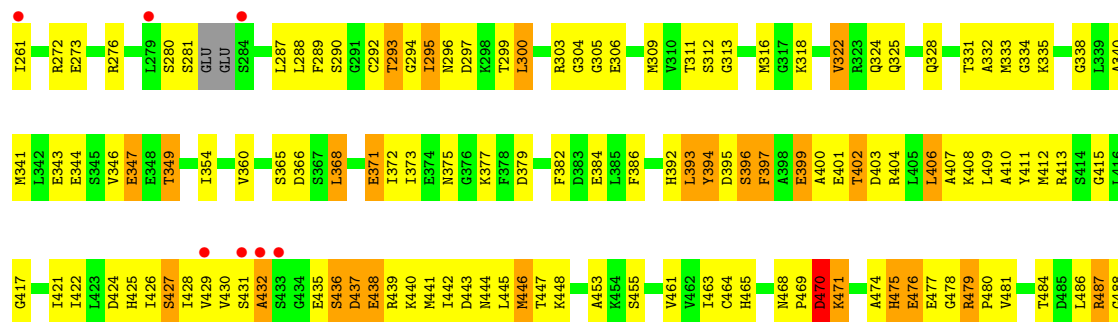




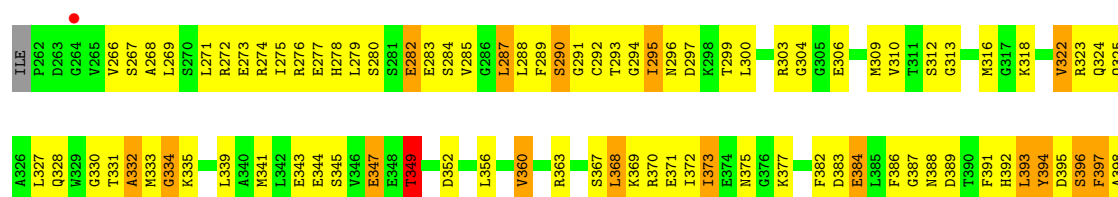
● Molecule 1: DNA HELICASE

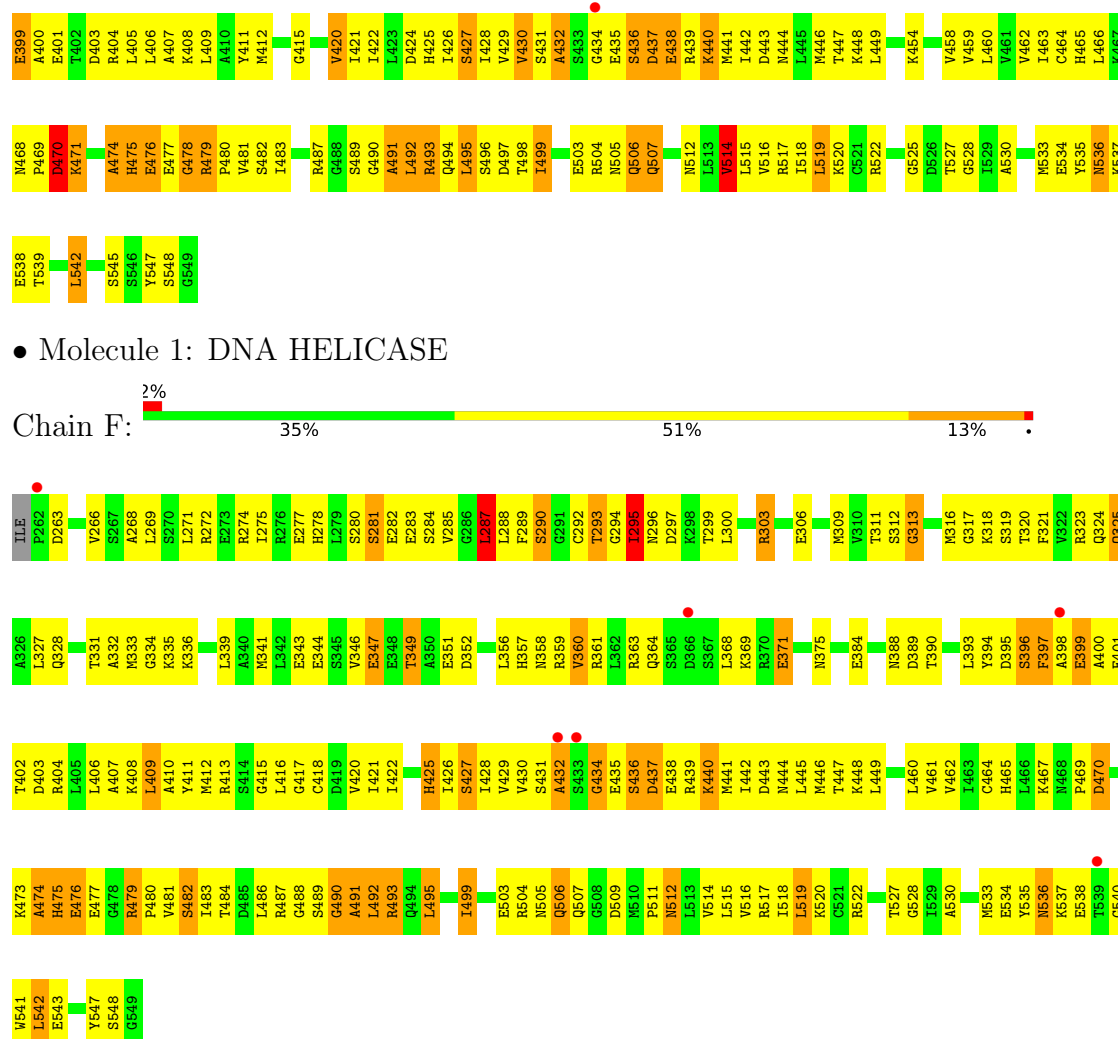


● Molecule 1: DNA HELICASE



● Molecule 1: DNA HELICASE





● Molecule 1: DNA HELICASE

Chain F: 2% 35% 51% 13%

4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	119.18Å 119.18Å 283.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00 20.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	96.7 (20.00-3.00) 97.5 (20.00-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.55 (at 2.98Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.253 , 0.304 0.244 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	72.3	Xtriage
Anisotropy	0.058	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 37.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	13392	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.45% of the height of the origin peak. No significant pseudotranslation is detected.*

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: MG, ANP

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	0.52	0/2233	1.08	13/2999 (0.4%)
1	B	0.54	0/2244	1.06	11/3014 (0.4%)
1	C	0.54	0/2244	1.08	12/3014 (0.4%)
1	D	0.49	0/2233	1.02	9/2999 (0.3%)
1	E	0.50	0/2244	1.05	12/3014 (0.4%)
1	F	0.53	0/2244	1.09	10/3014 (0.3%)
All	All	0.52	0/13442	1.06	67/18054 (0.4%)

There are no bond length outliers.

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	295	ILE	N-CA-C	-12.34	98.03	110.62
1	E	295	ILE	N-CA-C	-11.84	98.54	110.62
1	B	295	ILE	N-CA-C	-11.81	98.58	110.62
1	F	474	ALA	N-CA-C	11.78	127.02	109.24
1	C	474	ALA	N-CA-C	11.51	127.36	109.52
1	C	295	ILE	N-CA-C	-11.49	98.90	110.62
1	A	474	ALA	N-CA-C	11.43	126.95	110.14
1	E	474	ALA	N-CA-C	11.39	126.11	109.14
1	B	474	ALA	N-CA-C	11.11	125.69	109.14
1	D	474	ALA	N-CA-C	10.94	126.22	110.14
1	F	491	ALA	N-CA-C	-9.65	101.64	113.41
1	A	295	ILE	N-CA-C	-9.60	100.83	110.62
1	C	491	ALA	N-CA-C	-9.59	101.71	113.41
1	C	427	SER	N-CA-C	-9.51	102.48	114.56
1	A	261	ILE	CA-C-N	9.49	131.70	119.84
1	A	261	ILE	C-N-CA	9.49	131.70	119.84
1	F	427	SER	N-CA-C	-9.45	102.56	114.56
1	D	427	SER	N-CA-C	-9.27	103.07	114.75

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	427	SER	N-CA-C	-9.17	103.20	114.75
1	D	295	ILE	N-CA-C	-9.15	101.29	110.62
1	A	491	ALA	N-CA-C	-8.82	102.64	113.41
1	D	491	ALA	N-CA-C	-8.51	103.03	113.41
1	A	264	GLY	N-CA-C	8.50	127.27	114.61
1	A	394	TYR	N-CA-C	-8.29	99.35	110.55
1	F	293	THR	N-CA-C	-8.19	99.76	110.33
1	D	394	TYR	N-CA-C	-8.12	99.58	110.55
1	C	293	THR	N-CA-C	-8.10	99.89	110.33
1	B	293	THR	N-CA-C	-7.88	98.61	110.28
1	E	283	GLU	N-CA-C	7.87	122.27	109.76
1	F	283	GLU	N-CA-C	7.81	122.18	109.76
1	A	262	PRO	N-CA-C	7.73	128.40	112.47
1	B	394	TYR	N-CA-C	-7.15	101.09	110.53
1	E	293	THR	N-CA-C	-6.99	99.93	110.28
1	E	394	TYR	N-CA-C	-6.98	101.13	110.55
1	D	293	THR	N-CA-C	-6.84	101.47	110.43
1	F	409	LEU	N-CA-C	-6.67	104.02	111.28
1	E	491	ALA	N-CA-C	-6.66	103.19	112.45
1	A	304	GLY	N-CA-C	-6.66	104.02	112.54
1	B	283	GLU	N-CA-C	6.65	119.53	108.96
1	C	409	LEU	N-CA-C	-6.65	104.04	111.28
1	A	293	THR	N-CA-C	-6.59	101.79	110.43
1	B	427	SER	N-CA-C	-6.42	105.20	114.12
1	B	491	ALA	N-CA-C	-6.22	103.81	112.45
1	C	263	ASP	N-CA-C	6.05	118.39	108.52
1	E	427	SER	N-CA-C	-6.05	105.71	114.12
1	E	304	GLY	N-CA-C	-6.04	104.98	111.93
1	C	283	GLU	N-CA-C	5.94	119.21	109.76
1	E	349	THR	N-CA-C	-5.89	104.98	111.82
1	B	349	THR	N-CA-C	-5.89	104.99	111.82
1	B	478	GLY	N-CA-C	-5.75	102.41	112.53
1	F	313	GLY	N-CA-C	-5.68	106.08	112.33
1	C	473	LYS	N-CA-C	-5.59	99.31	108.76
1	D	510	MET	CA-C-N	5.44	125.27	119.28
1	D	510	MET	C-N-CA	5.44	125.27	119.28
1	F	473	LYS	N-CA-C	-5.36	99.71	108.76
1	B	304	GLY	N-CA-C	-5.31	105.83	111.93
1	E	478	GLY	N-CA-C	-5.25	102.70	112.37
1	E	525	GLY	N-CA-C	-5.19	107.83	115.30
1	C	342	LEU	N-CA-C	5.13	117.61	111.71
1	C	264	GLY	N-CA-C	-5.12	101.06	113.18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	510	MET	CA-C-N	5.11	124.90	119.28
1	A	510	MET	C-N-CA	5.11	124.90	119.28
1	F	263	ASP	N-CA-C	5.09	116.81	108.52
1	E	514	VAL	N-CA-C	5.08	115.44	108.12
1	D	304	GLY	N-CA-C	-5.06	105.62	112.14
1	B	393	LEU	N-CA-C	5.03	117.03	109.23
1	C	313	GLY	N-CA-C	-5.03	106.15	111.93

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	2204	0	2214	184	0
1	B	2214	0	2216	225	0
1	C	2214	0	2217	199	0
1	D	2204	0	2214	182	0
1	E	2214	0	2217	223	0
1	F	2214	0	2217	176	0
2	A	31	0	13	2	0
2	B	31	0	13	3	0
2	D	31	0	13	2	0
2	E	31	0	13	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
All	All	13392	0	13347	1116	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 42.

All (1116) 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:E:290:SER:H	1:E:325:GLN:NE2	1.46	1.14
1:D:476:GLU:HG3	1:E:483:ILE:HD12	1.25	1.10
1:A:290:SER:H	1:A:325:GLN:NE2	1.49	1.08
1:F:327:LEU:HD22	1:F:356:LEU:HD23	1.32	1.07
1:B:290:SER:H	1:B:325:GLN:NE2	1.51	1.05
1:C:327:LEU:HD22	1:C:356:LEU:HD23	1.38	1.03
1:B:476:GLU:HG3	1:C:483:ILE:HD12	1.40	1.03
1:D:290:SER:H	1:D:325:GLN:NE2	1.57	1.02
1:E:324:GLN:HE22	1:E:542:LEU:H	1.07	1.01
1:E:476:GLU:HG3	1:F:483:ILE:HD12	1.43	1.01
1:B:324:GLN:HE22	1:B:542:LEU:H	1.08	0.99
1:E:367:SER:HA	1:E:370:ARG:HH12	1.26	0.99
1:F:344:GLU:HG3	1:F:349:THR:HG22	1.45	0.98
1:B:367:SER:HA	1:B:370:ARG:HH12	1.26	0.98
1:F:290:SER:H	1:F:325:GLN:NE2	1.62	0.98
1:C:344:GLU:HG3	1:C:349:THR:HG22	1.47	0.96
1:A:476:GLU:HG3	1:B:483:ILE:HD12	1.49	0.94
1:A:324:GLN:HE22	1:A:542:LEU:H	1.08	0.94
1:D:506:GLN:HB2	1:E:527:THR:OG1	1.68	0.94
1:D:324:GLN:HE22	1:D:542:LEU:H	1.01	0.93
1:D:290:SER:H	1:D:325:GLN:HE22	1.08	0.93
1:C:290:SER:H	1:C:325:GLN:NE2	1.66	0.92
1:B:344:GLU:HG3	1:B:349:THR:HG22	1.52	0.92
1:C:440:LYS:HZ2	1:C:444:ASN:HB2	1.35	0.92
1:A:506:GLN:HB2	1:B:527:THR:OG1	1.71	0.91
1:E:440:LYS:HZ2	1:E:444:ASN:HB2	1.32	0.91
1:D:324:GLN:HE22	1:D:542:LEU:N	1.69	0.90
1:E:344:GLU:HG3	1:E:349:THR:HG22	1.53	0.90
1:E:290:SER:H	1:E:325:GLN:HE22	1.16	0.90
1:E:266:VAL:HG11	1:E:271:LEU:HD21	1.52	0.88
1:E:285:VAL:HG22	1:E:300:LEU:HD22	1.55	0.87
1:A:425:HIS:HE1	1:A:427:SER:HB2	1.40	0.87
1:A:290:SER:H	1:A:325:GLN:HE22	0.91	0.87
1:D:425:HIS:CE1	1:D:427:SER:HB2	2.10	0.87
1:B:266:VAL:HG11	1:B:271:LEU:HD21	1.55	0.86
1:D:324:GLN:NE2	1:D:542:LEU:H	1.73	0.86
1:D:425:HIS:HE1	1:D:427:SER:HB2	1.40	0.86
1:A:425:HIS:CE1	1:A:427:SER:HB2	2.11	0.86
1:A:290:SER:N	1:A:325:GLN:HE22	1.74	0.85
1:A:518:ILE:CD1	1:A:530:ALA:HB2	2.08	0.84
1:F:440:LYS:HZ2	1:F:444:ASN:HB2	1.41	0.84
1:A:324:GLN:HE22	1:A:542:LEU:N	1.74	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:429:VAL:HG23	1:F:430:VAL:H	1.41	0.84
1:C:425:HIS:CE1	1:C:427:SER:HB2	2.12	0.83
1:C:491:ALA:O	1:C:495:LEU:HD22	1.77	0.83
1:A:429:VAL:HG23	1:A:430:VAL:H	1.44	0.82
1:E:425:HIS:HE1	1:E:427:SER:HB2	1.43	0.82
1:B:370:ARG:HH11	1:B:370:ARG:HB3	1.44	0.82
1:E:309:MET:HE1	1:E:462:VAL:HG12	1.61	0.82
1:D:429:VAL:HG23	1:D:430:VAL:H	1.44	0.82
1:F:425:HIS:CE1	1:F:427:SER:HB2	2.13	0.82
1:F:491:ALA:O	1:F:495:LEU:HD22	1.80	0.82
1:C:404:ARG:NH1	1:C:408:LYS:HE3	1.95	0.82
1:C:429:VAL:HG23	1:C:430:VAL:H	1.43	0.81
1:D:477:GLU:OE2	1:E:482:SER:HB2	1.80	0.81
1:B:290:SER:H	1:B:325:GLN:HE21	1.28	0.81
1:B:309:MET:HE1	1:B:462:VAL:HG12	1.61	0.81
1:A:324:GLN:NE2	1:A:542:LEU:H	1.78	0.81
1:D:518:ILE:CD1	1:D:530:ALA:HB2	2.11	0.81
1:F:401:GLU:HA	1:F:430:VAL:O	1.80	0.81
1:B:425:HIS:HE1	1:B:427:SER:HB2	1.44	0.80
1:B:477:GLU:HA	1:B:505:ASN:HD22	1.46	0.80
1:B:290:SER:N	1:B:325:GLN:NE2	2.29	0.80
1:E:534:GLU:HG3	1:E:545:SER:HB2	1.63	0.80
1:E:477:GLU:HA	1:E:505:ASN:HD22	1.45	0.80
1:C:536:ASN:HD21	1:C:538:GLU:HB2	1.47	0.80
1:B:399:GLU:HB3	1:B:430:VAL:HG21	1.64	0.79
1:C:401:GLU:HA	1:C:430:VAL:O	1.81	0.79
1:E:399:GLU:HB3	1:E:430:VAL:HG21	1.64	0.79
1:B:440:LYS:HZ2	1:B:444:ASN:HB2	1.48	0.79
1:A:484:THR:HA	1:A:493:ARG:NH2	1.98	0.79
1:F:404:ARG:NH1	1:F:408:LYS:HE3	1.97	0.79
1:D:468:ASN:HD21	1:E:493:ARG:HD2	1.48	0.78
1:A:477:GLU:OE2	1:B:482:SER:HB2	1.84	0.78
1:C:425:HIS:HE1	1:C:427:SER:HB2	1.48	0.78
1:D:289:PHE:H	1:D:296:ASN:HD21	1.32	0.78
1:E:370:ARG:HH11	1:E:370:ARG:HB3	1.48	0.78
1:E:536:ASN:HD22	1:E:538:GLU:H	1.32	0.77
1:F:425:HIS:HE1	1:F:427:SER:HB2	1.49	0.77
1:B:534:GLU:HG3	1:B:545:SER:HB2	1.67	0.77
1:B:429:VAL:HG23	1:B:430:VAL:H	1.50	0.77
1:A:468:ASN:HD21	1:B:493:ARG:HD2	1.50	0.76
1:E:425:HIS:CE1	1:E:427:SER:HB2	2.20	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:339:LEU:HD22	1:B:341:MET:HE3	1.66	0.76
1:E:429:VAL:HG23	1:E:430:VAL:H	1.50	0.76
1:E:406:LEU:HD21	1:E:448:LYS:HB3	1.66	0.75
1:B:266:VAL:HG11	1:B:271:LEU:CD2	2.15	0.75
1:B:285:VAL:HG22	1:B:300:LEU:HD22	1.68	0.75
1:B:425:HIS:CE1	1:B:427:SER:HB2	2.22	0.75
1:A:290:SER:N	1:A:325:GLN:NE2	2.31	0.75
1:B:406:LEU:HD21	1:B:448:LYS:HB3	1.68	0.74
1:C:285:VAL:HG22	1:C:300:LEU:HD22	1.68	0.74
1:F:440:LYS:O	1:F:440:LYS:HD3	1.87	0.74
1:E:339:LEU:HD22	1:E:341:MET:HE3	1.68	0.74
1:B:536:ASN:HD22	1:B:538:GLU:H	1.36	0.74
1:D:484:THR:HA	1:D:493:ARG:NH2	2.03	0.74
1:C:289:PHE:H	1:C:296:ASN:HD21	1.36	0.73
1:C:440:LYS:O	1:C:440:LYS:HD3	1.88	0.73
1:D:290:SER:N	1:D:325:GLN:HE22	1.84	0.73
1:C:404:ARG:HH12	1:C:408:LYS:CE	2.02	0.73
1:E:367:SER:HA	1:E:370:ARG:NH1	2.04	0.73
1:C:404:ARG:HH12	1:C:408:LYS:HE3	1.52	0.73
1:E:536:ASN:ND2	1:E:538:GLU:H	1.87	0.73
1:C:316:MET:HA	1:C:504:ARG:NH1	2.05	0.72
1:C:313:GLY:HA3	1:C:316:MET:SD	2.29	0.72
1:E:536:ASN:ND2	1:E:539:THR:H	1.87	0.72
1:F:404:ARG:HH12	1:F:408:LYS:CE	2.02	0.72
1:B:290:SER:H	1:B:325:GLN:HE22	1.35	0.72
1:B:367:SER:HA	1:B:370:ARG:NH1	2.04	0.72
1:B:476:GLU:O	1:B:506:GLN:HG2	1.89	0.72
1:A:510:MET:HE1	1:A:547:TYR:CE1	2.25	0.72
1:E:375:ASN:HD21	1:E:377:LYS:CG	2.02	0.72
1:F:518:ILE:HD13	1:F:530:ALA:HB2	1.69	0.72
1:F:316:MET:HA	1:F:504:ARG:NH1	2.05	0.72
1:F:536:ASN:HD21	1:F:538:GLU:HB2	1.54	0.72
1:B:324:GLN:NE2	1:B:542:LEU:H	1.87	0.72
1:F:404:ARG:HH12	1:F:408:LYS:HE3	1.54	0.72
1:C:331:THR:HG22	1:C:332:ALA:N	2.04	0.72
1:B:489:SER:O	1:B:491:ALA:N	2.23	0.71
1:D:438:GLU:HA	1:D:441:MET:HG2	1.72	0.71
1:E:489:SER:O	1:E:491:ALA:N	2.23	0.71
1:C:399:GLU:HB3	1:C:430:VAL:HG21	1.72	0.71
1:D:309:MET:HE2	1:D:464:CYS:SG	2.31	0.71
1:F:313:GLY:HA3	1:F:316:MET:SD	2.31	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:536:ASN:C	1:C:536:ASN:HD22	1.97	0.71
1:E:476:GLU:O	1:E:506:GLN:HG2	1.91	0.71
1:A:438:GLU:HA	1:A:441:MET:HG2	1.73	0.71
1:B:395:ASP:O	1:B:396:SER:HB2	1.90	0.71
1:F:489:SER:O	1:F:491:ALA:N	2.24	0.70
1:E:284:SER:O	1:E:303:ARG:HD2	1.90	0.70
1:B:536:ASN:ND2	1:B:539:THR:H	1.89	0.70
1:E:393:LEU:N	1:E:393:LEU:HD12	2.06	0.70
1:F:404:ARG:HH12	1:F:408:LYS:NZ	1.89	0.70
1:E:324:GLN:NE2	1:E:542:LEU:H	1.87	0.70
1:B:375:ASN:HD21	1:B:377:LYS:CG	2.04	0.70
1:D:492:LEU:C	1:D:494:GLN:H	1.98	0.69
1:E:536:ASN:HD22	1:E:536:ASN:C	1.99	0.69
1:B:536:ASN:HD22	1:B:536:ASN:C	2.00	0.69
1:E:404:ARG:NH1	1:E:408:LYS:HE3	2.08	0.69
1:E:426:ILE:CD1	1:E:446:MET:HE3	2.22	0.69
1:F:476:GLU:O	1:F:506:GLN:HG2	1.92	0.69
1:A:492:LEU:C	1:A:494:GLN:H	1.98	0.69
1:F:331:THR:HG22	1:F:332:ALA:N	2.07	0.69
1:B:394:TYR:HE1	1:B:408:LYS:HD2	1.58	0.69
1:D:440:LYS:HD3	1:D:440:LYS:O	1.93	0.69
1:F:399:GLU:HB3	1:F:430:VAL:HG21	1.75	0.69
1:A:354:ILE:HD11	1:A:386:PHE:HE2	1.56	0.68
1:B:324:GLN:HE22	1:B:542:LEU:N	1.88	0.68
1:B:404:ARG:NH1	1:B:408:LYS:HE3	2.08	0.68
1:C:311:THR:HG21	1:C:486:LEU:HD21	1.74	0.68
1:C:489:SER:O	1:C:491:ALA:N	2.26	0.68
1:C:404:ARG:HH12	1:C:408:LYS:NZ	1.90	0.68
1:C:469:PRO:HG3	1:C:474:ALA:CB	2.23	0.68
1:D:510:MET:HE1	1:D:547:TYR:CE1	2.28	0.68
1:E:395:ASP:O	1:E:396:SER:HB2	1.93	0.68
1:F:280:SER:O	1:F:281:SER:HB2	1.92	0.68
1:C:518:ILE:HD13	1:C:530:ALA:HB2	1.73	0.68
1:E:536:ASN:HD21	1:E:538:GLU:HB2	1.59	0.68
1:B:429:VAL:HG23	1:B:430:VAL:N	2.08	0.68
1:E:394:TYR:HE1	1:E:408:LYS:HD2	1.58	0.68
1:E:429:VAL:HG23	1:E:430:VAL:N	2.08	0.68
1:E:290:SER:N	1:E:325:GLN:NE2	2.31	0.68
1:F:509:ASP:O	1:F:511:PRO:HD3	1.94	0.68
1:C:476:GLU:O	1:C:506:GLN:HG2	1.93	0.67
1:C:439:ARG:O	1:C:442:ILE:HG22	1.93	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:437:ASP:C	1:A:439:ARG:H	2.03	0.67
1:B:426:ILE:CD1	1:B:446:MET:HE3	2.24	0.67
1:B:394:TYR:CE1	1:B:408:LYS:HD2	2.30	0.67
1:C:343:GLU:HG3	1:C:428:ILE:HD11	1.76	0.67
1:C:484:THR:HA	1:C:493:ARG:NH2	2.09	0.67
1:F:285:VAL:HG22	1:F:300:LEU:HD22	1.75	0.67
1:F:444:ASN:OD1	1:F:448:LYS:HE2	1.95	0.67
1:A:383:ASP:CG	1:B:272:ARG:HH22	2.01	0.67
1:B:393:LEU:N	1:B:393:LEU:HD12	2.10	0.67
1:F:439:ARG:O	1:F:442:ILE:HG22	1.95	0.67
1:D:375:ASN:HD21	1:D:377:LYS:CG	2.07	0.67
1:B:370:ARG:HB3	1:B:370:ARG:NH1	2.07	0.67
1:C:509:ASP:O	1:C:511:PRO:HD3	1.95	0.67
1:D:354:ILE:HD11	1:D:386:PHE:HE2	1.60	0.67
1:F:400:ALA:O	1:F:430:VAL:HB	1.95	0.67
1:A:375:ASN:HD21	1:A:377:LYS:CG	2.08	0.66
1:C:444:ASN:OD1	1:C:448:LYS:HE2	1.94	0.66
1:A:477:GLU:HA	1:A:505:ASN:HD22	1.61	0.66
1:B:478:GLY:O	1:B:479:ARG:HB3	1.96	0.66
1:B:536:ASN:ND2	1:B:538:GLU:H	1.92	0.66
1:D:468:ASN:HD21	1:E:493:ARG:CD	2.08	0.66
1:F:429:VAL:HG23	1:F:430:VAL:N	2.11	0.66
1:A:534:GLU:HG3	1:A:545:SER:HB2	1.76	0.66
1:B:507:GLN:NE2	1:C:528:GLY:HA2	2.10	0.66
1:E:394:TYR:CE1	1:E:408:LYS:HD2	2.31	0.66
1:E:370:ARG:HB3	1:E:370:ARG:NH1	2.10	0.66
1:A:478:GLY:O	1:A:479:ARG:HB3	1.95	0.66
1:B:506:GLN:HB2	1:C:527:THR:OG1	1.96	0.66
1:E:375:ASN:HD21	1:E:377:LYS:HG3	1.60	0.66
1:D:437:ASP:C	1:D:439:ARG:H	2.04	0.65
1:F:446:MET:HE2	1:F:449:LEU:HD12	1.77	0.65
1:B:440:LYS:NZ	1:B:444:ASN:HB2	2.09	0.65
1:C:309:MET:HE2	1:C:464:CYS:HB3	1.78	0.65
1:C:477:GLU:HA	1:C:505:ASN:ND2	2.11	0.65
1:C:429:VAL:HG23	1:C:430:VAL:N	2.11	0.65
1:F:290:SER:H	1:F:325:GLN:HE21	1.41	0.65
1:F:469:PRO:HG3	1:F:474:ALA:CB	2.25	0.65
1:E:324:GLN:HE22	1:E:542:LEU:N	1.87	0.65
1:F:309:MET:HE2	1:F:464:CYS:HB3	1.79	0.65
1:D:477:GLU:HA	1:D:505:ASN:HD22	1.60	0.65
1:E:290:SER:N	1:E:325:GLN:HE22	1.92	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:311:THR:HG21	1:F:486:LEU:HD21	1.78	0.65
1:A:440:LYS:O	1:A:440:LYS:HD3	1.97	0.65
1:B:536:ASN:HD21	1:B:538:GLU:HB2	1.61	0.65
1:F:536:ASN:C	1:F:536:ASN:HD22	2.02	0.65
1:E:477:GLU:OE2	1:F:482:SER:HB2	1.96	0.64
1:E:478:GLY:O	1:E:479:ARG:HB3	1.97	0.64
1:C:422:ILE:HD13	1:C:461:VAL:HB	1.78	0.64
1:B:468:ASN:HD21	1:C:493:ARG:CZ	2.11	0.64
1:E:446:MET:HE2	1:E:446:MET:HA	1.79	0.64
1:D:401:GLU:HA	1:D:430:VAL:O	1.97	0.64
1:A:305:GLY:HA2	1:A:453:ALA:O	1.98	0.64
1:A:429:VAL:HG23	1:A:430:VAL:N	2.12	0.64
1:A:492:LEU:C	1:A:494:GLN:N	2.56	0.64
1:A:489:SER:O	1:A:491:ALA:N	2.31	0.64
1:B:446:MET:HE2	1:B:446:MET:HA	1.80	0.64
1:C:402:THR:HG23	1:C:445:LEU:HD13	1.79	0.64
1:C:400:ALA:O	1:C:430:VAL:HB	1.98	0.64
1:D:492:LEU:C	1:D:494:GLN:N	2.56	0.64
1:D:290:SER:N	1:D:325:GLN:NE2	2.39	0.63
1:E:536:ASN:HD22	1:E:538:GLU:N	1.95	0.63
1:F:343:GLU:C	1:F:397:PHE:HE1	2.06	0.63
1:B:470:ASP:OD2	1:C:467:LYS:NZ	2.31	0.63
1:D:489:SER:O	1:D:491:ALA:N	2.32	0.63
1:E:290:SER:H	1:E:325:GLN:HE21	1.38	0.63
1:F:343:GLU:HG3	1:F:428:ILE:HD11	1.80	0.63
1:E:476:GLU:CG	1:F:483:ILE:HD12	2.26	0.63
1:B:480:PRO:HA	1:B:503:GLU:CD	2.22	0.63
1:C:446:MET:HE2	1:C:449:LEU:HD12	1.80	0.63
1:E:440:LYS:O	1:E:440:LYS:HD3	1.97	0.63
1:E:480:PRO:HA	1:E:503:GLU:CD	2.23	0.63
1:B:382:PHE:HE1	1:C:275:ILE:HD12	1.63	0.63
1:D:429:VAL:HG23	1:D:430:VAL:N	2.12	0.63
1:E:446:MET:HE2	1:E:449:LEU:HD12	1.81	0.63
1:C:328:GLN:HG3	1:C:333:MET:HE3	1.80	0.63
1:E:426:ILE:HG12	1:E:426:ILE:O	1.97	0.63
1:E:518:ILE:HD13	1:E:530:ALA:HB2	1.81	0.63
1:C:480:PRO:HA	1:C:503:GLU:CD	2.24	0.63
1:C:536:ASN:ND2	1:C:538:GLU:H	1.96	0.63
1:F:289:PHE:H	1:F:296:ASN:HD21	1.46	0.63
1:D:309:MET:HE2	1:D:464:CYS:HB3	1.80	0.62
1:D:373:ILE:HD11	1:E:279:LEU:HB2	1.80	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:290:SER:N	1:F:325:GLN:NE2	2.42	0.62
1:D:395:ASP:O	1:D:396:SER:HB2	1.98	0.62
1:B:375:ASN:HD21	1:B:377:LYS:HG3	1.63	0.62
1:F:536:ASN:ND2	1:F:538:GLU:H	1.98	0.62
1:D:375:ASN:HD21	1:D:377:LYS:HG3	1.65	0.62
1:A:401:GLU:HA	1:A:430:VAL:O	1.99	0.62
1:C:440:LYS:HZ2	1:C:444:ASN:CB	2.10	0.62
1:F:484:THR:HA	1:F:493:ARG:NH2	2.15	0.62
1:B:446:MET:HE2	1:B:449:LEU:HD12	1.82	0.62
1:E:444:ASN:OD1	1:E:448:LYS:HE2	1.98	0.62
1:F:406:LEU:HD21	1:F:448:LYS:HB3	1.82	0.62
1:A:469:PRO:O	1:A:470:ASP:C	2.43	0.62
1:F:292:CYS:SG	1:F:295:ILE:CD1	2.88	0.62
1:D:399:GLU:HB3	1:D:430:VAL:HG21	1.82	0.62
1:E:360:VAL:HG11	1:E:368:LEU:HD11	1.81	0.61
1:A:262:PRO:O	1:A:263:ASP:HB2	1.99	0.61
1:A:344:GLU:OE2	1:A:349:THR:HB	2.00	0.61
1:A:382:PHE:CZ	1:B:272:ARG:HB2	2.34	0.61
1:D:534:GLU:HG3	1:D:545:SER:HB2	1.81	0.61
1:A:309:MET:HE2	1:A:464:CYS:HB3	1.81	0.61
1:D:468:ASN:ND2	1:E:493:ARG:HD2	2.15	0.61
1:F:395:ASP:O	1:F:396:SER:HB2	2.00	0.61
1:A:395:ASP:O	1:A:396:SER:HB2	1.98	0.61
1:D:509:ASP:C	1:D:511:PRO:HD3	2.24	0.61
1:F:440:LYS:HD3	1:F:440:LYS:C	2.23	0.61
1:F:443:ASP:O	1:F:447:THR:HG23	2.00	0.61
1:A:294:GLY:HA2	1:A:297:ASP:HB2	1.82	0.61
1:A:426:ILE:HG12	1:A:426:ILE:O	2.00	0.61
1:C:440:LYS:HD3	1:C:440:LYS:C	2.25	0.61
1:D:465:HIS:O	1:D:487:ARG:HB2	2.00	0.61
1:F:328:GLN:HG3	1:F:333:MET:HE3	1.81	0.61
1:F:438:GLU:HA	1:F:441:MET:HG2	1.82	0.61
1:F:477:GLU:HA	1:F:505:ASN:ND2	2.14	0.61
1:B:273:GLU:OE2	1:B:276:ARG:NH1	2.34	0.61
1:C:321:PHE:CD1	1:C:533:MET:HE1	2.35	0.61
1:C:343:GLU:C	1:C:397:PHE:HE1	2.09	0.61
1:A:289:PHE:HA	1:A:325:GLN:HE21	1.65	0.61
1:C:275:ILE:O	1:C:278:HIS:HB3	2.00	0.61
1:C:438:GLU:HA	1:C:441:MET:HG2	1.83	0.61
1:E:426:ILE:HD12	1:E:446:MET:HE3	1.83	0.61
1:C:395:ASP:O	1:C:396:SER:HB2	2.01	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:392:HIS:ND1	1:E:267:SER:HB2	2.15	0.61
1:B:444:ASN:OD1	1:B:448:LYS:HE2	2.01	0.60
1:A:397:PHE:HZ	1:B:454:LYS:HE3	1.66	0.60
1:A:402:THR:HG23	1:A:445:LEU:HD13	1.83	0.60
1:B:344:GLU:CG	1:B:349:THR:HG22	2.29	0.60
1:F:422:ILE:HD13	1:F:461:VAL:HB	1.82	0.60
1:B:518:ILE:HD13	1:B:530:ALA:HB2	1.83	0.60
1:C:309:MET:HE2	1:C:464:CYS:SG	2.41	0.60
1:C:443:ASP:O	1:C:447:THR:HG23	2.01	0.60
1:D:289:PHE:N	1:D:296:ASN:HD21	1.99	0.60
1:D:394:TYR:CE1	1:D:408:LYS:HD2	2.37	0.60
1:E:514:VAL:HG13	1:E:533:MET:HB2	1.81	0.60
1:B:351:GLU:HG3	1:C:279:LEU:HD21	1.83	0.60
1:E:278:HIS:O	1:E:282:GLU:HB3	2.01	0.60
1:F:266:VAL:HG11	1:F:271:LEU:HD21	1.83	0.60
1:B:292:CYS:HB2	1:B:533:MET:HG2	1.83	0.60
1:E:344:GLU:CG	1:E:349:THR:HG22	2.29	0.60
1:E:470:ASP:OD2	1:F:467:LYS:NZ	2.34	0.60
1:B:313:GLY:HA3	1:B:316:MET:SD	2.41	0.60
1:D:375:ASN:ND2	1:D:377:LYS:HG3	2.17	0.60
1:E:392:HIS:C	1:E:393:LEU:HD12	2.26	0.60
1:A:509:ASP:C	1:A:511:PRO:HD3	2.27	0.60
1:B:440:LYS:O	1:B:440:LYS:HD3	2.01	0.60
1:C:324:GLN:HE22	1:C:542:LEU:H	1.49	0.60
1:F:321:PHE:CD1	1:F:533:MET:HE1	2.37	0.60
1:A:375:ASN:ND2	1:A:377:LYS:HG3	2.17	0.60
1:A:518:ILE:HD11	1:A:530:ALA:HB2	1.84	0.60
1:B:290:SER:N	1:B:325:GLN:HE22	1.96	0.60
1:B:446:MET:SD	1:B:492:LEU:HB3	2.42	0.60
1:D:426:ILE:HG12	1:D:426:ILE:O	2.01	0.60
1:B:331:THR:O	1:B:334:GLY:N	2.30	0.60
1:B:536:ASN:HD22	1:B:538:GLU:N	2.00	0.60
1:D:469:PRO:O	1:D:470:ASP:C	2.45	0.59
1:F:402:THR:HG23	1:F:445:LEU:HD13	1.83	0.59
1:B:309:MET:HE2	1:B:464:CYS:HB3	1.82	0.59
1:C:358:ASN:O	1:C:360:VAL:HG22	2.01	0.59
1:F:480:PRO:HA	1:F:503:GLU:CD	2.27	0.59
1:C:290:SER:N	1:C:325:GLN:NE2	2.44	0.59
1:E:375:ASN:ND2	1:E:377:LYS:HG3	2.18	0.59
1:C:303:ARG:O	1:C:306:GLU:HB2	2.02	0.59
1:F:358:ASN:O	1:F:360:VAL:HG22	2.02	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:287:LEU:HD11	1:F:335:LYS:HG3	1.84	0.59
1:D:311:THR:HG21	1:D:486:LEU:HD21	1.85	0.59
1:E:375:ASN:HD21	1:E:377:LYS:CB	2.15	0.59
1:D:402:THR:HG23	1:D:445:LEU:HD13	1.85	0.59
1:E:309:MET:HE2	1:E:464:CYS:HB3	1.85	0.59
1:F:440:LYS:HZ2	1:F:444:ASN:CB	2.14	0.59
1:A:439:ARG:O	1:A:442:ILE:HG22	2.03	0.59
1:A:262:PRO:O	1:A:263:ASP:CB	2.50	0.59
1:E:382:PHE:HE1	1:F:275:ILE:HD12	1.68	0.58
1:A:375:ASN:HD21	1:A:377:LYS:HG3	1.68	0.58
1:A:394:TYR:CE1	1:A:408:LYS:HD2	2.39	0.58
1:A:399:GLU:HB3	1:A:430:VAL:HG21	1.85	0.58
1:D:397:PHE:CZ	1:E:454:LYS:HE3	2.38	0.58
1:E:331:THR:HG22	1:E:332:ALA:N	2.17	0.58
1:D:477:GLU:HA	1:D:505:ASN:ND2	2.18	0.58
1:F:303:ARG:O	1:F:306:GLU:HB2	2.04	0.58
1:A:303:ARG:HB2	1:A:306:GLU:CD	2.28	0.58
1:A:484:THR:HA	1:A:493:ARG:HH22	1.69	0.58
1:B:469:PRO:HG3	1:B:474:ALA:CB	2.34	0.58
1:F:320:THR:HG22	1:F:324:GLN:HE21	1.69	0.58
1:A:333:MET:O	1:A:335:LYS:HG2	2.03	0.58
1:B:477:GLU:HA	1:B:505:ASN:ND2	2.16	0.58
1:C:278:HIS:O	1:C:282:GLU:HB2	2.03	0.58
1:C:491:ALA:O	1:C:495:LEU:CD2	2.50	0.58
1:E:437:ASP:C	1:E:439:ARG:H	2.12	0.58
1:E:409:LEU:HA	1:E:412:MET:HE3	1.86	0.58
1:A:444:ASN:OD1	1:A:448:LYS:HE2	2.04	0.58
1:E:282:GLU:O	1:E:282:GLU:HG3	2.03	0.58
1:E:477:GLU:HA	1:E:505:ASN:ND2	2.16	0.58
1:E:440:LYS:NZ	1:E:444:ASN:HB2	2.13	0.57
1:B:319:SER:OG	2:B:700:ANP:O1B	2.22	0.57
1:C:406:LEU:HD21	1:C:448:LYS:HB3	1.86	0.57
1:D:305:GLY:HA2	1:D:453:ALA:O	2.03	0.57
1:D:444:ASN:OD1	1:D:448:LYS:HE2	2.04	0.57
1:F:394:TYR:OH	1:F:400:ALA:HB2	2.04	0.57
1:C:394:TYR:OH	1:C:400:ALA:HB2	2.04	0.57
1:E:372:ILE:HA	1:E:375:ASN:OD1	2.03	0.57
1:E:534:GLU:HG3	1:E:545:SER:CB	2.34	0.57
1:B:437:ASP:C	1:B:439:ARG:H	2.13	0.57
1:C:476:GLU:H	1:C:476:GLU:CD	2.11	0.57
1:D:303:ARG:HB2	1:D:306:GLU:CD	2.29	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:327:LEU:HD22	1:E:356:LEU:HD23	1.86	0.57
1:E:401:GLU:HA	1:E:430:VAL:O	2.04	0.57
1:A:524:THR:C	1:A:526:ASP:H	2.10	0.57
1:B:312:SER:OG	1:B:318:LYS:HG3	2.03	0.57
1:B:360:VAL:HG11	1:B:368:LEU:HD11	1.85	0.57
1:C:290:SER:H	1:C:325:GLN:HE21	1.46	0.57
1:A:477:GLU:HA	1:A:505:ASN:ND2	2.19	0.57
1:B:491:ALA:O	1:B:495:LEU:HD22	2.05	0.57
1:E:289:PHE:H	1:E:296:ASN:HD21	1.50	0.57
1:A:309:MET:HE2	1:A:464:CYS:SG	2.44	0.57
1:D:443:ASP:O	1:D:447:THR:HG23	2.05	0.57
1:D:331:THR:HG22	1:D:332:ALA:N	2.20	0.57
1:E:404:ARG:HH12	1:E:408:LYS:CE	2.17	0.57
1:A:311:THR:HG21	1:A:486:LEU:HD21	1.87	0.57
1:C:399:GLU:HB3	1:C:430:VAL:CG2	2.34	0.57
1:D:439:ARG:O	1:D:442:ILE:HG22	2.05	0.57
1:D:524:THR:C	1:D:526:ASP:H	2.12	0.57
1:E:292:CYS:HB2	1:E:533:MET:HG2	1.86	0.57
1:A:296:ASN:O	1:A:300:LEU:N	2.31	0.57
1:C:284:SER:HB2	1:C:523:PHE:HZ	1.70	0.57
1:F:426:ILE:O	1:F:426:ILE:HG23	2.05	0.56
1:A:536:ASN:HD21	1:A:538:GLU:HB2	1.70	0.56
1:C:287:LEU:HD11	1:C:335:LYS:HG3	1.86	0.56
1:C:399:GLU:HB3	1:C:430:VAL:HG11	1.87	0.56
1:C:536:ASN:ND2	1:C:538:GLU:HB2	2.17	0.56
1:D:478:GLY:O	1:D:479:ARG:HB3	2.04	0.56
1:E:394:TYR:OH	1:E:400:ALA:HB2	2.04	0.56
1:E:399:GLU:HB3	1:E:430:VAL:CG2	2.33	0.56
1:A:379:ASP:OD1	1:B:276:ARG:NH2	2.38	0.56
1:A:507:GLN:HE21	1:B:517:ARG:HH11	1.53	0.56
1:A:515:LEU:HD23	1:A:515:LEU:C	2.30	0.56
1:B:375:ASN:HD21	1:B:377:LYS:CB	2.18	0.56
1:B:392:HIS:C	1:B:393:LEU:HD12	2.31	0.56
1:B:426:ILE:HD12	1:B:446:MET:HE3	1.87	0.56
1:B:426:ILE:HG12	1:B:426:ILE:O	2.04	0.56
1:B:468:ASN:HD21	1:C:493:ARG:CD	2.17	0.56
1:C:512:ASN:O	1:C:534:GLU:HA	2.05	0.56
1:E:420:VAL:HG13	1:E:459:VAL:CG1	2.35	0.56
1:F:512:ASN:O	1:F:534:GLU:HA	2.04	0.56
1:C:407:ALA:O	1:C:410:ALA:HB3	2.05	0.56
1:B:266:VAL:HG12	1:B:267:SER:N	2.20	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:396:SER:O	1:C:397:PHE:CB	2.54	0.56
1:D:294:GLY:HA2	1:D:297:ASP:HB2	1.85	0.56
1:F:399:GLU:HB3	1:F:430:VAL:CG2	2.35	0.56
1:B:375:ASN:ND2	1:B:377:LYS:HG3	2.21	0.56
1:C:273:GLU:OE2	1:C:276:ARG:NH1	2.38	0.56
1:E:309:MET:HE3	1:E:462:VAL:O	2.05	0.56
1:F:290:SER:H	1:F:325:GLN:HE22	1.52	0.56
1:F:492:LEU:HD12	1:F:492:LEU:H	1.70	0.56
1:B:404:ARG:HH12	1:B:408:LYS:CE	2.18	0.56
1:B:468:ASN:HD21	1:C:493:ARG:NE	2.03	0.56
1:D:309:MET:HE2	1:D:464:CYS:CB	2.35	0.56
1:D:393:LEU:N	1:D:393:LEU:HD12	2.21	0.56
1:E:331:THR:O	1:E:334:GLY:N	2.29	0.56
1:F:399:GLU:HB3	1:F:430:VAL:HG11	1.86	0.56
1:A:399:GLU:HB3	1:A:430:VAL:HG11	1.88	0.56
1:B:289:PHE:H	1:B:296:ASN:HD21	1.53	0.56
1:A:273:GLU:OE1	1:A:276:ARG:NH1	2.39	0.56
1:D:366:ASP:OD1	1:E:284:SER:HB3	2.06	0.56
1:E:477:GLU:CA	1:E:505:ASN:HD22	2.17	0.56
1:B:344:GLU:HG3	1:B:349:THR:CG2	2.33	0.56
1:A:289:PHE:H	1:A:296:ASN:HD21	1.54	0.55
1:B:401:GLU:HB3	1:B:404:ARG:HB2	1.88	0.55
1:D:261:ILE:HG22	1:D:261:ILE:O	2.06	0.55
1:B:394:TYR:OH	1:B:400:ALA:HB2	2.06	0.55
1:D:379:ASP:OD1	1:E:276:ARG:NH2	2.39	0.55
1:A:365:SER:OG	1:A:368:LEU:HB2	2.07	0.55
1:B:468:ASN:HD21	1:C:493:ARG:HD2	1.70	0.55
1:D:289:PHE:HA	1:D:325:GLN:HE21	1.70	0.55
1:C:469:PRO:HG3	1:C:474:ALA:HB1	1.88	0.55
1:E:375:ASN:HD21	1:E:377:LYS:HB2	1.71	0.55
1:A:303:ARG:HB2	1:A:306:GLU:OE2	2.06	0.55
1:A:412:MET:HE3	1:A:421:ILE:HD12	1.87	0.55
1:A:422:ILE:HD13	1:A:461:VAL:HB	1.89	0.55
1:B:409:LEU:HA	1:B:412:MET:HE3	1.88	0.55
1:D:312:SER:HB2	1:D:502:LEU:O	2.06	0.55
1:E:399:GLU:HB3	1:E:430:VAL:HG11	1.87	0.55
1:C:294:GLY:HA2	1:C:297:ASP:HB2	1.88	0.55
1:C:363:ARG:HA	1:C:369:LYS:HE2	1.89	0.55
1:D:344:GLU:OE2	1:D:349:THR:HB	2.05	0.55
1:D:399:GLU:HB3	1:D:430:VAL:HG11	1.88	0.55
1:A:413:ARG:O	1:A:417:GLY:HA2	2.06	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:401:GLU:HA	1:B:430:VAL:O	2.07	0.55
1:E:469:PRO:O	1:E:470:ASP:C	2.50	0.55
1:F:346:VAL:HG23	1:F:347:GLU:N	2.21	0.55
1:B:284:SER:O	1:B:303:ARG:HD2	2.07	0.55
1:B:477:GLU:CA	1:B:505:ASN:HD22	2.15	0.55
1:E:313:GLY:HA3	1:E:316:MET:SD	2.47	0.55
1:F:536:ASN:ND2	1:F:538:GLU:HB2	2.22	0.55
1:B:351:GLU:OE1	1:C:278:HIS:NE2	2.40	0.55
1:B:399:GLU:HB3	1:B:430:VAL:CG2	2.33	0.55
1:D:536:ASN:HD21	1:D:538:GLU:HB2	1.72	0.55
1:F:396:SER:O	1:F:397:PHE:CB	2.55	0.55
1:B:420:VAL:HG13	1:B:459:VAL:CG1	2.37	0.54
1:C:492:LEU:HD12	1:C:492:LEU:H	1.70	0.54
1:D:446:MET:HG3	1:D:492:LEU:HB3	1.89	0.54
1:D:468:ASN:HD21	1:E:493:ARG:CZ	2.19	0.54
1:B:439:ARG:O	1:B:442:ILE:HG22	2.07	0.54
1:C:309:MET:HE2	1:C:464:CYS:CB	2.36	0.54
1:C:536:ASN:C	1:C:536:ASN:ND2	2.65	0.54
1:D:492:LEU:HD12	1:D:493:ARG:H	1.73	0.54
1:F:476:GLU:H	1:F:476:GLU:CD	2.13	0.54
1:C:426:ILE:HG23	1:C:426:ILE:O	2.07	0.54
1:E:446:MET:SD	1:E:492:LEU:HB3	2.48	0.54
1:F:324:GLN:HE22	1:F:542:LEU:H	1.55	0.54
1:F:393:LEU:HD12	1:F:393:LEU:N	2.22	0.54
1:A:393:LEU:HD12	1:A:393:LEU:N	2.23	0.54
1:A:437:ASP:C	1:A:439:ARG:N	2.66	0.54
1:D:413:ARG:O	1:D:417:GLY:HA2	2.07	0.54
1:E:440:LYS:HD3	1:E:440:LYS:C	2.33	0.54
1:B:400:ALA:O	1:B:430:VAL:HB	2.08	0.54
1:D:536:ASN:ND2	1:D:538:GLU:HB2	2.23	0.54
1:E:345:SER:OG	1:E:347:GLU:HG2	2.08	0.54
1:E:439:ARG:O	1:E:442:ILE:HG22	2.07	0.54
1:E:469:PRO:HG3	1:E:474:ALA:CB	2.37	0.54
1:B:534:GLU:HG3	1:B:545:SER:CB	2.37	0.54
1:C:547:TYR:CG	1:C:548:SER:N	2.76	0.54
1:E:506:GLN:HB2	1:F:527:THR:OG1	2.08	0.54
1:A:536:ASN:ND2	1:A:538:GLU:HB2	2.23	0.54
1:C:426:ILE:O	1:C:426:ILE:HG12	2.08	0.54
1:D:518:ILE:HD11	1:D:530:ALA:HB2	1.90	0.54
1:E:303:ARG:O	1:E:306:GLU:HB2	2.07	0.54
1:E:273:GLU:OE1	1:E:276:ARG:NH1	2.40	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:331:THR:HG22	1:B:332:ALA:N	2.22	0.53
1:B:383:ASP:CG	1:C:272:ARG:HH22	2.16	0.53
1:B:425:HIS:NE2	1:B:465:HIS:NE2	2.56	0.53
1:B:469:PRO:O	1:B:470:ASP:C	2.50	0.53
1:B:514:VAL:HG13	1:B:533:MET:HB2	1.90	0.53
1:D:288:LEU:HD12	1:D:288:LEU:H	1.73	0.53
1:F:324:GLN:HE22	1:F:542:LEU:HB2	1.71	0.53
1:A:266:VAL:HG11	1:A:271:LEU:HD21	1.89	0.53
1:A:300:LEU:HD12	1:A:524:THR:CG2	2.38	0.53
1:B:443:ASP:O	1:B:447:THR:HG23	2.08	0.53
1:F:344:GLU:CG	1:F:349:THR:HG22	2.31	0.53
1:B:303:ARG:O	1:B:306:GLU:HB2	2.08	0.53
1:B:370:ARG:NH1	1:B:370:ARG:CB	2.71	0.53
1:C:268:ALA:HA	1:C:271:LEU:HD12	1.90	0.53
1:D:470:ASP:OD1	1:E:493:ARG:NH2	2.41	0.53
1:A:288:LEU:H	1:A:288:LEU:HD12	1.73	0.53
1:B:327:LEU:HD22	1:B:356:LEU:HD23	1.90	0.53
1:B:399:GLU:HB3	1:B:430:VAL:HG11	1.89	0.53
1:D:386:PHE:CD1	1:E:268:ALA:HB1	2.44	0.53
1:F:413:ARG:O	1:F:417:GLY:HA2	2.09	0.53
1:B:379:ASP:OD2	1:C:276:ARG:NH2	2.41	0.53
1:D:412:MET:HE3	1:D:421:ILE:HD12	1.89	0.53
1:E:401:GLU:HB3	1:E:404:ARG:HB2	1.90	0.53
1:E:536:ASN:ND2	1:E:538:GLU:N	2.53	0.53
1:F:278:HIS:O	1:F:282:GLU:HB2	2.08	0.53
1:A:446:MET:HG3	1:A:492:LEU:HB3	1.90	0.53
1:D:300:LEU:HD12	1:D:524:THR:CG2	2.39	0.53
1:D:437:ASP:C	1:D:439:ARG:N	2.67	0.53
1:E:278:HIS:O	1:E:282:GLU:CB	2.56	0.53
1:E:491:ALA:O	1:E:495:LEU:HD22	2.09	0.53
1:A:324:GLN:HE22	1:A:542:LEU:HB2	1.74	0.53
1:C:271:LEU:O	1:C:275:ILE:HG13	2.08	0.53
1:E:344:GLU:HG3	1:E:349:THR:CG2	2.32	0.53
1:A:506:GLN:CB	1:B:527:THR:OG1	2.53	0.53
1:C:411:TYR:OH	1:C:416:LEU:HD21	2.09	0.53
1:D:343:GLU:HG3	1:D:428:ILE:HD11	1.89	0.53
1:E:476:GLU:CD	1:E:476:GLU:H	2.16	0.53
1:B:397:PHE:CE1	1:C:454:LYS:HE3	2.43	0.52
1:C:339:LEU:HD22	1:C:341:MET:HE3	1.91	0.52
1:A:292:CYS:HB2	1:A:533:MET:HG2	1.90	0.52
1:C:344:GLU:CG	1:C:349:THR:HG22	2.32	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:363:ARG:HA	1:F:369:LYS:HE2	1.91	0.52
1:B:440:LYS:HD3	1:B:440:LYS:C	2.34	0.52
1:C:469:PRO:O	1:C:470:ASP:C	2.52	0.52
1:D:375:ASN:HD21	1:D:377:LYS:CB	2.23	0.52
1:E:312:SER:OG	1:E:318:LYS:HG3	2.10	0.52
1:F:339:LEU:HD22	1:F:341:MET:HE3	1.89	0.52
1:F:351:GLU:OE2	1:F:363:ARG:HG3	2.09	0.52
1:D:382:PHE:CE1	1:E:272:ARG:HA	2.45	0.52
1:E:440:LYS:HZ2	1:E:444:ASN:CB	2.15	0.52
1:A:401:GLU:HB3	1:A:404:ARG:HB2	1.90	0.52
1:D:401:GLU:HB3	1:D:404:ARG:HB2	1.92	0.52
1:F:469:PRO:O	1:F:470:ASP:C	2.51	0.52
1:B:375:ASN:HD21	1:B:377:LYS:HB2	1.73	0.52
1:B:478:GLY:O	1:B:479:ARG:CB	2.57	0.52
1:B:535:TYR:HD1	1:B:542:LEU:HD13	1.75	0.52
1:C:434:GLY:C	1:C:435:GLU:HG3	2.35	0.52
1:D:422:ILE:HD13	1:D:461:VAL:HB	1.90	0.52
1:F:292:CYS:SG	1:F:295:ILE:HD12	2.50	0.52
1:A:331:THR:HG22	1:A:332:ALA:N	2.24	0.52
1:A:343:GLU:HG3	1:A:428:ILE:HD11	1.92	0.52
1:F:407:ALA:O	1:F:410:ALA:HB3	2.10	0.52
1:F:469:PRO:HG3	1:F:474:ALA:HB1	1.91	0.52
1:F:547:TYR:CG	1:F:548:SER:N	2.77	0.52
1:B:372:ILE:HA	1:B:375:ASN:OD1	2.09	0.52
1:C:324:GLN:HE22	1:C:542:LEU:N	2.07	0.52
1:D:311:THR:O	1:D:312:SER:HB3	2.09	0.52
1:F:491:ALA:O	1:F:495:LEU:CD2	2.54	0.52
1:A:396:SER:O	1:A:397:PHE:CB	2.58	0.52
1:C:394:TYR:HE2	1:C:408:LYS:HD2	1.75	0.52
1:D:280:SER:O	1:D:281:SER:HB2	2.09	0.52
1:F:434:GLY:C	1:F:435:GLU:HG3	2.35	0.52
1:B:404:ARG:HH12	1:B:408:LYS:HE3	1.75	0.51
1:D:303:ARG:HB2	1:D:306:GLU:OE2	2.11	0.51
1:E:370:ARG:NH1	1:E:370:ARG:CB	2.74	0.51
1:F:536:ASN:C	1:F:536:ASN:ND2	2.68	0.51
1:A:300:LEU:HD12	1:A:524:THR:HG21	1.92	0.51
1:E:468:ASN:HD21	1:F:493:ARG:CZ	2.23	0.51
1:A:346:VAL:HG23	1:A:347:GLU:N	2.25	0.51
1:B:425:HIS:CE1	1:B:465:HIS:CD2	2.98	0.51
1:C:324:GLN:HE22	1:C:542:LEU:HB2	1.75	0.51
1:D:515:LEU:HD23	1:D:515:LEU:C	2.36	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:411:TYR:OH	1:F:416:LEU:HD21	2.11	0.51
1:A:366:ASP:OD1	1:B:284:SER:HB3	2.11	0.51
1:B:285:VAL:HG22	1:B:300:LEU:CD2	2.37	0.51
1:B:347:GLU:OE1	1:C:274:ARG:HD2	2.11	0.51
1:C:290:SER:H	1:C:325:GLN:HE22	1.56	0.51
1:A:443:ASP:O	1:A:447:THR:HG23	2.11	0.51
1:B:476:GLU:CD	1:B:476:GLU:H	2.18	0.51
1:D:300:LEU:HD12	1:D:524:THR:HG21	1.93	0.51
1:E:352:ASP:OD2	1:E:363:ARG:NH2	2.44	0.51
1:F:396:SER:O	1:F:397:PHE:HB2	2.10	0.51
1:C:396:SER:O	1:C:397:PHE:HB2	2.10	0.51
1:C:536:ASN:HD22	1:C:538:GLU:H	1.57	0.51
1:F:309:MET:HE2	1:F:464:CYS:CB	2.40	0.51
1:A:492:LEU:HD12	1:A:493:ARG:H	1.76	0.51
1:D:292:CYS:HB2	1:D:533:MET:HG2	1.92	0.51
1:D:322:VAL:CG1	1:D:422:ILE:HG21	2.41	0.51
1:A:426:ILE:O	1:A:426:ILE:HG23	2.11	0.50
1:D:290:SER:OG	1:D:328:GLN:HG2	2.11	0.50
1:D:468:ASN:HD21	1:E:493:ARG:NE	2.09	0.50
1:E:478:GLY:O	1:E:479:ARG:CB	2.58	0.50
1:A:290:SER:OG	1:A:328:GLN:HG2	2.11	0.50
1:A:524:THR:C	1:A:526:ASP:N	2.70	0.50
1:D:340:ALA:C	1:D:341:MET:HE2	2.35	0.50
1:D:372:ILE:HA	1:D:375:ASN:OD1	2.11	0.50
1:D:536:ASN:HD22	1:D:538:GLU:H	1.59	0.50
1:E:333:MET:O	1:E:335:LYS:HG2	2.11	0.50
1:E:341:MET:HE1	1:E:422:ILE:CG2	2.41	0.50
1:A:517:ARG:HD2	1:A:519:LEU:HD11	1.94	0.50
1:B:306:GLU:HA	1:B:497:ASP:OD2	2.12	0.50
1:B:352:ASP:OD2	1:B:363:ARG:NH2	2.44	0.50
1:E:299:THR:O	1:E:300:LEU:HB2	2.11	0.50
1:A:397:PHE:CZ	1:B:454:LYS:HE3	2.45	0.50
1:F:309:MET:HE2	1:F:464:CYS:SG	2.51	0.50
1:C:320:THR:HG22	1:C:324:GLN:HE21	1.77	0.50
1:D:394:TYR:OH	1:D:400:ALA:HB2	2.12	0.50
1:E:404:ARG:HH12	1:E:408:LYS:HE3	1.75	0.50
1:F:426:ILE:O	1:F:426:ILE:HG12	2.11	0.50
1:F:483:ILE:HG12	1:F:519:LEU:HG	1.94	0.50
1:A:465:HIS:O	1:A:487:ARG:HB2	2.11	0.50
1:C:339:LEU:HB3	1:C:341:MET:HE3	1.93	0.50
1:E:341:MET:HB3	1:E:344:GLU:HG2	1.92	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:492:LEU:HD12	1:F:492:LEU:N	2.27	0.50
1:A:373:ILE:HD11	1:B:279:LEU:HB2	1.93	0.50
1:A:375:ASN:HD21	1:A:377:LYS:CB	2.25	0.50
1:D:411:TYR:O	1:D:415:GLY:N	2.45	0.50
1:A:468:ASN:ND2	1:B:493:ARG:HD2	2.24	0.50
1:D:476:GLU:CG	1:E:483:ILE:HD12	2.18	0.49
1:E:404:ARG:HG3	1:E:404:ARG:HH11	1.77	0.49
1:E:449:LEU:HD22	1:E:460:LEU:HD21	1.94	0.49
1:F:425:HIS:CD2	1:F:465:HIS:NE2	2.80	0.49
1:A:309:MET:HE2	1:A:464:CYS:CB	2.42	0.49
1:D:303:ARG:O	1:D:306:GLU:HB2	2.12	0.49
1:E:273:GLU:CD	1:E:276:ARG:NH1	2.70	0.49
1:A:509:ASP:O	1:A:511:PRO:HD3	2.13	0.49
1:C:331:THR:HG22	1:C:332:ALA:H	1.76	0.49
1:C:346:VAL:HG23	1:C:347:GLU:N	2.27	0.49
1:D:296:ASN:O	1:D:300:LEU:N	2.34	0.49
1:E:395:ASP:OD2	1:F:274:ARG:NH2	2.36	0.49
1:E:266:VAL:HG11	1:E:271:LEU:CD2	2.33	0.49
1:E:400:ALA:O	1:E:430:VAL:HB	2.12	0.49
1:A:309:MET:CE	1:A:464:CYS:HB3	2.42	0.49
1:C:266:VAL:HG11	1:C:271:LEU:HD21	1.95	0.49
1:C:413:ARG:O	1:C:417:GLY:HA2	2.12	0.49
1:C:499:ILE:HG13	1:C:520:LYS:HB3	1.95	0.49
1:D:346:VAL:HG23	1:D:347:GLU:N	2.27	0.49
1:E:515:LEU:C	1:E:515:LEU:HD23	2.37	0.49
1:A:404:ARG:O	1:A:408:LYS:HG3	2.12	0.49
1:A:475:HIS:H	1:A:479:ARG:HD2	1.77	0.49
1:B:409:LEU:HA	1:B:412:MET:CE	2.43	0.49
1:E:425:HIS:CE1	1:E:465:HIS:CD2	3.00	0.49
1:C:469:PRO:CG	1:C:474:ALA:CB	2.91	0.49
1:D:394:TYR:HE1	1:D:408:LYS:HD2	1.73	0.49
1:D:404:ARG:NH1	1:D:408:LYS:HE3	2.28	0.49
1:A:273:GLU:CD	1:A:276:ARG:NH1	2.71	0.49
2:A:700:ANP:O4'	1:B:525:GLY:HA3	2.12	0.49
1:B:309:MET:HE3	1:B:462:VAL:O	2.12	0.49
1:D:309:MET:CE	1:D:464:CYS:HB3	2.43	0.49
1:F:483:ILE:HD11	1:F:519:LEU:O	2.13	0.49
1:A:372:ILE:HA	1:A:375:ASN:OD1	2.12	0.49
1:A:404:ARG:NH1	1:A:408:LYS:HE3	2.28	0.49
1:D:484:THR:HA	1:D:493:ARG:HH22	1.74	0.49
1:F:294:GLY:HA2	1:F:297:ASP:HB2	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:309:MET:HE1	1:B:462:VAL:CG1	2.39	0.48
1:F:499:ILE:HG13	1:F:520:LYS:HB3	1.96	0.48
1:B:493:ARG:O	1:B:493:ARG:HG3	2.09	0.48
1:E:285:VAL:CG2	1:E:300:LEU:HD22	2.34	0.48
1:A:312:SER:HB2	1:A:502:LEU:O	2.13	0.48
2:B:700:ANP:O3G	1:C:522:ARG:NH1	2.46	0.48
1:C:313:GLY:CA	1:C:316:MET:SD	2.99	0.48
1:D:426:ILE:O	1:D:426:ILE:HG23	2.12	0.48
1:E:306:GLU:HA	1:E:497:ASP:OD2	2.14	0.48
1:E:387:GLY:C	1:E:389:ASP:H	2.22	0.48
1:E:420:VAL:HG13	1:E:459:VAL:HG12	1.95	0.48
1:A:480:PRO:HA	1:A:503:GLU:CD	2.37	0.48
1:C:536:ASN:HB2	1:C:543:GLU:OE1	2.13	0.48
1:D:316:MET:HA	1:D:504:ARG:NH1	2.28	0.48
1:D:396:SER:O	1:D:397:PHE:CB	2.61	0.48
1:F:399:GLU:HB3	1:F:430:VAL:CG1	2.44	0.48
1:A:411:TYR:OH	1:A:416:LEU:HD21	2.12	0.48
1:A:470:ASP:OD1	1:B:493:ARG:NH2	2.46	0.48
1:B:383:ASP:OD1	1:C:272:ARG:NH2	2.44	0.48
1:B:411:TYR:O	1:B:415:GLY:N	2.46	0.48
1:D:480:PRO:HA	1:D:503:GLU:CD	2.39	0.48
1:D:516:VAL:HG22	1:D:533:MET:HE2	1.96	0.48
1:B:536:ASN:ND2	1:B:538:GLU:N	2.59	0.48
1:C:483:ILE:HG12	1:C:519:LEU:HG	1.96	0.48
1:D:402:THR:HG23	1:D:445:LEU:CD1	2.44	0.48
1:E:492:LEU:HD12	1:E:493:ARG:H	1.79	0.48
1:F:289:PHE:HA	1:F:325:GLN:HE21	1.79	0.48
1:F:434:GLY:O	1:F:435:GLU:HG3	2.13	0.48
1:B:536:ASN:ND2	1:B:536:ASN:C	2.70	0.48
1:C:312:SER:OG	1:C:318:LYS:CG	2.61	0.48
1:C:492:LEU:HD12	1:C:492:LEU:N	2.29	0.48
1:D:436:SER:O	1:D:437:ASP:C	2.56	0.48
1:E:387:GLY:O	1:E:389:ASP:N	2.47	0.48
1:A:316:MET:HA	1:A:504:ARG:NH1	2.29	0.48
1:A:402:THR:HG23	1:A:445:LEU:CD1	2.43	0.48
1:A:436:SER:O	1:A:437:ASP:C	2.55	0.48
1:D:517:ARG:HD2	1:D:519:LEU:HD11	1.96	0.48
1:E:396:SER:O	1:E:397:PHE:CB	2.62	0.48
1:F:292:CYS:C	1:F:293:THR:O	2.49	0.48
1:F:312:SER:OG	1:F:318:LYS:CG	2.62	0.48
1:F:317:GLY:O	1:F:318:LYS:C	2.57	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:MET:HE1	1:A:422:ILE:CG2	2.43	0.47
1:A:394:TYR:HE1	1:A:408:LYS:HD2	1.78	0.47
1:B:404:ARG:NH1	1:B:408:LYS:CE	2.77	0.47
1:B:449:LEU:HD22	1:B:460:LEU:HD21	1.96	0.47
1:C:393:LEU:HD12	1:C:393:LEU:N	2.29	0.47
1:C:434:GLY:O	1:C:435:GLU:HG3	2.14	0.47
1:D:509:ASP:O	1:D:511:PRO:HD3	2.13	0.47
1:D:535:TYR:HD1	1:D:542:LEU:HD13	1.78	0.47
1:E:474:ALA:HA	1:E:479:ARG:HD2	1.96	0.47
1:F:299:THR:O	1:F:300:LEU:HB2	2.13	0.47
1:A:536:ASN:HD22	1:A:538:GLU:H	1.62	0.47
1:B:345:SER:OG	1:B:347:GLU:HG2	2.14	0.47
1:B:474:ALA:HA	1:B:479:ARG:HD2	1.94	0.47
1:C:292:CYS:SG	1:C:295:ILE:CD1	3.02	0.47
1:E:536:ASN:ND2	1:E:536:ASN:C	2.70	0.47
1:F:394:TYR:HE2	1:F:408:LYS:HD2	1.79	0.47
1:F:356:LEU:HG	1:F:541:TRP:NE1	2.29	0.47
1:B:396:SER:O	1:B:397:PHE:CB	2.62	0.47
2:B:700:ANP:O3G	1:C:522:ARG:CZ	2.62	0.47
1:C:343:GLU:HG3	1:C:428:ILE:CD1	2.44	0.47
1:E:271:LEU:O	1:E:275:ILE:HG13	2.14	0.47
1:E:425:HIS:NE2	1:E:465:HIS:NE2	2.63	0.47
1:F:361:ARG:NH1	1:F:535:TYR:OH	2.48	0.47
1:B:492:LEU:HD12	1:B:493:ARG:H	1.79	0.47
1:B:506:GLN:CB	1:C:527:THR:OG1	2.63	0.47
1:D:429:VAL:CG2	1:D:430:VAL:H	2.23	0.47
1:E:443:ASP:O	1:E:447:THR:HG23	2.13	0.47
1:F:536:ASN:HD22	1:F:538:GLU:H	1.62	0.47
1:A:322:VAL:CG1	1:A:422:ILE:HG21	2.44	0.47
1:A:324:GLN:NE2	1:A:542:LEU:HB2	2.30	0.47
1:A:516:VAL:HG22	1:A:533:MET:HE2	1.96	0.47
1:B:429:VAL:CG2	1:B:430:VAL:H	2.22	0.47
1:D:292:CYS:SG	1:D:295:ILE:CD1	3.03	0.47
1:E:426:ILE:HD12	1:E:446:MET:CE	2.43	0.47
1:E:496:SER:O	1:E:520:LYS:HE2	2.14	0.47
1:F:492:LEU:HD12	1:F:493:ARG:H	1.80	0.47
1:A:311:THR:O	1:A:312:SER:HB3	2.14	0.47
1:C:361:ARG:NH1	1:C:535:TYR:OH	2.48	0.47
1:D:538:GLU:HA	1:D:538:GLU:OE1	2.13	0.47
1:E:309:MET:HE2	1:E:464:CYS:SG	2.55	0.47
1:F:421:ILE:HB	1:F:460:LEU:HD12	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:426:ILE:O	1:B:426:ILE:HG23	2.14	0.47
1:D:475:HIS:H	1:D:479:ARG:HD2	1.80	0.47
1:F:409:LEU:HA	1:F:412:MET:HE3	1.95	0.47
1:F:509:ASP:C	1:F:511:PRO:HD3	2.40	0.47
1:B:469:PRO:HG3	1:B:474:ALA:HB1	1.96	0.46
1:C:344:GLU:OE2	1:C:349:THR:HB	2.14	0.46
1:D:475:HIS:C	1:D:477:GLU:H	2.23	0.46
1:E:436:SER:O	1:E:437:ASP:O	2.32	0.46
1:E:537:LYS:HE2	1:E:537:LYS:HB3	1.72	0.46
1:D:306:GLU:HG2	1:D:497:ASP:HB2	1.97	0.46
1:E:393:LEU:N	1:E:393:LEU:CD1	2.77	0.46
1:E:411:TYR:O	1:E:415:GLY:N	2.47	0.46
1:E:535:TYR:HD1	1:E:542:LEU:HD13	1.80	0.46
1:F:388:ASN:O	1:F:389:ASP:C	2.57	0.46
1:A:341:MET:HE1	1:A:422:ILE:HG22	1.96	0.46
1:A:357:HIS:CG	1:A:385:LEU:HD13	2.50	0.46
1:B:343:GLU:HG3	1:B:428:ILE:HD11	1.97	0.46
1:D:299:THR:O	1:D:300:LEU:HB2	2.14	0.46
1:D:407:ALA:O	1:D:410:ALA:HB3	2.14	0.46
1:D:425:HIS:NE2	1:D:465:HIS:NE2	2.62	0.46
1:D:502:LEU:HD23	1:D:514:VAL:HG21	1.97	0.46
1:E:399:GLU:OE1	1:E:430:VAL:HG22	2.16	0.46
1:E:404:ARG:NH1	1:E:408:LYS:CE	2.76	0.46
1:F:313:GLY:CA	1:F:316:MET:SD	3.02	0.46
1:B:405:LEU:O	1:B:406:LEU:C	2.58	0.46
1:C:317:GLY:O	1:C:318:LYS:C	2.58	0.46
1:C:399:GLU:HB3	1:C:430:VAL:CG1	2.45	0.46
1:C:483:ILE:HD11	1:C:519:LEU:O	2.15	0.46
1:D:365:SER:OG	1:D:368:LEU:HB2	2.15	0.46
1:F:395:ASP:O	1:F:396:SER:CB	2.64	0.46
1:A:394:TYR:OH	1:A:400:ALA:HB2	2.15	0.46
1:B:436:SER:O	1:B:437:ASP:O	2.33	0.46
1:C:263:ASP:OD1	1:C:263:ASP:N	2.46	0.46
1:D:468:ASN:OD1	1:E:493:ARG:CZ	2.63	0.46
1:F:437:ASP:C	1:F:439:ARG:H	2.22	0.46
1:F:537:LYS:HB3	1:F:537:LYS:HE2	1.70	0.46
1:B:429:VAL:CG2	1:B:430:VAL:N	2.78	0.46
1:C:492:LEU:HD12	1:C:493:ARG:H	1.81	0.46
1:E:273:GLU:OE2	1:E:276:ARG:NH1	2.48	0.46
1:A:306:GLU:HG2	1:A:497:ASP:HB2	1.97	0.46
1:A:309:MET:HB3	1:A:499:ILE:HG12	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:386:PHE:CD1	1:B:268:ALA:HB1	2.50	0.46
1:D:324:GLN:HE22	1:D:542:LEU:HB2	1.81	0.46
1:D:475:HIS:C	1:D:477:GLU:N	2.72	0.46
1:E:429:VAL:CG2	1:E:430:VAL:N	2.77	0.46
1:C:442:ILE:HG23	1:C:443:ASP:OD1	2.16	0.46
1:F:295:ILE:HD11	1:F:516:VAL:HG11	1.97	0.46
1:A:346:VAL:CG2	1:A:347:GLU:N	2.79	0.46
1:C:426:ILE:HD13	1:C:446:MET:HE3	1.98	0.46
1:E:309:MET:HE2	1:E:464:CYS:CB	2.45	0.46
1:E:429:VAL:CG2	1:E:430:VAL:H	2.22	0.46
1:E:434:GLY:C	1:E:435:GLU:HG3	2.41	0.46
1:A:292:CYS:O	1:A:295:ILE:HD13	2.16	0.46
1:A:537:LYS:HB3	1:A:537:LYS:HE2	1.74	0.46
1:C:289:PHE:HB3	1:C:325:GLN:NE2	2.30	0.46
1:D:524:THR:C	1:D:526:ASP:N	2.72	0.46
1:A:289:PHE:N	1:A:296:ASN:HD21	2.13	0.45
1:D:404:ARG:O	1:D:408:LYS:HG3	2.16	0.45
1:A:340:ALA:C	1:A:341:MET:HE2	2.41	0.45
1:A:475:HIS:C	1:A:477:GLU:H	2.24	0.45
1:C:285:VAL:HG22	1:C:300:LEU:CD2	2.43	0.45
1:E:295:ILE:HG13	1:E:516:VAL:HG11	1.97	0.45
1:E:542:LEU:HD12	1:E:542:LEU:HA	1.88	0.45
1:A:320:THR:OG1	2:A:700:ANP:H8	2.16	0.45
1:C:395:ASP:O	1:C:396:SER:CB	2.64	0.45
1:D:476:GLU:O	1:D:506:GLN:HG2	2.16	0.45
1:E:409:LEU:HD23	1:E:412:MET:CE	2.46	0.45
1:F:442:ILE:HG23	1:F:443:ASP:OD1	2.16	0.45
1:C:292:CYS:C	1:C:293:THR:O	2.53	0.45
1:C:437:ASP:C	1:C:439:ARG:H	2.24	0.45
1:D:392:HIS:HA	1:E:267:SER:HA	1.98	0.45
1:E:421:ILE:HG12	1:E:458:VAL:HG21	1.99	0.45
1:A:411:TYR:O	1:A:415:GLY:N	2.49	0.45
1:B:316:MET:HA	1:B:504:ARG:NH1	2.32	0.45
1:C:312:SER:OG	1:C:318:LYS:HG2	2.16	0.45
1:C:324:GLN:NE2	1:C:542:LEU:H	2.15	0.45
1:C:425:HIS:CD2	1:C:465:HIS:NE2	2.85	0.45
1:D:399:GLU:HB3	1:D:430:VAL:CG2	2.47	0.45
1:D:425:HIS:H	1:D:463:ILE:HB	1.81	0.45
1:A:510:MET:SD	1:A:513:LEU:HD22	2.56	0.45
1:B:404:ARG:HG3	1:B:404:ARG:HH11	1.82	0.45
1:C:295:ILE:HD11	1:C:516:VAL:HG11	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:398:ALA:O	1:C:399:GLU:C	2.60	0.45
1:C:436:SER:O	1:C:437:ASP:O	2.35	0.45
1:D:401:GLU:O	1:D:404:ARG:HB3	2.16	0.45
1:E:438:GLU:HA	1:E:441:MET:HG2	1.99	0.45
1:F:437:ASP:C	1:F:439:ARG:N	2.75	0.45
1:A:292:CYS:HB3	1:A:295:ILE:HD13	1.98	0.45
1:A:401:GLU:O	1:A:404:ARG:HB3	2.16	0.45
1:B:398:ALA:O	1:B:399:GLU:C	2.60	0.45
1:B:480:PRO:HB3	1:B:517:ARG:NH2	2.32	0.45
1:C:352:ASP:OD2	1:C:363:ARG:NH2	2.50	0.45
1:C:477:GLU:HA	1:C:505:ASN:HD22	1.80	0.45
1:C:509:ASP:C	1:C:511:PRO:HD3	2.41	0.45
1:D:311:THR:HG21	1:D:486:LEU:CD2	2.46	0.45
1:D:431:SER:O	1:D:432:ALA:C	2.59	0.45
1:D:510:MET:SD	1:D:513:LEU:HD22	2.57	0.45
1:A:425:HIS:H	1:A:463:ILE:HB	1.81	0.45
1:B:492:LEU:C	1:B:494:GLN:H	2.25	0.45
1:F:436:SER:O	1:F:437:ASP:O	2.35	0.45
1:A:538:GLU:OE1	1:A:538:GLU:HA	2.17	0.45
1:B:292:CYS:O	1:B:295:ILE:HD13	2.16	0.45
1:B:310:VAL:O	1:B:463:ILE:HA	2.17	0.45
1:B:399:GLU:OE1	1:B:430:VAL:HG22	2.16	0.45
1:B:295:ILE:HG13	1:B:516:VAL:HG11	1.99	0.45
1:B:309:MET:HE2	1:B:464:CYS:CB	2.45	0.45
1:B:339:LEU:CD2	1:B:341:MET:HE3	2.43	0.45
1:C:319:SER:O	1:C:323:ARG:HB2	2.17	0.45
1:E:292:CYS:O	1:E:295:ILE:HD13	2.17	0.45
1:E:405:LEU:O	1:E:406:LEU:C	2.58	0.45
1:A:407:ALA:O	1:A:410:ALA:HB3	2.16	0.44
1:A:436:SER:O	1:A:437:ASP:O	2.35	0.44
1:B:440:LYS:HZ2	1:B:444:ASN:HD22	1.63	0.44
1:D:333:MET:O	1:D:335:LYS:HG2	2.16	0.44
1:D:521:CYS:O	1:D:525:GLY:N	2.43	0.44
1:A:273:GLU:OE2	1:A:276:ARG:NH1	2.50	0.44
1:C:309:MET:CE	1:C:464:CYS:HB3	2.45	0.44
1:D:375:ASN:HD21	1:D:377:LYS:HB2	1.81	0.44
1:E:398:ALA:O	1:E:399:GLU:C	2.61	0.44
1:E:493:ARG:O	1:E:493:ARG:HG3	2.12	0.44
1:F:321:PHE:CE1	1:F:533:MET:HE1	2.53	0.44
1:F:469:PRO:CG	1:F:474:ALA:CB	2.93	0.44
1:F:515:LEU:HD23	1:F:515:LEU:C	2.42	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:542:LEU:HD12	1:D:542:LEU:HA	1.89	0.44
1:E:328:GLN:HG3	1:E:333:MET:HE3	1.98	0.44
1:E:469:PRO:HG3	1:E:474:ALA:HB1	1.98	0.44
1:E:471:LYS:O	1:E:471:LYS:HD3	2.18	0.44
1:F:356:LEU:O	1:F:357:HIS:C	2.61	0.44
1:A:299:THR:O	1:A:300:LEU:HB2	2.17	0.44
1:D:346:VAL:CG2	1:D:347:GLU:N	2.81	0.44
1:E:409:LEU:HA	1:E:412:MET:CE	2.46	0.44
1:E:480:PRO:HA	1:E:503:GLU:OE2	2.17	0.44
1:A:431:SER:O	1:A:432:ALA:C	2.60	0.44
1:C:309:MET:HE3	1:C:462:VAL:O	2.17	0.44
1:E:387:GLY:O	1:F:269:LEU:HD11	2.16	0.44
1:F:339:LEU:HB3	1:F:341:MET:HE3	1.99	0.44
1:F:429:VAL:CG2	1:F:430:VAL:H	2.21	0.44
1:A:475:HIS:C	1:A:477:GLU:N	2.73	0.44
1:A:536:ASN:HD22	1:A:536:ASN:C	2.26	0.44
1:B:328:GLN:HG3	1:B:333:MET:HE3	1.99	0.44
1:B:471:LYS:HD3	1:B:471:LYS:O	2.18	0.44
1:C:289:PHE:CD1	1:C:295:ILE:HG21	2.53	0.44
1:C:299:THR:O	1:C:300:LEU:HB2	2.17	0.44
1:C:359:ARG:HD3	1:C:541:TRP:NE1	2.33	0.44
1:C:547:TYR:CD2	1:C:548:SER:N	2.86	0.44
1:D:318:LYS:NZ	2:D:700:ANP:O1G	2.40	0.44
1:E:404:ARG:O	1:E:408:LYS:HG3	2.17	0.44
1:E:431:SER:O	1:E:432:ALA:C	2.60	0.44
1:E:498:THR:HA	1:E:520:LYS:O	2.18	0.44
1:A:287:LEU:HD11	1:A:335:LYS:HG3	1.98	0.44
1:A:289:PHE:CA	1:A:325:GLN:HE21	2.30	0.44
1:B:431:SER:O	1:B:432:ALA:C	2.60	0.44
1:C:289:PHE:N	1:C:296:ASN:HD21	2.11	0.44
1:C:476:GLU:CD	1:C:476:GLU:N	2.75	0.44
1:E:424:ASP:O	1:E:425:HIS:CB	2.66	0.44
1:C:409:LEU:HA	1:C:412:MET:HE3	2.00	0.44
1:C:431:SER:O	1:C:432:ALA:C	2.61	0.44
1:D:273:GLU:OE2	1:D:276:ARG:NH1	2.50	0.44
1:D:382:PHE:HE1	1:E:275:ILE:HD12	1.82	0.44
1:D:436:SER:O	1:D:437:ASP:O	2.36	0.44
1:D:537:LYS:HE2	1:D:537:LYS:HB3	1.75	0.44
1:F:547:TYR:CD2	1:F:548:SER:N	2.86	0.44
1:A:303:ARG:O	1:A:306:GLU:HB2	2.18	0.44
1:B:438:GLU:HA	1:B:441:MET:HG2	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:466:LEU:HD13	1:B:475:HIS:CE1	2.53	0.44
1:C:437:ASP:C	1:C:439:ARG:N	2.76	0.44
1:D:292:CYS:O	1:D:295:ILE:HD13	2.18	0.44
1:A:396:SER:OG	1:A:398:ALA:HB3	2.18	0.43
1:A:491:ALA:O	1:A:494:GLN:HB2	2.17	0.43
1:A:502:LEU:HD23	1:A:514:VAL:HG21	1.99	0.43
1:B:442:ILE:HG23	1:B:443:ASP:N	2.32	0.43
1:B:517:ARG:HD2	1:B:519:LEU:CD1	2.48	0.43
1:C:291:GLY:O	1:C:292:CYS:HB2	2.18	0.43
1:C:475:HIS:C	1:C:477:GLU:N	2.72	0.43
1:E:310:VAL:O	1:E:463:ILE:HA	2.18	0.43
1:B:341:MET:HE1	1:B:422:ILE:CG2	2.48	0.43
1:C:289:PHE:CD1	1:C:295:ILE:CG2	3.01	0.43
1:D:386:PHE:O	1:E:269:LEU:HG	2.17	0.43
2:E:700:ANP:O3G	1:F:522:ARG:NH1	2.50	0.43
1:F:406:LEU:CD2	1:F:448:LYS:HB3	2.48	0.43
1:D:400:ALA:O	1:D:430:VAL:HB	2.17	0.43
1:F:312:SER:OG	1:F:318:LYS:HG2	2.18	0.43
1:E:383:ASP:CG	1:F:272:ARG:HH22	2.26	0.43
1:F:319:SER:O	1:F:323:ARG:HB2	2.18	0.43
1:B:358:ASN:O	1:B:360:VAL:HG22	2.18	0.43
1:E:294:GLY:HA2	1:E:297:ASP:HB2	2.00	0.43
1:F:431:SER:O	1:F:432:ALA:C	2.61	0.43
1:A:375:ASN:HD21	1:A:377:LYS:HB2	1.82	0.43
1:B:324:GLN:HE22	1:B:542:LEU:HB2	1.84	0.43
1:B:434:GLY:C	1:B:435:GLU:HG3	2.43	0.43
1:B:515:LEU:C	1:B:515:LEU:HD23	2.44	0.43
1:D:341:MET:HE1	1:D:422:ILE:CG2	2.48	0.43
1:E:322:VAL:HG12	1:E:323:ARG:N	2.33	0.43
1:F:493:ARG:O	1:F:493:ARG:HG3	2.17	0.43
1:A:425:HIS:NE2	1:A:465:HIS:NE2	2.67	0.43
1:C:289:PHE:CA	1:C:325:GLN:HE21	2.32	0.43
1:F:344:GLU:OE2	1:F:349:THR:HB	2.18	0.43
1:A:280:SER:O	1:A:281:SER:HB2	2.19	0.43
1:B:468:ASN:ND2	1:C:493:ARG:HD2	2.33	0.43
1:B:537:LYS:HE2	1:B:537:LYS:HB3	1.70	0.43
1:C:321:PHE:CE1	1:C:533:MET:HE1	2.54	0.43
2:D:700:ANP:O3G	1:E:522:ARG:NH2	2.51	0.43
1:F:359:ARG:HD3	1:F:541:TRP:NE1	2.33	0.43
1:F:476:GLU:CD	1:F:476:GLU:N	2.76	0.43
1:D:408:LYS:O	1:D:412:MET:HG3	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:442:ILE:HG23	1:E:443:ASP:N	2.33	0.43
1:A:399:GLU:HB3	1:A:430:VAL:CG2	2.49	0.43
1:A:437:ASP:O	1:A:439:ARG:N	2.52	0.43
1:A:476:GLU:O	1:A:506:GLN:HG2	2.19	0.43
1:D:516:VAL:CG2	1:D:533:MET:HE2	2.49	0.43
1:A:266:VAL:HG12	1:A:267:SER:N	2.34	0.42
1:A:450:LYS:HB2	1:A:495:LEU:HB3	2.01	0.42
1:A:480:PRO:HB3	1:A:517:ARG:NH2	2.34	0.42
1:B:426:ILE:HD13	1:B:446:MET:HE3	2.01	0.42
1:B:480:PRO:HB3	1:B:517:ARG:HH21	1.84	0.42
1:C:289:PHE:HA	1:C:325:GLN:HE21	1.84	0.42
1:C:356:LEU:HG	1:C:541:TRP:NE1	2.33	0.42
1:C:388:ASN:O	1:C:389:ASP:C	2.62	0.42
1:C:421:ILE:HB	1:C:460:LEU:HD12	2.01	0.42
1:C:475:HIS:C	1:C:477:GLU:H	2.27	0.42
1:D:313:GLY:HA3	1:D:316:MET:SD	2.59	0.42
1:D:435:GLU:O	1:D:436:SER:O	2.37	0.42
1:D:480:PRO:HB3	1:D:517:ARG:NH2	2.34	0.42
1:A:408:LYS:O	1:A:412:MET:HG3	2.20	0.42
1:C:394:TYR:CE2	1:C:408:LYS:HD2	2.53	0.42
1:E:369:LYS:NZ	1:F:282:GLU:HG3	2.33	0.42
1:A:396:SER:O	1:A:397:PHE:HB3	2.19	0.42
1:A:542:LEU:HD12	1:A:542:LEU:HA	1.88	0.42
1:B:266:VAL:CG1	1:B:267:SER:N	2.81	0.42
1:B:341:MET:HB3	1:B:344:GLU:HG2	2.00	0.42
1:D:491:ALA:O	1:D:494:GLN:HB2	2.19	0.42
1:E:399:GLU:HB3	1:E:430:VAL:CG1	2.49	0.42
1:A:404:ARG:HG3	1:A:404:ARG:HH11	1.84	0.42
1:B:426:ILE:HD12	1:B:446:MET:CE	2.48	0.42
1:C:537:LYS:HB3	1:C:537:LYS:HE2	1.69	0.42
1:E:463:ILE:HG22	1:E:464:CYS:N	2.33	0.42
1:F:320:THR:HG22	1:F:324:GLN:NE2	2.33	0.42
1:B:424:ASP:O	1:B:425:HIS:CB	2.68	0.42
1:B:484:THR:HA	1:B:493:ARG:NH2	2.34	0.42
1:C:273:GLU:OE1	1:C:273:GLU:HA	2.19	0.42
1:D:507:GLN:NE2	1:E:528:GLY:HA2	2.35	0.42
1:F:359:ARG:CZ	1:F:541:TRP:CZ2	3.02	0.42
1:C:424:ASP:OD1	1:C:424:ASP:C	2.63	0.42
1:F:309:MET:HE1	1:F:462:VAL:HG12	2.02	0.42
1:D:409:LEU:HA	1:D:412:MET:HE2	2.01	0.42
1:F:344:GLU:HA	1:F:397:PHE:CE1	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:404:ARG:O	1:B:408:LYS:HG3	2.20	0.42
1:B:507:GLN:NE2	1:C:528:GLY:CA	2.80	0.42
1:C:404:ARG:HG3	1:C:404:ARG:HH11	1.84	0.42
1:E:426:ILE:O	1:E:426:ILE:HG23	2.19	0.42
1:E:492:LEU:C	1:E:494:GLN:H	2.27	0.42
1:F:477:GLU:HA	1:F:505:ASN:HD22	1.82	0.42
1:A:261:ILE:HA	1:A:262:PRO:HD2	1.84	0.42
1:A:521:CYS:O	1:A:525:GLY:N	2.43	0.42
1:B:387:GLY:C	1:B:389:ASP:H	2.28	0.42
1:B:496:SER:OG	1:B:499:ILE:HD11	2.20	0.42
1:C:278:HIS:O	1:C:282:GLU:CB	2.66	0.42
1:C:443:ASP:CG	1:C:491:ALA:HB2	2.45	0.42
1:A:294:GLY:O	1:A:295:ILE:C	2.63	0.42
1:A:311:THR:HG21	1:A:486:LEU:CD2	2.48	0.42
1:B:401:GLU:HB3	1:B:404:ARG:CB	2.49	0.42
1:B:405:LEU:O	1:B:408:LYS:N	2.53	0.42
1:C:344:GLU:HA	1:C:397:PHE:CE1	2.55	0.42
1:E:343:GLU:HG3	1:E:428:ILE:HD11	2.00	0.42
1:E:517:ARG:HD2	1:E:519:LEU:CD1	2.50	0.42
1:F:336:LYS:HB3	1:F:418:CYS:HA	2.02	0.42
1:F:398:ALA:O	1:F:399:GLU:C	2.62	0.42
1:F:399:GLU:CB	1:F:430:VAL:HG11	2.49	0.42
1:B:322:VAL:CG1	1:B:422:ILE:HG21	2.50	0.41
1:B:420:VAL:HG13	1:B:459:VAL:HG12	2.02	0.41
1:C:269:LEU:HA	1:C:269:LEU:HD23	1.84	0.41
1:C:536:ASN:HD22	1:C:537:LYS:N	2.18	0.41
1:D:506:GLN:HG2	1:D:506:GLN:H	1.68	0.41
1:A:535:TYR:HD1	1:A:542:LEU:HD13	1.84	0.41
1:B:383:ASP:O	1:B:385:LEU:N	2.53	0.41
1:B:401:GLU:OE1	1:B:404:ARG:N	2.36	0.41
1:C:336:LYS:HB3	1:C:418:CYS:HA	2.02	0.41
1:D:368:LEU:O	1:D:371:GLU:HB2	2.20	0.41
1:E:322:VAL:CG1	1:E:422:ILE:HG21	2.50	0.41
1:F:343:GLU:HG3	1:F:428:ILE:CD1	2.48	0.41
1:F:411:TYR:O	1:F:415:GLY:N	2.49	0.41
1:B:309:MET:HE2	1:B:464:CYS:SG	2.60	0.41
1:B:322:VAL:HG13	1:B:422:ILE:HG21	2.01	0.41
1:B:465:HIS:O	1:B:487:ARG:HB2	2.20	0.41
1:C:424:ASP:O	1:C:425:HIS:CB	2.68	0.41
1:C:515:LEU:HB2	1:C:532:TYR:CE2	2.55	0.41
1:C:515:LEU:HD12	1:C:532:TYR:CE2	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:517:ARG:HD2	1:C:519:LEU:CD1	2.50	0.41
1:D:341:MET:HE1	1:D:422:ILE:HG22	2.02	0.41
1:E:330:GLY:HA3	1:E:391:PHE:CZ	2.56	0.41
1:E:492:LEU:C	1:E:494:GLN:N	2.78	0.41
1:E:506:GLN:HG2	1:E:506:GLN:H	1.54	0.41
1:E:536:ASN:HD21	1:E:538:GLU:CB	2.32	0.41
1:B:299:THR:O	1:B:300:LEU:HB2	2.20	0.41
1:B:333:MET:O	1:B:335:LYS:HG2	2.20	0.41
1:B:358:ASN:ND2	1:B:381:TRP:CE2	2.88	0.41
1:B:496:SER:O	1:B:520:LYS:HE2	2.20	0.41
1:D:492:LEU:HD12	1:D:493:ARG:N	2.35	0.41
1:E:466:LEU:HD13	1:E:475:HIS:CE1	2.56	0.41
1:E:496:SER:OG	1:E:499:ILE:HD11	2.20	0.41
1:F:346:VAL:CG2	1:F:347:GLU:N	2.83	0.41
1:F:401:GLU:OE1	1:F:404:ARG:N	2.43	0.41
1:F:536:ASN:HB2	1:F:543:GLU:OE1	2.20	0.41
1:A:409:LEU:HA	1:A:412:MET:HE2	2.01	0.41
1:A:481:VAL:HG12	1:A:503:GLU:HG2	2.01	0.41
1:D:404:ARG:HG3	1:D:404:ARG:HH11	1.86	0.41
1:D:437:ASP:O	1:D:439:ARG:N	2.54	0.41
1:E:309:MET:HE1	1:E:462:VAL:CG1	2.41	0.41
1:E:480:PRO:HB3	1:E:517:ARG:NH2	2.35	0.41
1:F:535:TYR:HE1	1:F:540:GLY:O	2.03	0.41
1:A:510:MET:HE1	1:A:547:TYR:HE1	1.82	0.41
1:B:282:GLU:O	1:B:282:GLU:HG3	2.20	0.41
1:B:443:ASP:OD1	1:B:491:ALA:HB2	2.21	0.41
1:B:468:ASN:ND2	1:C:493:ARG:CZ	2.82	0.41
1:E:316:MET:HA	1:E:504:ARG:NH1	2.35	0.41
1:E:386:PHE:CD1	1:F:268:ALA:HB1	2.55	0.41
1:F:352:ASP:OD2	1:F:363:ARG:NH2	2.53	0.41
1:F:475:HIS:C	1:F:477:GLU:N	2.75	0.41
1:B:483:ILE:CG2	1:B:493:ARG:HB2	2.50	0.41
1:D:440:LYS:HD3	1:D:440:LYS:C	2.45	0.41
1:D:536:ASN:HD22	1:D:536:ASN:C	2.28	0.41
1:F:489:SER:O	1:F:490:GLY:C	2.63	0.41
1:A:435:GLU:O	1:A:436:SER:O	2.39	0.41
1:A:517:ARG:HD2	1:A:519:LEU:CD1	2.50	0.41
1:B:278:HIS:O	1:B:282:GLU:CB	2.69	0.41
1:C:359:ARG:CZ	1:C:541:TRP:CZ2	3.04	0.41
1:D:471:LYS:O	1:D:471:LYS:HD3	2.21	0.41
1:E:476:GLU:HB3	1:E:506:GLN:NE2	2.36	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:271:LEU:O	1:F:272:ARG:C	2.64	0.41
1:B:295:ILE:HD12	1:B:295:ILE:N	2.35	0.41
1:B:330:GLY:HA3	1:B:391:PHE:CZ	2.55	0.41
1:B:476:GLU:CG	1:C:483:ILE:HD12	2.28	0.41
1:B:506:GLN:HG2	1:B:506:GLN:H	1.52	0.41
1:C:265:VAL:O	1:C:265:VAL:HG12	2.21	0.41
1:C:273:GLU:O	1:C:274:ARG:C	2.64	0.41
1:D:324:GLN:NE2	1:D:542:LEU:HB2	2.35	0.41
1:D:406:LEU:HD21	1:D:448:LYS:HB3	2.02	0.41
1:E:406:LEU:O	1:E:407:ALA:C	2.64	0.41
1:E:442:ILE:HG23	1:E:443:ASP:OD1	2.20	0.41
1:E:507:GLN:NE2	1:F:528:GLY:HA2	2.35	0.41
1:F:339:LEU:O	1:F:393:LEU:HA	2.21	0.41
1:A:429:VAL:CG2	1:A:430:VAL:H	2.23	0.41
1:B:485:ASP:O	1:B:486:LEU:C	2.62	0.41
1:B:492:LEU:C	1:B:494:GLN:N	2.77	0.41
1:E:291:GLY:HA2	1:E:542:LEU:O	2.21	0.41
1:E:547:TYR:CG	1:E:548:SER:N	2.89	0.41
1:A:306:GLU:HG2	1:A:497:ASP:CB	2.51	0.40
1:A:396:SER:HB3	1:A:397:PHE:H	1.72	0.40
1:A:400:ALA:O	1:A:430:VAL:HB	2.21	0.40
1:B:480:PRO:HA	1:B:503:GLU:OE2	2.21	0.40
1:C:399:GLU:CB	1:C:430:VAL:HG11	2.49	0.40
1:B:421:ILE:HG12	1:B:458:VAL:HG21	2.03	0.40
1:D:396:SER:O	1:D:397:PHE:HB3	2.22	0.40
1:D:399:GLU:HB3	1:D:430:VAL:CG1	2.51	0.40
1:E:316:MET:O	1:E:504:ARG:NH1	2.53	0.40
1:F:309:MET:CE	1:F:464:CYS:HB3	2.50	0.40
1:B:411:TYR:CD1	1:B:415:GLY:HA3	2.56	0.40
1:B:442:ILE:HG23	1:B:443:ASP:OD1	2.21	0.40
1:D:340:ALA:H	1:D:341:MET:HE2	1.86	0.40
1:D:368:LEU:HD23	1:D:368:LEU:HA	1.86	0.40
1:E:373:ILE:HD13	1:F:280:SER:HB3	2.03	0.40
1:E:436:SER:O	1:E:437:ASP:C	2.63	0.40
1:F:404:ARG:HH11	1:F:404:ARG:HG3	1.86	0.40
1:F:443:ASP:CG	1:F:491:ALA:HB2	2.47	0.40
1:A:516:VAL:CG2	1:A:533:MET:HE2	2.50	0.40
1:A:536:ASN:ND2	1:A:538:GLU:H	2.19	0.40
1:B:492:LEU:HD12	1:B:493:ARG:N	2.36	0.40
1:C:401:GLU:OE1	1:C:404:ARG:N	2.42	0.40
1:D:341:MET:HA	1:D:424:ASP:HB3	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:292:CYS:HB3	1:E:295:ILE:HD13	2.02	0.40
1:A:411:TYR:CD1	1:A:415:GLY:HA3	2.57	0.40
1:C:313:GLY:H	1:C:316:MET:CE	2.34	0.40
1:C:366:ASP:N	1:C:366:ASP:OD1	2.54	0.40
1:D:338:GLY:HA3	1:D:421:ILE:HD13	2.04	0.40
1:D:425:HIS:CE1	1:D:465:HIS:CD2	3.10	0.40
1:F:324:GLN:HE22	1:F:542:LEU:N	2.17	0.40
1:F:517:ARG:HD2	1:F:519:LEU:CD1	2.50	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran 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 backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	283/289 (98%)	231 (82%)	32 (11%)	20 (7%)	1	4
1	B	286/289 (99%)	242 (85%)	26 (9%)	18 (6%)	1	6
1	C	286/289 (99%)	234 (82%)	35 (12%)	17 (6%)	1	7
1	D	283/289 (98%)	231 (82%)	34 (12%)	18 (6%)	1	6
1	E	286/289 (99%)	243 (85%)	24 (8%)	19 (7%)	1	5
1	F	286/289 (99%)	232 (81%)	37 (13%)	17 (6%)	1	7
All	All	1710/1734 (99%)	1413 (83%)	188 (11%)	109 (6%)	1	6

All (109) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	262	PRO
1	A	263	ASP
1	A	396	SER
1	A	436	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	437	ASP
1	A	475	HIS
1	A	490	GLY
1	B	396	SER
1	B	436	SER
1	B	437	ASP
1	B	475	HIS
1	B	490	GLY
1	C	396	SER
1	C	436	SER
1	C	437	ASP
1	C	475	HIS
1	C	490	GLY
1	D	396	SER
1	D	436	SER
1	D	437	ASP
1	D	475	HIS
1	D	490	GLY
1	E	388	ASN
1	E	396	SER
1	E	436	SER
1	E	437	ASP
1	E	475	HIS
1	E	490	GLY
1	F	396	SER
1	F	436	SER
1	F	437	ASP
1	F	475	HIS
1	F	490	GLY
1	A	287	LEU
1	A	397	PHE
1	A	399	GLU
1	A	432	ALA
1	A	488	GLY
1	A	489	SER
1	B	334	GLY
1	B	388	ASN
1	B	397	PHE
1	B	399	GLU
1	B	432	ALA
1	C	334	GLY
1	C	397	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	397	PHE
1	D	399	GLU
1	D	432	ALA
1	D	488	GLY
1	D	489	SER
1	E	334	GLY
1	E	397	PHE
1	E	399	GLU
1	E	432	ALA
1	F	287	LEU
1	F	334	GLY
1	F	371	GLU
1	F	397	PHE
1	A	334	GLY
1	A	438	GLU
1	B	384	GLU
1	B	479	ARG
1	C	287	LEU
1	C	292	CYS
1	C	399	GLU
1	C	432	ALA
1	D	287	LEU
1	E	479	ARG
1	F	399	GLU
1	F	432	ALA
1	F	479	ARG
1	A	470	ASP
1	A	471	LYS
1	A	479	ARG
1	B	287	LEU
1	B	438	GLU
1	C	364	GLN
1	C	371	GLU
1	C	425	HIS
1	C	479	ARG
1	D	334	GLY
1	D	371	GLU
1	D	438	GLU
1	D	471	LYS
1	D	479	ARG
1	E	332	ALA
1	E	384	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	438	GLU
1	F	281	SER
1	F	364	GLN
1	F	425	HIS
1	A	371	GLU
1	A	402	THR
1	B	332	ALA
1	B	470	ASP
1	D	402	THR
1	D	470	ASP
1	E	287	LEU
1	E	470	ASP
1	E	471	LYS
1	F	488	GLY
1	B	402	THR
1	C	488	GLY
1	E	371	GLU
1	F	434	GLY
1	C	434	GLY
1	B	430	VAL
1	E	430	VAL

5.3.2 Protein sidechains ⓘ

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	240/242 (99%)	214 (89%)	26 (11%)	6	26
1	B	241/242 (100%)	209 (87%)	32 (13%)	4	18
1	C	241/242 (100%)	204 (85%)	37 (15%)	2	13
1	D	240/242 (99%)	214 (89%)	26 (11%)	6	26
1	E	241/242 (100%)	208 (86%)	33 (14%)	3	17
1	F	241/242 (100%)	205 (85%)	36 (15%)	3	15
All	All	1444/1452 (99%)	1254 (87%)	190 (13%)	4	18

All (190) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	277	GLU
1	A	293	THR
1	A	300	LEU
1	A	322	VAL
1	A	347	GLU
1	A	349	THR
1	A	360	VAL
1	A	368	LEU
1	A	384	GLU
1	A	393	LEU
1	A	403	ASP
1	A	406	LEU
1	A	446	MET
1	A	455	SER
1	A	470	ASP
1	A	476	GLU
1	A	481	VAL
1	A	487	ARG
1	A	492	LEU
1	A	495	LEU
1	A	500	ILE
1	A	507	GLN
1	A	512	ASN
1	A	514	VAL
1	A	522	ARG
1	A	542	LEU
1	B	267	SER
1	B	277	GLU
1	B	287	LEU
1	B	288	LEU
1	B	290	SER
1	B	322	VAL
1	B	347	GLU
1	B	349	THR
1	B	360	VAL
1	B	368	LEU
1	B	373	ILE
1	B	384	GLU
1	B	393	LEU
1	B	403	ASP
1	B	420	VAL
1	B	440	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	470	ASP
1	B	476	GLU
1	B	481	VAL
1	B	487	ARG
1	B	492	LEU
1	B	493	ARG
1	B	495	LEU
1	B	499	ILE
1	B	504	ARG
1	B	506	GLN
1	B	507	GLN
1	B	512	ASN
1	B	514	VAL
1	B	519	LEU
1	B	536	ASN
1	B	542	LEU
1	C	263	ASP
1	C	277	GLU
1	C	287	LEU
1	C	288	LEU
1	C	290	SER
1	C	295	ILE
1	C	303	ARG
1	C	325	GLN
1	C	347	GLU
1	C	349	THR
1	C	360	VAL
1	C	368	LEU
1	C	371	GLU
1	C	375	ASN
1	C	384	GLU
1	C	390	THR
1	C	393	LEU
1	C	403	ASP
1	C	440	LYS
1	C	470	ASP
1	C	476	GLU
1	C	479	ARG
1	C	481	VAL
1	C	482	SER
1	C	487	ARG
1	C	492	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	493	ARG
1	C	495	LEU
1	C	499	ILE
1	C	506	GLN
1	C	507	GLN
1	C	512	ASN
1	C	514	VAL
1	C	515	LEU
1	C	519	LEU
1	C	536	ASN
1	C	542	LEU
1	D	272	ARG
1	D	293	THR
1	D	300	LEU
1	D	322	VAL
1	D	347	GLU
1	D	349	THR
1	D	360	VAL
1	D	368	LEU
1	D	384	GLU
1	D	393	LEU
1	D	403	ASP
1	D	406	LEU
1	D	446	MET
1	D	455	SER
1	D	470	ASP
1	D	476	GLU
1	D	481	VAL
1	D	487	ARG
1	D	492	LEU
1	D	495	LEU
1	D	500	ILE
1	D	507	GLN
1	D	512	ASN
1	D	514	VAL
1	D	522	ARG
1	D	542	LEU
1	E	274	ARG
1	E	277	GLU
1	E	280	SER
1	E	282	GLU
1	E	287	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	288	LEU
1	E	290	SER
1	E	322	VAL
1	E	347	GLU
1	E	349	THR
1	E	360	VAL
1	E	368	LEU
1	E	373	ILE
1	E	384	GLU
1	E	393	LEU
1	E	403	ASP
1	E	420	VAL
1	E	440	LYS
1	E	470	ASP
1	E	476	GLU
1	E	481	VAL
1	E	487	ARG
1	E	492	LEU
1	E	493	ARG
1	E	495	LEU
1	E	499	ILE
1	E	506	GLN
1	E	507	GLN
1	E	512	ASN
1	E	514	VAL
1	E	519	LEU
1	E	536	ASN
1	E	542	LEU
1	F	277	GLU
1	F	284	SER
1	F	287	LEU
1	F	288	LEU
1	F	290	SER
1	F	295	ILE
1	F	303	ARG
1	F	325	GLN
1	F	347	GLU
1	F	349	THR
1	F	360	VAL
1	F	368	LEU
1	F	371	GLU
1	F	375	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	384	GLU
1	F	390	THR
1	F	403	ASP
1	F	420	VAL
1	F	440	LYS
1	F	470	ASP
1	F	476	GLU
1	F	479	ARG
1	F	481	VAL
1	F	482	SER
1	F	487	ARG
1	F	492	LEU
1	F	493	ARG
1	F	495	LEU
1	F	499	ILE
1	F	506	GLN
1	F	507	GLN
1	F	512	ASN
1	F	514	VAL
1	F	519	LEU
1	F	536	ASN
1	F	542	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (71) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	296	ASN
1	A	324	GLN
1	A	325	GLN
1	A	358	ASN
1	A	375	ASN
1	A	392	HIS
1	A	475	HIS
1	A	494	GLN
1	A	505	ASN
1	A	507	GLN
1	A	512	ASN
1	A	536	ASN
1	B	296	ASN
1	B	324	GLN
1	B	325	GLN
1	B	358	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	375	ASN
1	B	392	HIS
1	B	425	HIS
1	B	444	ASN
1	B	468	ASN
1	B	475	HIS
1	B	494	GLN
1	B	505	ASN
1	B	507	GLN
1	B	536	ASN
1	C	296	ASN
1	C	324	GLN
1	C	325	GLN
1	C	358	ASN
1	C	375	ASN
1	C	392	HIS
1	C	425	HIS
1	C	494	GLN
1	C	505	ASN
1	C	536	ASN
1	D	296	ASN
1	D	324	GLN
1	D	325	GLN
1	D	375	ASN
1	D	475	HIS
1	D	494	GLN
1	D	505	ASN
1	D	507	GLN
1	D	512	ASN
1	D	536	ASN
1	E	296	ASN
1	E	324	GLN
1	E	325	GLN
1	E	358	ASN
1	E	375	ASN
1	E	388	ASN
1	E	392	HIS
1	E	444	ASN
1	E	468	ASN
1	E	475	HIS
1	E	494	GLN
1	E	505	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	506	GLN
1	E	507	GLN
1	E	536	ASN
1	F	296	ASN
1	F	324	GLN
1	F	325	GLN
1	F	358	ASN
1	F	375	ASN
1	F	392	HIS
1	F	425	HIS
1	F	494	GLN
1	F	505	ASN
1	F	536	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 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	$\# Z > 2$
2	ANP	A	700	3	33,33,33	1.53	5 (15%)	45,52,52	1.50	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ANP	E	700	3	33,33,33	1.46	3 (9%)	45,52,52	1.50	3 (6%)
2	ANP	D	700	3	33,33,33	1.51	4 (12%)	45,52,52	1.48	4 (8%)
2	ANP	B	700	3	33,33,33	1.19	4 (12%)	45,52,52	1.44	3 (6%)

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
2	ANP	A	700	3	-	6/18/38/38	0/3/3/3
2	ANP	E	700	3	-	6/18/38/38	0/3/3/3
2	ANP	D	700	3	-	6/18/38/38	0/3/3/3
2	ANP	B	700	3	-	6/18/38/38	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	700	ANP	PB-O1B	5.86	1.55	1.46
2	E	700	ANP	PB-O1B	5.28	1.54	1.46
2	A	700	ANP	PB-O1B	4.59	1.53	1.46
2	B	700	ANP	PB-O1B	2.98	1.50	1.46
2	D	700	ANP	PB-O2B	-2.85	1.49	1.56
2	A	700	ANP	PG-N3B	-2.85	1.55	1.63
2	B	700	ANP	PB-O2B	-2.80	1.49	1.56
2	A	700	ANP	PB-O2B	-2.75	1.49	1.56
2	E	700	ANP	PB-O2B	-2.68	1.49	1.56
2	D	700	ANP	PG-N3B	-2.35	1.57	1.63
2	B	700	ANP	PG-N3B	-2.26	1.57	1.63
2	D	700	ANP	PG-O2G	-2.21	1.50	1.56
2	E	700	ANP	C4-N3	2.16	1.38	1.34
2	B	700	ANP	PG-O2G	-2.10	1.51	1.56
2	A	700	ANP	C8-N9	2.03	1.41	1.37
2	A	700	ANP	C2-N1	2.01	1.37	1.33

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	700	ANP	O1G-PG-N3B	-7.78	100.31	111.77
2	A	700	ANP	O1G-PG-N3B	-7.71	100.41	111.77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	700	ANP	O1G-PG-N3B	-7.61	100.56	111.77
2	B	700	ANP	O1G-PG-N3B	-7.35	100.94	111.77
2	A	700	ANP	O2B-PB-O1B	4.77	120.09	109.87
2	E	700	ANP	O2B-PB-O1B	4.65	119.84	109.87
2	B	700	ANP	O2B-PB-O1B	4.62	119.77	109.87
2	D	700	ANP	O2B-PB-O1B	4.61	119.77	109.87
2	D	700	ANP	O2G-PG-O3G	2.49	114.27	107.59
2	B	700	ANP	O2G-PG-O3G	2.48	114.25	107.59
2	A	700	ANP	O2G-PG-O3G	2.45	114.19	107.59
2	E	700	ANP	O2G-PG-O3G	2.36	113.94	107.59
2	D	700	ANP	O3A-PB-N3B	-2.10	100.78	106.59

There are no chirality outliers.

All (24) torsion outliers are listed below:

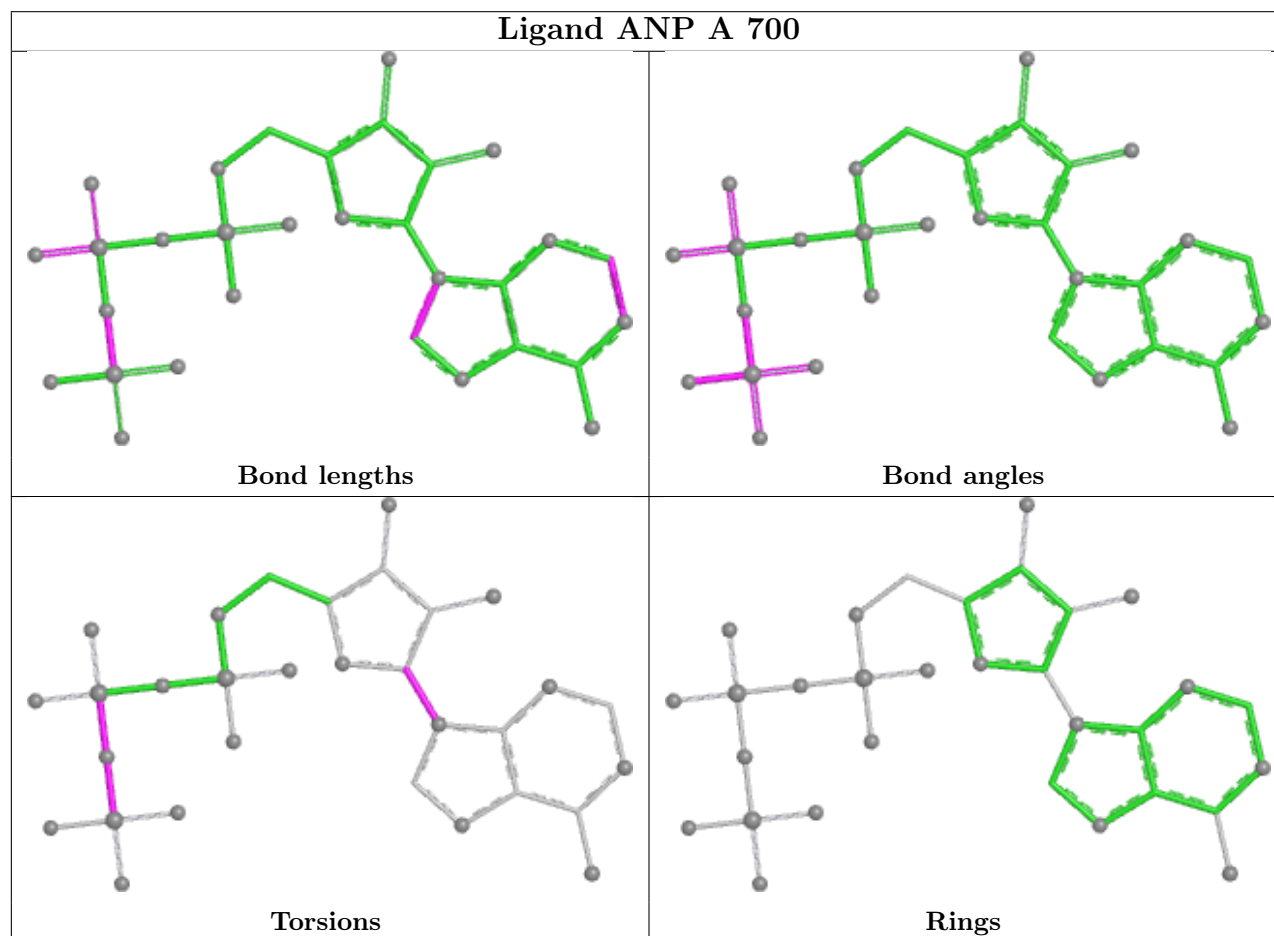
Mol	Chain	Res	Type	Atoms
2	A	700	ANP	PB-N3B-PG-O1G
2	A	700	ANP	PG-N3B-PB-O1B
2	A	700	ANP	PG-N3B-PB-O3A
2	B	700	ANP	PB-N3B-PG-O1G
2	B	700	ANP	PG-N3B-PB-O1B
2	B	700	ANP	PG-N3B-PB-O3A
2	D	700	ANP	PB-N3B-PG-O1G
2	D	700	ANP	PG-N3B-PB-O1B
2	D	700	ANP	PG-N3B-PB-O3A
2	E	700	ANP	PB-N3B-PG-O1G
2	E	700	ANP	PG-N3B-PB-O1B
2	E	700	ANP	PG-N3B-PB-O3A
2	A	700	ANP	C2'-C1'-N9-C8
2	B	700	ANP	C2'-C1'-N9-C8
2	D	700	ANP	C2'-C1'-N9-C8
2	E	700	ANP	C2'-C1'-N9-C8
2	B	700	ANP	C2'-C1'-N9-C4
2	B	700	ANP	O4'-C1'-N9-C8
2	D	700	ANP	O4'-C1'-N9-C8
2	E	700	ANP	O4'-C1'-N9-C8
2	A	700	ANP	O4'-C1'-N9-C8
2	A	700	ANP	C2'-C1'-N9-C4
2	D	700	ANP	C2'-C1'-N9-C4
2	E	700	ANP	C2'-C1'-N9-C4

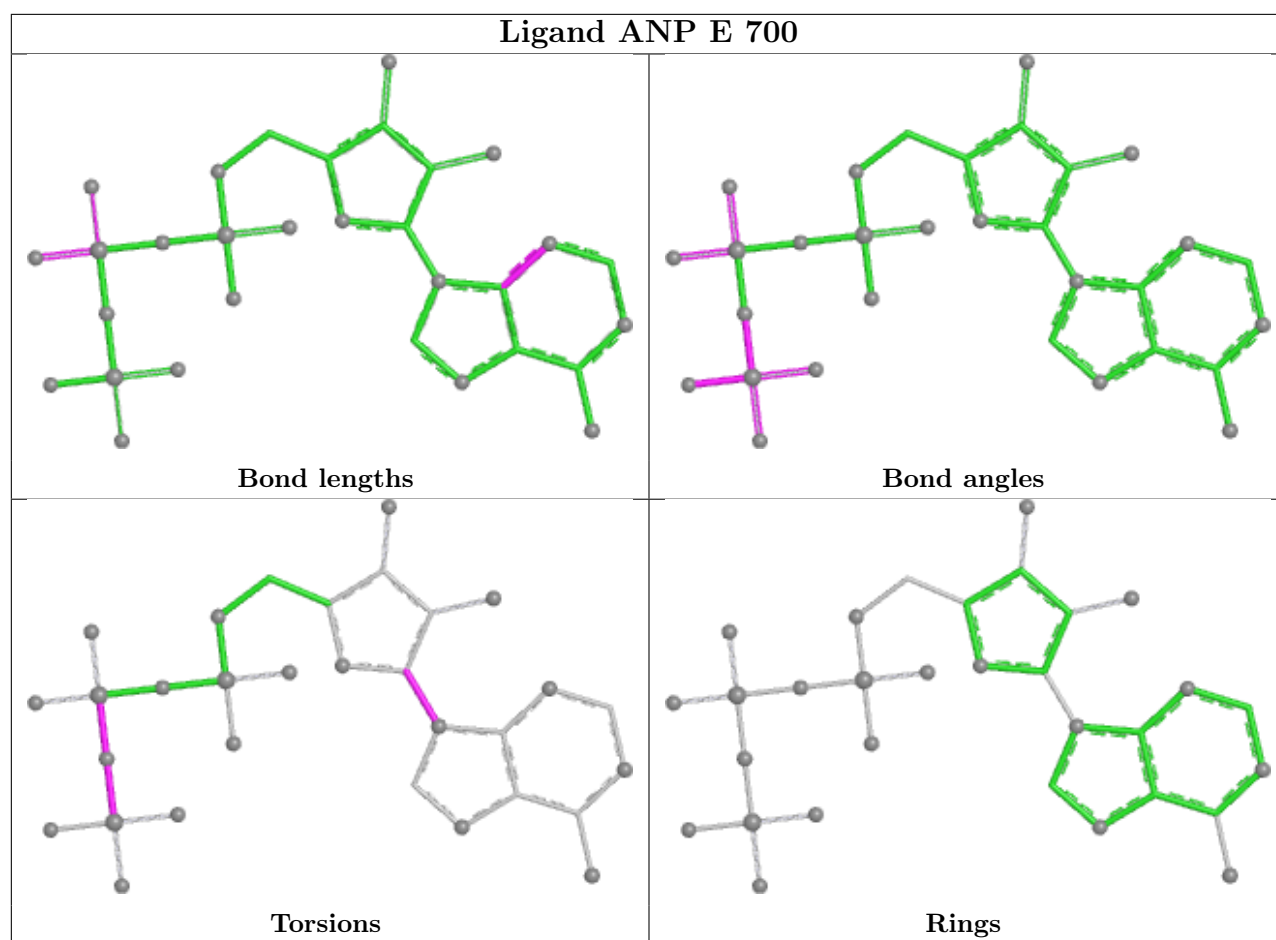
There are no ring outliers.

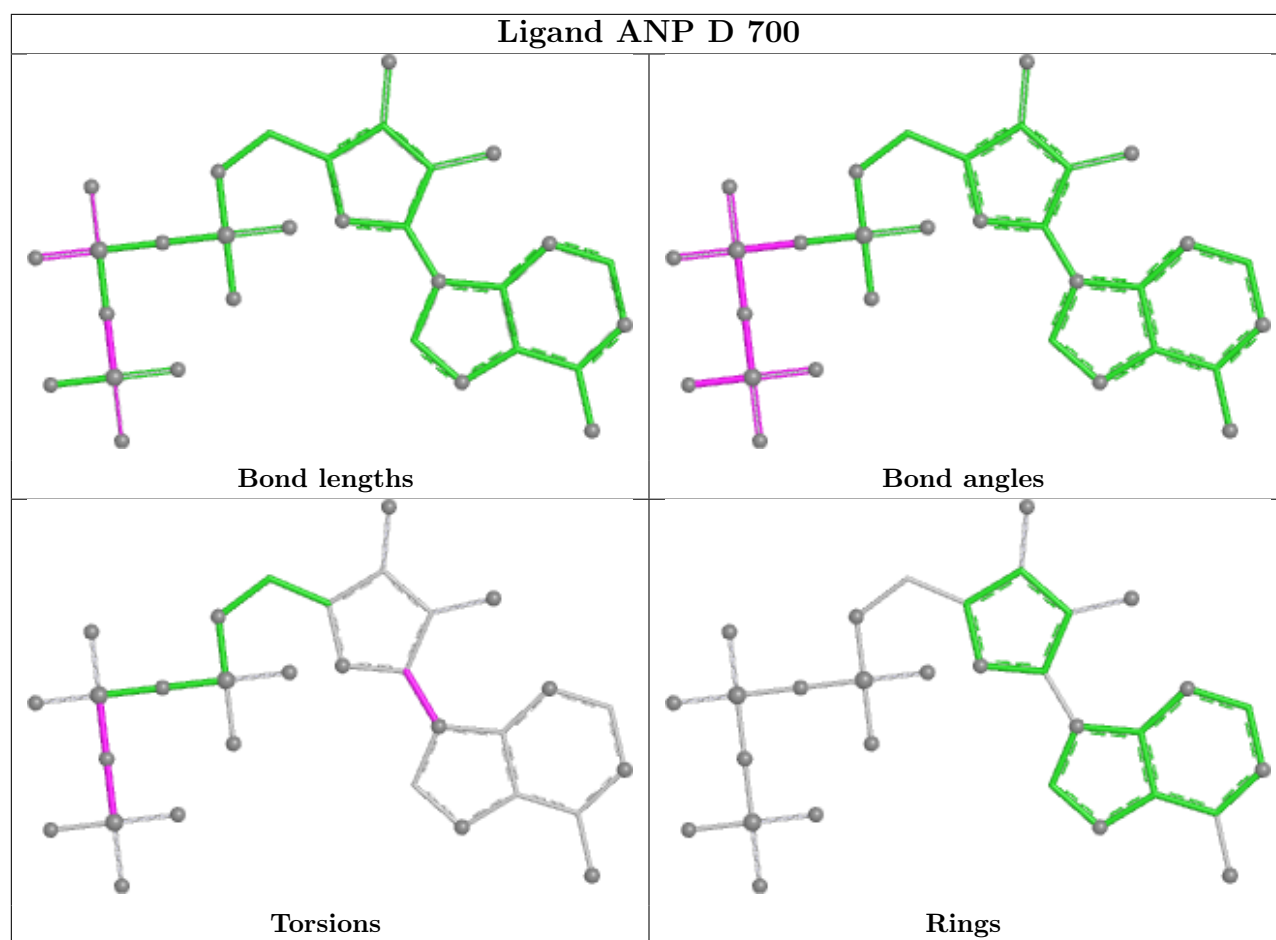
4 monomers are involved in 8 short contacts:

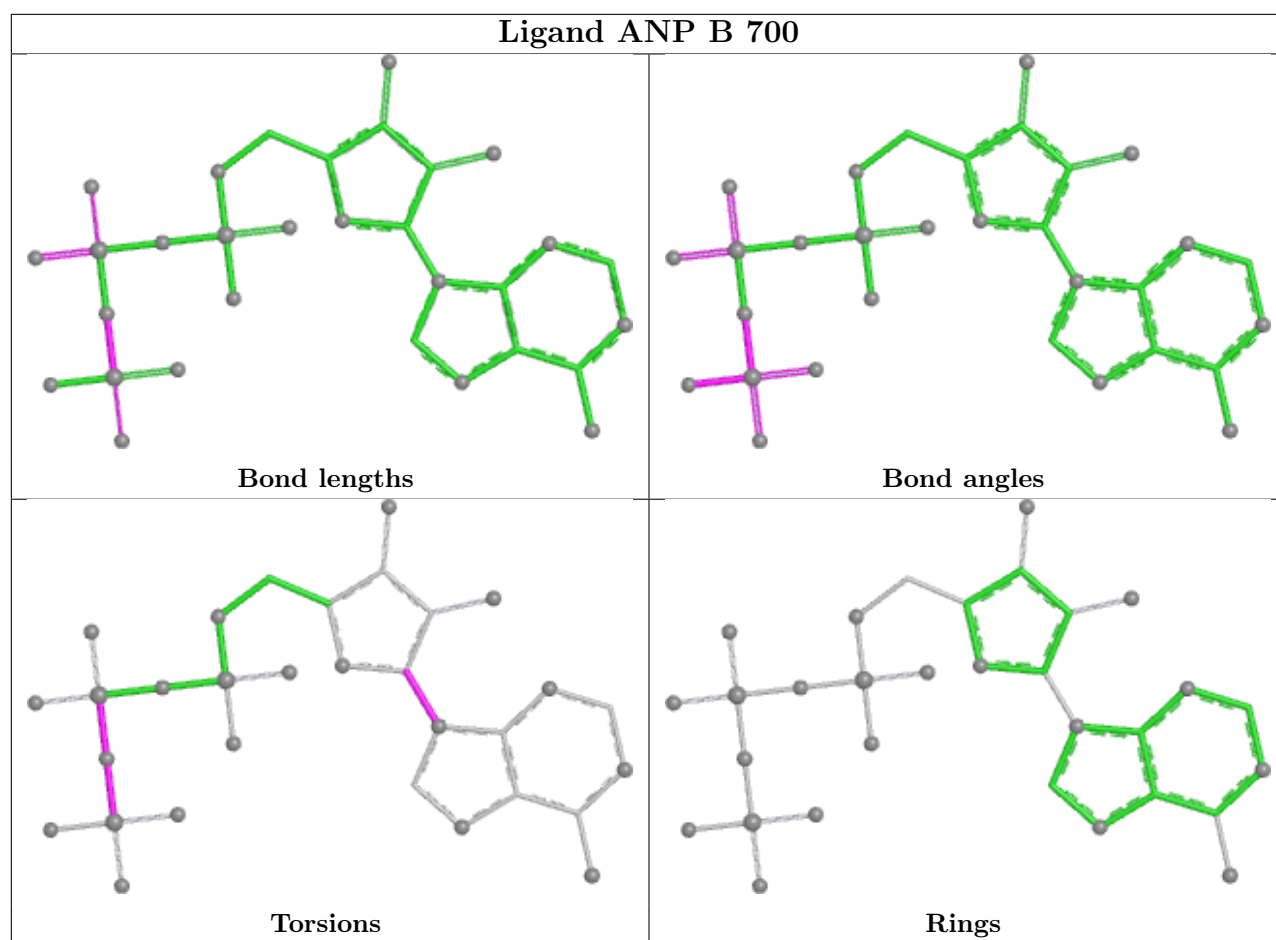
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	700	ANP	2	0
2	E	700	ANP	1	0
2	D	700	ANP	2	0
2	B	700	ANP	3	0

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.









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	287/289 (99%)	0.17	10 (3%)	47 27	40, 67, 132, 169	0
1	B	288/289 (99%)	-0.06	8 (2%)	55 32	33, 58, 124, 159	0
1	C	288/289 (99%)	-0.06	4 (1%)	73 51	34, 60, 126, 155	0
1	D	287/289 (99%)	0.07	7 (2%)	59 36	44, 69, 135, 166	0
1	E	288/289 (99%)	-0.07	2 (0%)	84 66	37, 62, 124, 161	0
1	F	288/289 (99%)	0.02	6 (2%)	63 40	38, 62, 128, 158	0
All	All	1726/1734 (99%)	0.01	37 (2%)	63 40	33, 64, 131, 169	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	284	SER	8.4
1	B	433	SER	5.1
1	D	432	ALA	4.0
1	D	429	VAL	3.4
1	C	470	ASP	3.4
1	C	429	VAL	3.3
1	F	433	SER	3.2
1	A	433	SER	3.1
1	D	279	LEU	3.0
1	E	434	GLY	3.0
1	D	261	ILE	3.0
1	A	429	VAL	3.0
1	A	436	SER	2.8
1	B	541	TRP	2.8
1	B	434	GLY	2.8
1	D	284	SER	2.7
1	D	433	SER	2.7
1	D	431	SER	2.7
1	B	281	SER	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	262	PRO	2.6
1	E	264	GLY	2.6
1	B	442	ILE	2.4
1	A	406	LEU	2.4
1	F	398	ALA	2.3
1	B	264	GLY	2.3
1	F	366	ASP	2.3
1	A	263	ASP	2.3
1	B	370	ARG	2.2
1	A	480	PRO	2.2
1	C	397	PHE	2.2
1	A	526	ASP	2.2
1	C	442	ILE	2.1
1	A	432	ALA	2.1
1	F	539	THR	2.1
1	B	432	ALA	2.1
1	A	546	SER	2.1
1	F	432	ALA	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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.

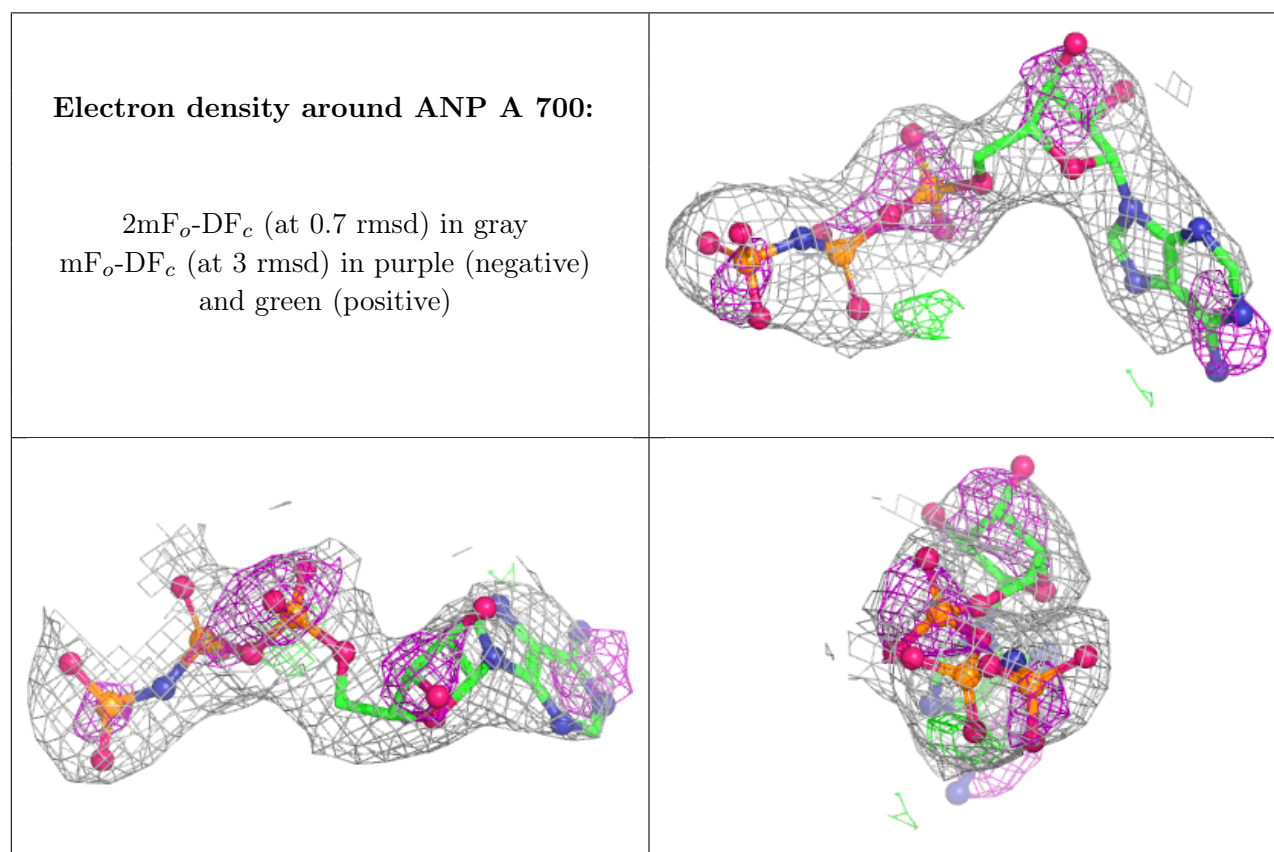
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MG	E	701	1/1	0.82	0.11	43,43,43,43	0
3	MG	B	701	1/1	0.86	0.16	38,38,38,38	0
2	ANP	A	700	31/31	0.88	0.09	32,39,51,55	0
3	MG	D	701	1/1	0.89	0.08	43,43,43,43	0
2	ANP	D	700	31/31	0.91	0.08	30,38,52,59	0

Continued on next page...

Continued from previous page...

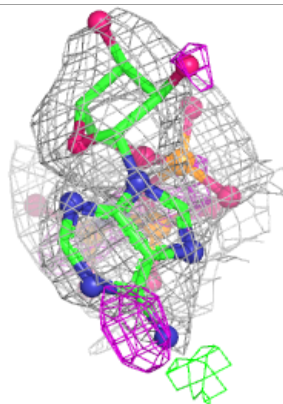
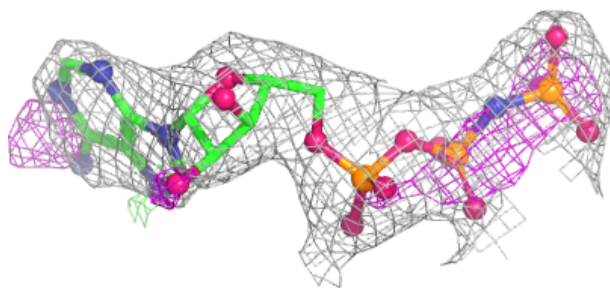
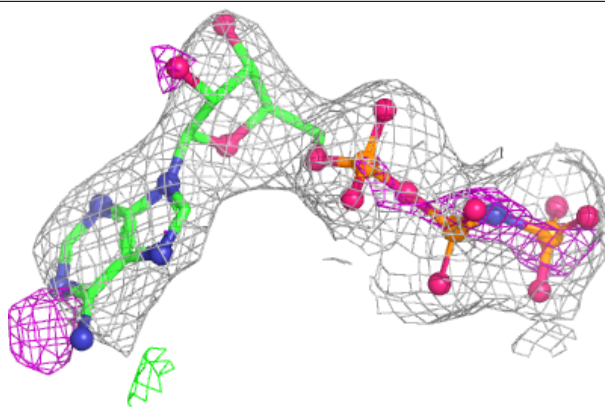
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ANP	B	700	31/31	0.92	0.08	32,36,49,57	0
2	ANP	E	700	31/31	0.94	0.07	33,36,53,55	0
3	MG	A	701	1/1	0.97	0.04	38,38,38,38	0

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.

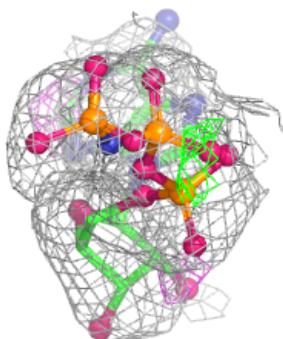
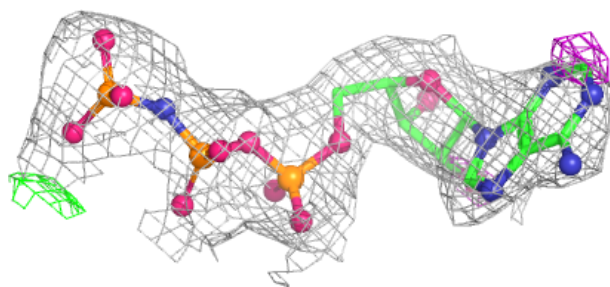
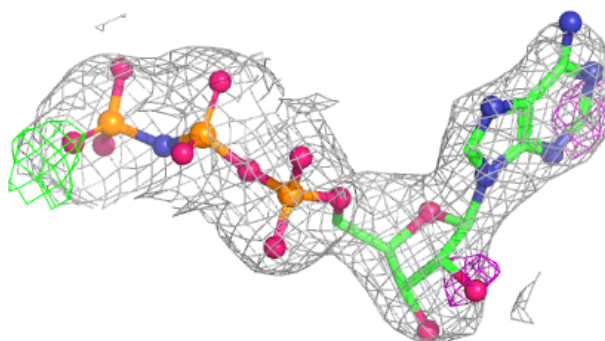


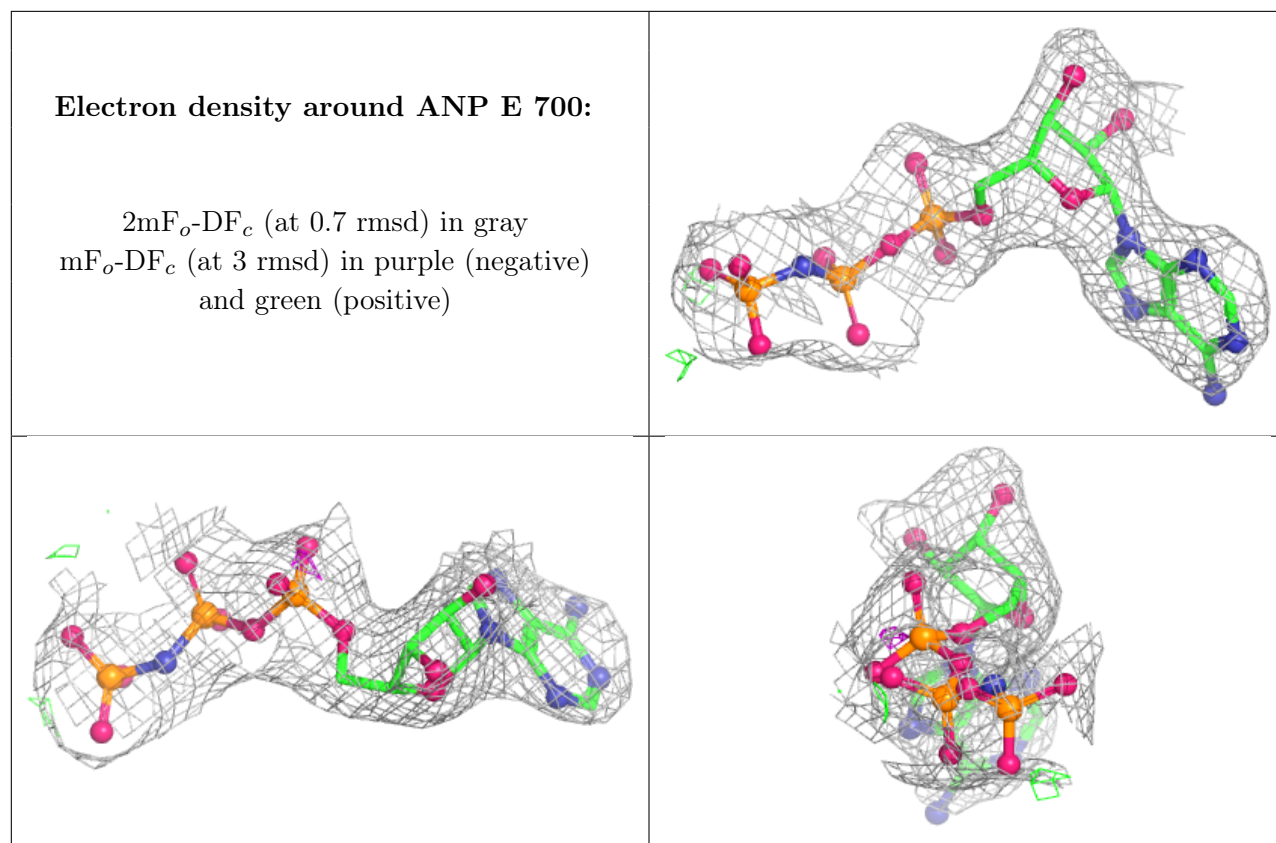
Electron density around ANP D 700:

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

**Electron density around ANP B 700:**

$2mF_o-DF_c$ (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.