



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:16 AM UTC

PDB ID : 5JR7 / pdb_00005jr7
Title : Crystal structure of an ACRDYS heterodimer [RIa(92-365):C] of PKA
Authors : Bruystens, J.G.H.; Wu, J.; Taylor, S.S.
Deposited on : 2016-05-05
Resolution : 3.56 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

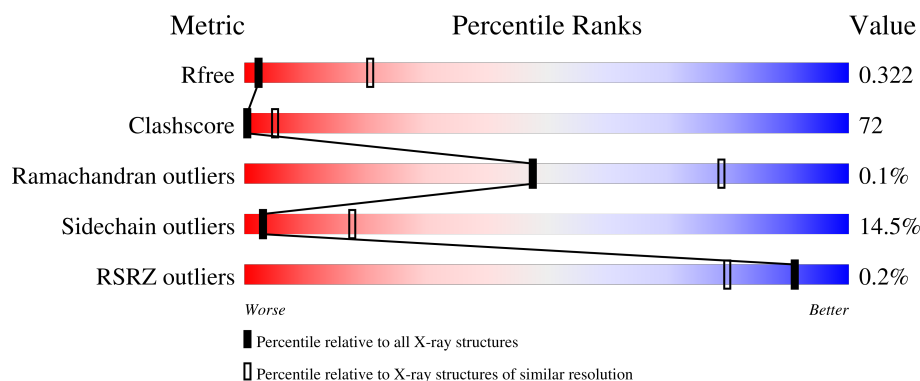
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.56 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	1410 (3.62-3.50)
Clashscore	190562	1480 (3.62-3.50)
Ramachandran outliers	187476	1440 (3.62-3.50)
Sidechain outliers	187428	1441 (3.62-3.50)
RSRZ outliers	180081	1409 (3.62-3.50)

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	350	
1	C	350	
2	B	275	
2	D	275	

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.

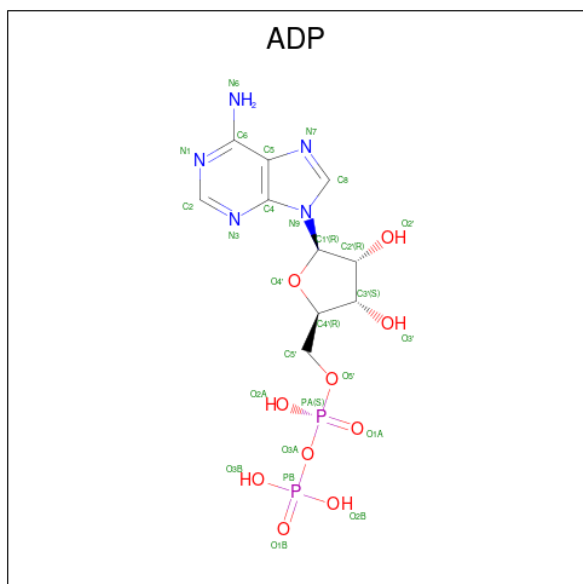
- Molecule 1 is a protein called cAMP-dependent protein kinase catalytic subunit alpha.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	338	Total	C	N	O	P	S	6	0	0
			2734	1773	451	499	3	8			
1	C	338	Total	C	N	O	P	S	0	0	0
			2729	1767	451	500	3	8			

- Molecule 2 is a protein called cAMP-dependent protein kinase type I-alpha regulatory subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	267	Total 2079	C 1321	N 354	O 397	S 7	1	0	0
2	D	266	Total 2069	C 1317	N 353	O 392	S 7	1	0	0

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

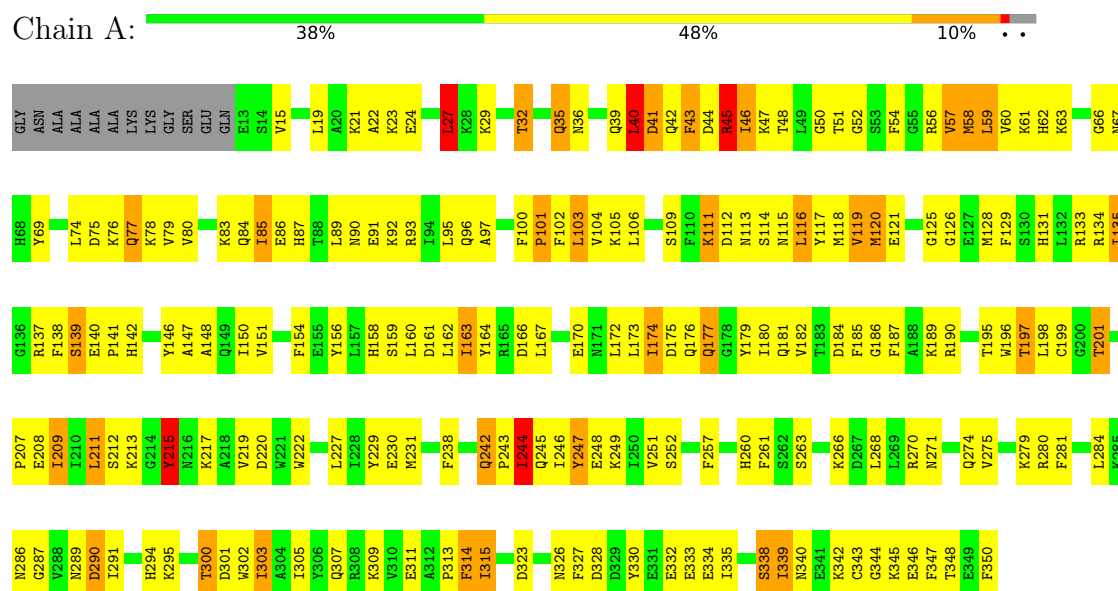


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

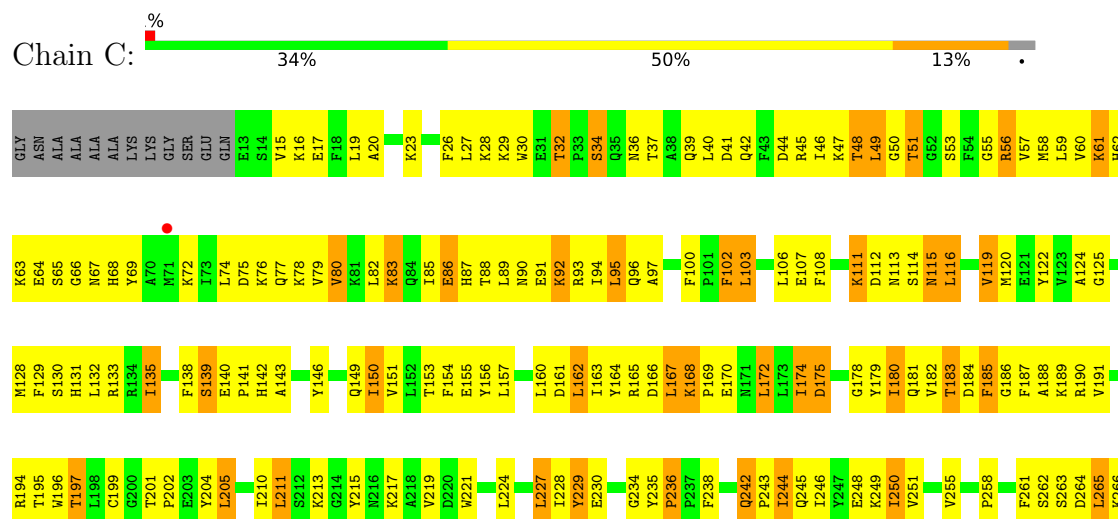
3 Residue-property plots

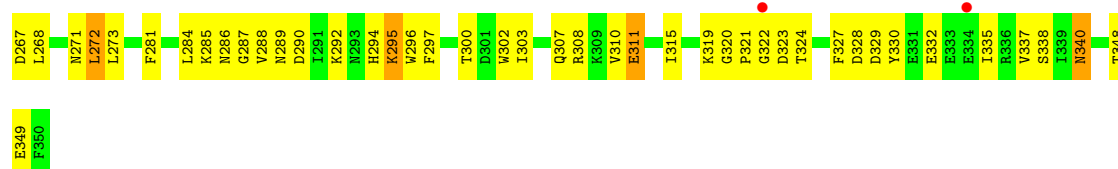
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

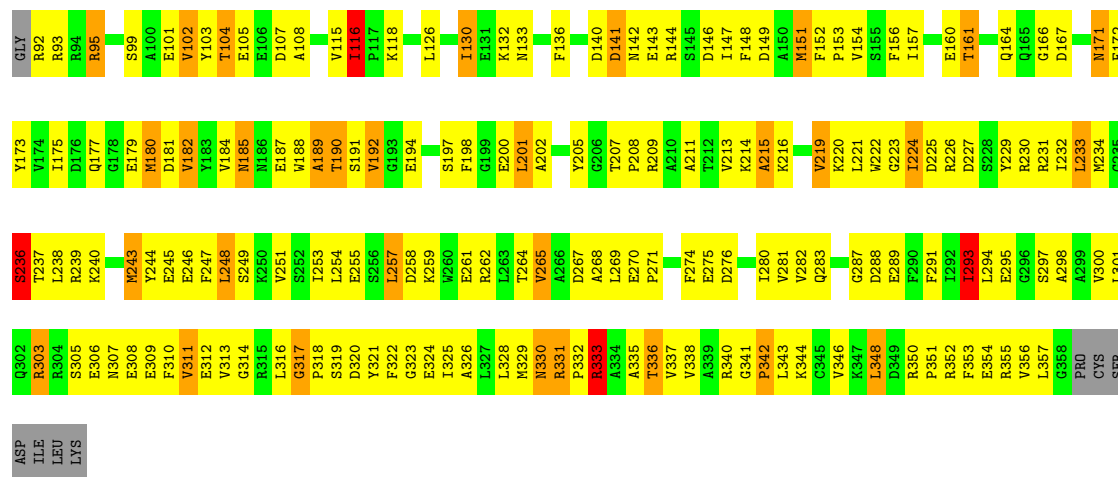


- Molecule 1: cAMP-dependent protein kinase catalytic subunit alpha

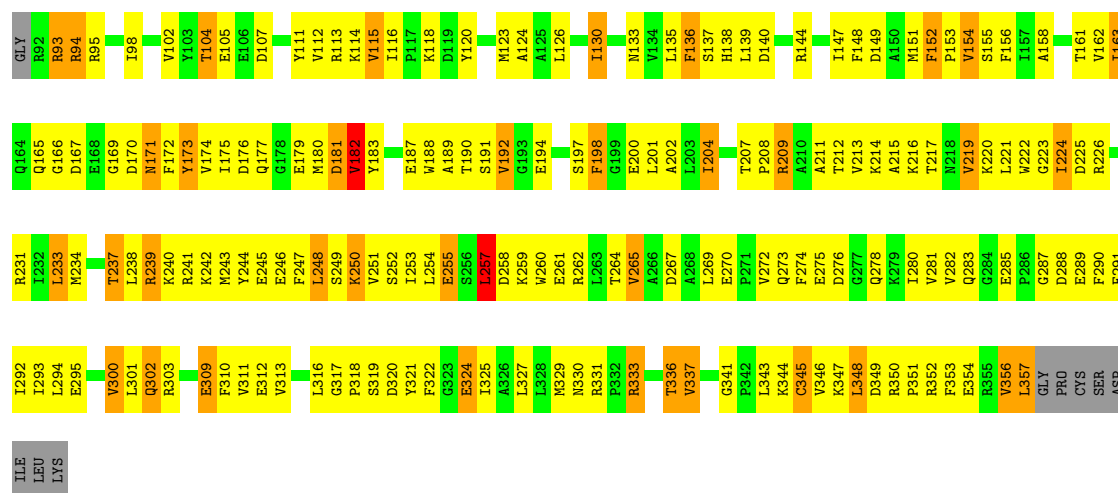




- Molecule 2: cAMP-dependent protein kinase type I-alpha regulatory subunit



- Molecule 2: cAMP-dependent protein kinase type I-alpha regulatory subunit



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	60.15Å 66.79Å 87.93Å 101.76° 89.37° 105.27°	Depositor
Resolution (Å)	49.11 – 3.56 49.11 – 3.56	Depositor EDS
% Data completeness (in resolution range)	97.4 (49.11-3.56) 97.4 (49.11-3.56)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.55 (at 3.48Å)	Xtriage
Refinement program	PHENIX 1.7_650	Depositor
R, R_{free}	0.266 , 0.322 0.258 , 0.322	Depositor DCC
R_{free} test set	797 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	82.1	Xtriage
Anisotropy	0.109	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 115.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	9665	wwPDB-VP
Average B, all atoms (Å ²)	109.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.61% 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: TPO, ADP, SEP

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	0.60	1/2771 (0.0%)	1.32	29/3745 (0.8%)
1	C	0.48	0/2765	1.04	18/3736 (0.5%)
2	B	0.66	1/2116 (0.0%)	1.40	28/2857 (1.0%)
2	D	0.65	4/2106 (0.2%)	1.08	12/2845 (0.4%)
All	All	0.59	6/9758 (0.1%)	1.22	87/13183 (0.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	333	ARG	NE-CZ	14.88	1.49	1.33
2	D	333	ARG	NE-CZ	14.72	1.49	1.33
2	D	181	ASP	CB-CG	-7.73	1.32	1.52
1	A	111	LYS	CE-NZ	-5.93	1.31	1.49
2	D	181	ASP	CA-C	5.74	1.59	1.52
2	D	181	ASP	N-CA	-5.22	1.39	1.46

All (87) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	61	LYS	CD-CE-NZ	-13.02	70.25	111.90
1	A	40	LEU	N-CA-C	10.28	122.49	111.28
1	A	27	LEU	CB-CG-CD1	-9.76	81.41	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	333	ARG	CD-NE-CZ	-9.66	110.87	124.40
1	A	77	GLN	N-CA-C	9.60	121.83	111.36
2	D	181	ASP	CB-CG-OD1	-9.29	97.02	118.40
1	A	101	PRO	CB-CA-C	-8.48	99.81	111.85
2	D	333	ARG	CD-NE-CZ	-8.29	112.80	124.40
2	D	171	ASN	N-CA-C	8.23	118.81	108.45
1	A	209	ILE	CB-CA-C	-7.88	101.70	112.02
2	B	236	SER	N-CA-C	7.66	119.27	111.07
2	B	141	ASP	N-CA-C	7.65	119.62	111.28
2	B	142	ASN	N-CA-C	7.57	119.17	111.07
2	D	257	LEU	N-CA-C	7.54	121.20	109.52
1	C	227	LEU	CB-CG-CD1	-7.33	88.71	110.70
2	D	181	ASP	CB-CG-OD2	7.29	135.17	118.40
1	A	36	ASN	N-CA-C	7.09	121.03	111.24
1	C	236	PRO	CA-C-N	7.06	127.04	119.28
1	C	236	PRO	C-N-CA	7.06	127.04	119.28
2	B	317	GLY	CA-C-N	7.03	127.07	119.90
2	B	317	GLY	C-N-CA	7.03	127.07	119.90
2	B	232	ILE	N-CA-C	7.02	117.16	110.42
1	A	15	VAL	N-CA-C	6.97	117.76	110.72
2	B	95	ARG	N-CA-C	-6.93	97.43	108.73
2	D	130	ILE	N-CA-C	6.82	119.58	112.83
1	C	102	PHE	N-CA-C	6.81	121.30	112.92
1	A	244	ILE	N-CA-C	6.73	117.52	110.72
2	B	102	VAL	N-CA-C	6.67	117.64	109.30
1	C	320	GLY	CA-C-N	-6.66	113.78	120.31
1	C	320	GLY	C-N-CA	-6.66	113.78	120.31
1	A	257	PHE	CA-C-N	6.51	126.49	119.78
1	A	257	PHE	C-N-CA	6.51	126.49	119.78
2	D	181	ASP	CA-CB-CG	-6.42	106.18	112.60
2	B	313	VAL	CB-CA-C	-6.32	103.36	111.20
2	B	192	VAL	N-CA-C	6.29	117.84	108.46
1	C	32	THR	CA-C-N	6.29	126.25	119.78
1	C	32	THR	C-N-CA	6.29	126.25	119.78
2	B	293	ILE	N-CA-C	6.28	117.18	108.89
2	B	180	MET	N-CA-C	6.25	119.37	109.50
1	A	45	ARG	N-CA-C	6.17	118.77	108.96
1	C	185	PHE	N-CA-C	6.10	120.34	113.02
2	B	116	ILE	CA-C-N	6.09	126.45	119.93
2	B	116	ILE	C-N-CA	6.09	126.45	119.93
2	D	270	GLU	CA-C-N	-5.99	113.59	119.76
2	D	270	GLU	C-N-CA	-5.99	113.59	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	111	LYS	CB-CA-C	-5.98	97.29	111.65
1	A	291	ILE	N-CA-C	5.94	116.11	110.53
2	D	198	PHE	N-CA-C	5.88	117.19	107.73
1	A	303	ILE	N-CA-C	5.84	116.62	110.72
1	C	49	LEU	N-CA-C	5.80	117.69	111.36
1	A	58	MET	N-CA-C	5.80	118.35	108.90
2	B	101	GLU	N-CA-C	5.78	118.16	110.53
1	C	115	ASN	N-CA-C	5.77	117.95	109.24
1	C	242	GLN	CA-C-N	-5.75	113.26	119.24
1	C	242	GLN	C-N-CA	-5.75	113.26	119.24
2	B	257	LEU	N-CA-C	5.72	119.42	110.32
2	B	215	ALA	N-CA-C	5.69	117.95	109.59
1	C	167	LEU	CB-CG-CD2	-5.68	93.65	110.70
1	A	21	LYS	N-CA-C	-5.66	105.19	111.36
1	A	35	GLN	N-CA-C	5.63	117.55	108.32
1	A	314	PHE	N-CA-C	5.60	118.60	108.69
2	B	306	GLU	N-CA-C	5.59	117.82	111.11
2	B	331	ARG	N-CA-C	-5.59	99.36	109.09
1	A	58	MET	CB-CA-C	5.56	119.89	109.71
1	C	168	LYS	CA-C-N	5.54	125.63	119.32
1	C	168	LYS	C-N-CA	5.54	125.63	119.32
2	B	175	ILE	N-CA-C	5.51	116.33	107.73
2	B	190	THR	N-CA-C	5.51	115.81	108.38
2	B	171	ASN	N-CA-C	5.50	118.19	109.50
2	B	307	ASN	N-CA-C	5.48	117.44	109.71
2	D	309	GLU	N-CA-C	5.46	118.82	110.36
1	A	46	ILE	N-CA-C	5.43	120.63	109.34
1	A	300	THR	N-CA-C	5.42	117.57	108.96
1	A	215	TYR	N-CA-C	5.40	116.48	108.60
1	A	246	ILE	CB-CA-C	-5.37	105.10	111.97
1	A	24	GLU	N-CA-C	5.36	117.21	111.36
2	B	303	ARG	N-CA-C	5.34	117.12	108.41
1	A	315	ILE	N-CA-C	5.29	116.07	107.71
1	C	128	MET	N-CA-C	-5.29	106.09	112.54
1	A	83	LYS	N-CA-C	5.27	118.90	111.52
2	B	219	VAL	N-CA-C	5.20	116.34	108.96
2	B	108	ALA	N-CA-C	5.20	116.63	111.07
2	D	182	VAL	N-CA-C	5.19	116.05	108.53
1	A	289	ASN	N-CA-C	5.09	118.59	112.38
2	B	342	PRO	CA-C-O	-5.05	115.58	121.34
1	A	242	GLN	CA-C-N	5.04	125.07	119.32
1	A	242	GLN	C-N-CA	5.04	125.07	119.32

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	189	ALA	Mainchain

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	2734	0	2640	382	0
1	C	2729	0	2631	385	0
2	B	2079	0	2030	273	0
2	D	2069	0	2023	359	0
3	A	27	0	12	5	0
3	C	27	0	12	1	0
All	All	9665	0	9348	1360	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 72.

All (1360) 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:A:79:VAL:HA	1:A:84:GLN:NE2	1.38	1.36
1:A:116:LEU:HD12	1:A:117:TYR:N	1.48	1.27
1:C:150:ILE:HG22	1:C:154:PHE:CE2	1.71	1.24
2:D:151:MET:HE3	2:D:152:PHE:O	1.41	1.20
1:A:48:THR:HG21	1:A:330:TYR:HB2	1.20	1.16
1:A:175:ASP:HB3	1:A:181:GLN:NE2	1.60	1.15
2:D:181:ASP:OD1	2:D:188:TRP:CZ3	1.99	1.15
1:C:95:LEU:HB3	1:C:106:LEU:HD23	1.29	1.13
1:A:91:GLU:O	1:A:95:LEU:HD13	1.48	1.13
2:B:325:ILE:CD1	2:B:331:ARG:HD3	1.78	1.12
1:A:92:LYS:HD3	1:A:350:PHE:CE2	1.84	1.11
2:B:308:GLU:HG2	2:B:309:GLU:H	1.01	1.10
1:C:56:ARG:HD2	1:C:57:VAL:N	1.65	1.10
2:D:151:MET:HE2	2:D:222:TRP:HB3	1.33	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:120:TYR:CE1	2:D:124:ALA:HB2	1.84	1.10
1:A:111:LYS:NZ	1:A:350:PHE:CD1	2.18	1.10
1:A:48:THR:CG2	1:A:330:TYR:HB2	1.83	1.08
2:D:188:TRP:CH2	2:D:190:THR:C	2.31	1.08
1:A:111:LYS:NZ	1:A:350:PHE:CG	2.22	1.08
1:C:56:ARG:HD2	1:C:57:VAL:H	0.97	1.07
2:B:325:ILE:HD13	2:B:331:ARG:HD3	1.18	1.07
1:C:167:LEU:HD21	1:C:227:LEU:HD11	1.36	1.07
1:C:50:GLY:H	1:C:56:ARG:NH1	1.52	1.06
2:D:154:VAL:HG23	2:D:221:LEU:HD11	1.33	1.05
1:C:100:PHE:HB3	1:C:103:LEU:HD13	1.34	1.05
1:A:35:GLN:HE22	1:A:350:PHE:C	1.63	1.05
2:D:172:PHE:HE1	2:D:198:PHE:N	1.55	1.05
1:C:95:LEU:HB3	1:C:106:LEU:CD2	1.86	1.04
1:A:46:ILE:HD11	1:A:59:LEU:HB3	1.38	1.04
1:C:30:TRP:HZ2	1:C:190:ARG:CZ	1.70	1.04
1:C:30:TRP:HE1	1:C:190:ARG:NH1	1.55	1.03
2:D:151:MET:HE1	2:D:223:GLY:N	1.73	1.03
2:D:181:ASP:OD1	2:D:188:TRP:CH2	2.12	1.03
1:A:46:ILE:HG12	1:A:59:LEU:HD22	1.39	1.03
2:B:151:MET:SD	2:B:224:ILE:HD11	1.98	1.02
1:A:61:LYS:HZ1	1:A:66:GLY:HA2	1.17	1.02
1:C:150:ILE:HG22	1:C:154:PHE:HE2	0.85	1.02
1:C:89:LEU:HG	1:C:92:LYS:HZ1	1.22	1.01
2:D:154:VAL:O	2:D:221:LEU:HG	1.59	1.00
1:A:61:LYS:NZ	1:A:66:GLY:HA2	1.76	1.00
1:A:131:HIS:CD2	1:A:134:ARG:HH11	1.81	0.98
2:D:252:SER:OG	2:D:253:ILE:HD12	1.64	0.98
1:C:113:ASN:HB3	1:C:340:ASN:O	1.62	0.98
2:D:172:PHE:HD1	2:D:198:PHE:O	1.46	0.97
1:A:131:HIS:HD2	1:A:134:ARG:NH1	1.60	0.97
2:D:169:GLY:HA2	2:D:209:ARG:CZ	1.93	0.97
2:B:331:ARG:HG3	2:B:332:PRO:HD2	1.44	0.96
1:C:29:LYS:HE2	1:C:97:ALA:HA	1.45	0.96
2:D:116:ILE:HD13	2:D:152:PHE:HB3	1.46	0.96
1:C:150:ILE:CG2	1:C:154:PHE:HE2	1.77	0.96
2:D:272:VAL:CG1	2:D:347:LYS:HE2	1.95	0.96
1:A:131:HIS:HD2	1:A:134:ARG:HH11	0.99	0.96
2:B:116:ILE:HD11	2:B:151:MET:O	1.66	0.95
2:D:257:LEU:HD11	2:D:262:ARG:CZ	1.96	0.95
2:D:144:ARG:O	2:D:147:ILE:HG13	1.66	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:50:GLY:H	1:C:56:ARG:HH12	1.10	0.95
1:A:215:TYR:HD1	1:A:219:VAL:HG11	1.28	0.95
1:C:169:PRO:HA	1:C:172:LEU:HD12	1.46	0.94
1:A:76:LYS:HD3	1:A:342:LYS:O	1.67	0.94
1:C:164:TYR:CE2	1:C:166:ASP:O	2.21	0.94
1:C:157:LEU:O	1:C:162:LEU:HD12	1.65	0.94
1:A:242:GLN:HE22	1:A:245:GLN:HB2	1.32	0.93
2:D:188:TRP:CH2	2:D:190:THR:O	2.22	0.92
2:D:175:ILE:HD13	2:D:192:VAL:HG21	1.49	0.92
1:C:30:TRP:HZ2	1:C:190:ARG:NE	1.66	0.92
1:A:48:THR:HG21	1:A:330:TYR:CB	1.98	0.92
2:D:257:LEU:CD1	2:D:262:ARG:HG3	2.00	0.92
2:D:171:ASN:CB	2:D:173:TYR:HE1	1.83	0.92
1:C:89:LEU:HG	1:C:92:LYS:NZ	1.85	0.92
1:C:129:PHE:HE1	1:C:133:ARG:CZ	1.82	0.92
1:A:116:LEU:HD12	1:A:117:TYR:H	1.17	0.91
2:B:308:GLU:HG2	2:B:309:GLU:N	1.81	0.91
2:B:104:THR:HG23	2:B:107:ASP:OD2	1.69	0.91
1:C:30:TRP:CZ2	1:C:190:ARG:CZ	2.53	0.91
2:B:191:SER:HB2	2:B:216:LYS:HZ1	1.36	0.91
1:A:79:VAL:CA	1:A:84:GLN:NE2	2.33	0.91
1:A:92:LYS:HD3	1:A:350:PHE:CD2	2.06	0.91
1:C:56:ARG:NH1	1:C:57:VAL:O	2.04	0.91
1:C:80:VAL:HA	1:C:85:ILE:HD11	1.51	0.91
1:C:243:PRO:HA	1:C:246:ILE:HD12	1.51	0.91
2:B:191:SER:HB2	2:B:216:LYS:NZ	1.86	0.91
1:A:95:LEU:HD11	1:A:185:PHE:HB2	1.51	0.90
2:D:257:LEU:HD12	2:D:257:LEU:C	1.97	0.90
2:B:259:LYS:HG2	2:B:262:ARG:HH21	1.35	0.90
1:A:79:VAL:HA	1:A:84:GLN:HE22	1.10	0.90
1:A:160:LEU:HB2	1:A:162:LEU:HD12	1.53	0.89
2:D:172:PHE:CZ	2:D:197:SER:HB2	2.07	0.89
1:A:116:LEU:HD12	1:A:116:LEU:C	1.79	0.89
1:A:43:PHE:O	1:A:45:ARG:NH1	2.05	0.89
1:A:175:ASP:CB	1:A:181:GLN:NE2	2.35	0.88
1:A:160:LEU:HB2	1:A:162:LEU:CD1	2.03	0.88
1:C:44:ASP:HB2	1:C:63:LYS:HE3	1.54	0.88
1:A:40:LEU:HD12	1:A:45:ARG:HH21	1.38	0.88
1:C:106:LEU:O	1:C:106:LEU:HD12	1.74	0.88
2:D:154:VAL:HB	2:D:221:LEU:HD21	1.54	0.88
1:A:46:ILE:HD12	1:A:47:LYS:N	1.89	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:290:PHE:CD1	2:D:291:PHE:N	2.42	0.87
1:A:111:LYS:CE	1:A:350:PHE:CD1	2.58	0.87
2:B:301:LEU:HB2	2:B:336:THR:HG23	1.56	0.87
1:C:87:HIS:O	1:C:90:ASN:HB3	1.74	0.86
1:A:131:HIS:HA	1:A:134:ARG:HE	1.39	0.86
2:D:350:ARG:HG3	2:D:351:PRO:HD3	1.57	0.86
1:A:61:LYS:HE2	1:A:66:GLY:C	1.99	0.86
2:B:107:ASP:HB3	2:B:231:ARG:HH22	1.38	0.86
1:C:90:ASN:HD21	1:C:189:LYS:HA	1.39	0.86
1:C:167:LEU:CD2	1:C:227:LEU:HD11	2.06	0.85
2:D:172:PHE:CD1	2:D:198:PHE:O	2.28	0.85
2:B:331:ARG:CG	2:B:332:PRO:HD2	2.05	0.85
2:B:188:TRP:CH2	2:B:190:THR:HA	2.11	0.85
1:C:48:THR:C	1:C:56:ARG:NH2	2.34	0.84
2:D:257:LEU:HD12	2:D:257:LEU:O	1.77	0.84
1:A:131:HIS:O	1:A:135:ILE:HD13	1.77	0.84
1:A:163:ILE:HD12	1:A:164:TYR:H	1.42	0.84
1:A:115:ASN:HB2	1:A:117:TYR:OH	1.77	0.84
2:B:188:TRP:CZ2	2:B:190:THR:HA	2.13	0.84
2:D:224:ILE:HG13	2:D:225:ASP:N	1.91	0.84
1:A:74:LEU:HB2	1:A:116:LEU:HB3	1.57	0.84
1:C:90:ASN:OD1	1:C:94:ILE:HD13	1.78	0.84
2:D:177:GLN:HB2	2:D:220:LYS:H	1.42	0.83
1:A:146:TYR:HD1	1:A:180:ILE:HD11	1.44	0.83
2:D:151:MET:HE1	2:D:222:TRP:C	2.02	0.83
1:A:315:ILE:O	1:A:315:ILE:HD12	1.78	0.83
1:A:175:ASP:CB	1:A:181:GLN:HE22	1.91	0.83
2:B:308:GLU:CG	2:B:309:GLU:H	1.89	0.83
1:C:87:HIS:O	1:C:90:ASN:N	2.11	0.83
2:D:111:TYR:CD1	2:D:231:ARG:HD2	2.14	0.83
2:B:251:VAL:HG11	2:B:254:LEU:HD12	1.60	0.83
1:C:164:TYR:HE2	1:C:166:ASP:O	1.62	0.83
1:A:111:LYS:NZ	1:A:350:PHE:CD2	2.44	0.83
1:C:61:LYS:HZ1	1:C:68:HIS:CE1	1.97	0.83
1:A:111:LYS:HE2	1:A:350:PHE:CD1	2.13	0.82
1:C:108:PHE:HB2	1:C:119:VAL:HG13	1.59	0.82
1:A:47:LYS:N	1:A:58:MET:HE3	1.93	0.82
1:C:61:LYS:NZ	1:C:68:HIS:CG	2.47	0.82
1:C:129:PHE:CE1	1:C:133:ARG:CZ	2.61	0.82
1:C:68:HIS:CE1	1:C:321:PRO:HB2	2.14	0.82
1:A:35:GLN:NE2	1:A:350:PHE:C	2.37	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:96:GLN:N	1:C:106:LEU:HD21	1.93	0.82
2:D:172:PHE:HE1	2:D:198:PHE:H	0.84	0.82
2:D:202:ALA:O	2:D:226:ARG:HD3	1.79	0.82
2:D:275:GLU:OE1	2:D:275:GLU:N	2.13	0.82
2:B:276:ASP:HB2	2:B:341:GLY:HA2	1.60	0.82
1:C:30:TRP:NE1	1:C:190:ARG:NH1	2.27	0.82
2:B:177:GLN:O	2:B:219:VAL:HG23	1.80	0.81
1:A:48:THR:HA	1:A:58:MET:HG2	1.62	0.81
1:C:166:ASP:HB2	1:C:187:PHE:HD2	1.46	0.81
1:A:131:HIS:HA	1:A:134:ARG:NE	1.96	0.81
1:A:111:LYS:CE	1:A:350:PHE:CG	2.64	0.81
1:C:50:GLY:N	1:C:56:ARG:NH2	2.28	0.81
1:C:56:ARG:HH11	1:C:57:VAL:H	1.26	0.81
2:B:259:LYS:HG2	2:B:262:ARG:NH2	1.94	0.80
1:A:133:ARG:NH2	2:B:95:ARG:HH22	1.79	0.80
1:A:328:ASP:OD2	2:B:92:ARG:NH2	2.13	0.80
1:A:334:GLU:CB	2:D:260:TRP:CZ2	2.64	0.80
1:C:204:TYR:CE2	1:C:227:LEU:HD23	2.17	0.80
2:B:171:ASN:ND2	2:B:173:TYR:CE1	2.50	0.80
1:A:27:LEU:HD12	1:A:27:LEU:N	1.95	0.80
1:C:90:ASN:HA	1:C:93:ARG:HG2	1.61	0.80
1:A:242:GLN:NE2	1:A:245:GLN:HB2	1.97	0.79
1:A:195:THR:HG22	1:A:197:TPO:O2P	1.81	0.79
1:C:50:GLY:H	1:C:56:ARG:CZ	1.96	0.79
2:D:346:VAL:C	2:D:347:LYS:HD3	2.07	0.79
1:A:85:ILE:HD12	1:A:86:GLU:H	1.48	0.79
1:C:80:VAL:HG12	1:C:85:ILE:HD11	1.64	0.79
2:B:236:SER:HA	2:B:239:ARG:NH1	1.98	0.79
2:D:272:VAL:CG1	2:D:347:LYS:CE	2.61	0.78
2:D:294:LEU:HD11	2:D:346:VAL:HG13	1.64	0.78
2:B:148:PHE:HA	2:B:151:MET:HE2	1.63	0.78
1:C:90:ASN:ND2	1:C:188:ALA:O	2.16	0.78
2:D:151:MET:HE2	2:D:222:TRP:CB	2.12	0.78
1:C:89:LEU:HD23	1:C:93:ARG:HD3	1.64	0.78
2:B:184:VAL:HG22	2:B:189:ALA:HB2	1.66	0.78
1:C:174:ILE:HD13	1:C:178:GLY:HA2	1.65	0.78
2:D:291:PHE:HD2	2:D:347:LYS:HZ2	1.31	0.78
2:D:300:VAL:O	2:D:301:LEU:HD23	1.83	0.78
1:A:61:LYS:HD2	1:A:67:ASN:O	1.84	0.78
1:C:150:ILE:O	1:C:154:PHE:HD2	1.67	0.78
1:C:319:LYS:O	1:C:323:ASP:HB2	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:174:ILE:CD1	1:C:178:GLY:HA2	2.13	0.78
1:A:42:GLN:C	1:A:63:LYS:HE2	2.07	0.78
2:B:293:ILE:HD13	2:B:318:PRO:HA	1.66	0.78
1:C:161:ASP:HA	1:C:217:LYS:HE2	1.66	0.78
2:B:293:ILE:HD11	2:B:320:ASP:H	1.48	0.78
1:A:40:LEU:HA	1:A:43:PHE:CE1	2.18	0.78
1:A:92:LYS:HG3	1:A:93:ARG:N	1.99	0.78
1:C:50:GLY:N	1:C:56:ARG:HH22	1.80	0.78
1:C:95:LEU:CB	1:C:106:LEU:HD23	2.12	0.78
2:D:151:MET:CE	2:D:222:TRP:C	2.56	0.78
2:D:171:ASN:CB	2:D:173:TYR:CE1	2.67	0.78
2:D:257:LEU:HD13	2:D:262:ARG:HG3	1.65	0.78
1:C:55:GLY:HA3	1:C:74:LEU:HD23	1.65	0.77
1:C:122:TYR:CE2	1:C:124:ALA:HB2	2.20	0.77
1:A:46:ILE:HD12	1:A:47:LYS:H	1.48	0.77
1:A:142:HIS:CE1	1:A:146:TYR:HE2	2.01	0.77
1:A:328:ASP:CG	2:B:92:ARG:NH2	2.41	0.77
1:C:30:TRP:CZ2	1:C:190:ARG:NE	2.51	0.77
1:A:332:GLU:OE1	1:A:332:GLU:HA	1.85	0.77
1:C:167:LEU:HD21	1:C:227:LEU:CD1	2.12	0.77
1:A:245:GLN:HA	1:A:248:GLU:CD	2.10	0.77
2:B:219:VAL:HG22	2:B:220:LYS:N	1.99	0.76
1:A:112:ASP:OD1	1:A:117:TYR:OH	2.03	0.76
2:B:187:GLU:HB3	1:C:37:THR:HG21	1.68	0.76
2:D:257:LEU:HD11	2:D:262:ARG:HG3	1.67	0.76
1:A:77:GLN:NE2	1:A:342:LYS:HD2	1.99	0.76
2:B:244:TYR:O	2:B:248:LEU:HD13	1.86	0.76
2:D:171:ASN:HB2	2:D:173:TYR:CE1	2.20	0.76
1:C:80:VAL:CG1	1:C:85:ILE:HD11	2.15	0.76
1:A:46:ILE:CD1	1:A:59:LEU:HD13	2.15	0.76
1:C:48:THR:HA	1:C:58:MET:HG3	1.66	0.76
2:D:177:GLN:CG	2:D:220:LYS:HG2	2.16	0.76
1:A:146:TYR:CD1	1:A:180:ILE:HD11	2.22	0.75
1:C:51:THR:HG23	1:C:56:ARG:HD3	1.68	0.75
1:A:23:LYS:O	1:A:27:LEU:CD1	2.35	0.75
2:D:116:ILE:CD1	2:D:152:PHE:HB3	2.16	0.75
2:D:180:MET:HG2	2:D:215:ALA:HA	1.67	0.75
1:C:102:PHE:C	1:C:103:LEU:HD12	2.10	0.75
1:C:107:GLU:O	1:C:108:PHE:CG	2.39	0.75
2:D:118:LYS:O	2:D:123:MET:HE2	1.87	0.75
2:D:151:MET:CE	2:D:152:PHE:O	2.30	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:180:MET:HG2	2:B:215:ALA:HA	1.68	0.75
1:C:62:HIS:HD1	1:C:65:SER:HG	1.33	0.75
1:C:68:HIS:NE2	1:C:322:GLY:N	2.35	0.75
1:A:76:LYS:CD	1:A:342:LYS:O	2.33	0.74
2:B:350:ARG:O	2:B:354:GLU:HG3	1.87	0.74
1:C:133:ARG:HH22	2:D:95:ARG:HH22	1.32	0.74
1:A:61:LYS:CD	1:A:67:ASN:O	2.34	0.74
2:D:147:ILE:HD12	2:D:148:PHE:N	2.01	0.74
1:A:77:GLN:HE22	1:A:342:LYS:NZ	1.84	0.74
1:A:244:ILE:HD11	2:B:201:LEU:HB2	1.70	0.74
2:D:171:ASN:HB3	2:D:173:TYR:HE1	1.50	0.74
1:A:175:ASP:CG	1:A:181:GLN:HE22	1.95	0.74
1:A:215:TYR:CD1	1:A:219:VAL:HG11	2.19	0.74
1:A:244:ILE:HG22	1:A:248:GLU:OE1	1.87	0.74
1:A:268:LEU:HD13	1:A:294:HIS:CD2	2.21	0.74
1:C:50:GLY:O	1:C:56:ARG:NH1	2.21	0.74
1:C:132:LEU:HD13	1:C:138:PHE:CE2	2.22	0.74
1:A:48:THR:HA	1:A:58:MET:CG	2.17	0.74
2:B:288:ASP:OD2	2:B:289:GLU:OE1	2.06	0.74
1:A:243:PRO:HB2	2:B:201:LEU:HD13	1.69	0.73
1:C:48:THR:OG1	1:C:56:ARG:NH2	2.21	0.73
1:A:46:ILE:HD12	1:A:47:LYS:HB2	1.70	0.73
1:C:16:LYS:O	1:C:19:LEU:HG	1.88	0.73
2:B:259:LYS:CG	2:B:262:ARG:NH2	2.51	0.73
2:D:290:PHE:HD1	2:D:291:PHE:H	1.33	0.73
1:A:47:LYS:CA	1:A:58:MET:HE3	2.19	0.73
1:A:100:PHE:CD2	1:A:101:PRO:HD2	2.23	0.73
2:B:130:ILE:HD12	2:B:130:ILE:C	2.14	0.73
2:B:144:ARG:O	2:B:147:ILE:HG13	1.89	0.73
2:B:182:VAL:HG13	2:B:189:ALA:HB3	1.71	0.73
2:B:352:ARG:HA	2:B:355:ARG:CZ	2.19	0.73
2:D:93:ARG:O	2:D:93:ARG:HG3	1.87	0.73
1:A:45:ARG:HG3	1:A:45:ARG:HH11	1.52	0.73
1:A:46:ILE:HG13	1:A:59:LEU:O	1.89	0.73
1:A:245:GLN:HA	1:A:248:GLU:OE2	1.88	0.73
2:B:249:SER:O	2:B:255:GLU:OE2	2.06	0.73
2:B:240:LYS:O	2:B:243:MET:HG3	1.89	0.73
1:C:48:THR:HG22	1:C:332:GLU:HG2	1.71	0.73
2:D:173:TYR:HA	2:D:222:TRP:O	1.88	0.73
1:A:266:LYS:O	1:A:270:ARG:HG3	1.89	0.73
1:C:297:PHE:O	1:C:300:THR:HG22	1.88	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:116:ILE:HD13	2:D:152:PHE:CB	2.16	0.72
1:A:116:LEU:CD1	1:A:117:TYR:H	2.00	0.72
2:B:243:MET:HE2	2:B:244:TYR:HD2	1.52	0.72
2:D:181:ASP:OD1	2:D:181:ASP:C	2.19	0.72
2:D:288:ASP:HA	2:D:350:ARG:NH1	2.04	0.72
2:B:240:LYS:HA	2:B:243:MET:HG2	1.69	0.72
2:B:224:ILE:N	2:B:224:ILE:HD12	2.04	0.72
1:C:166:ASP:HB2	1:C:187:PHE:CD2	2.25	0.72
2:B:293:ILE:HD11	2:B:317:GLY:O	1.89	0.72
1:A:109:SER:OG	1:A:350:PHE:HE1	1.73	0.72
2:D:154:VAL:CG2	2:D:221:LEU:HD11	2.17	0.72
1:C:184:ASP:HB2	3:C:400:ADP:O1A	1.90	0.72
2:B:223:GLY:C	2:B:224:ILE:HD12	2.14	0.71
1:C:201:THR:HG21	2:D:95:ARG:CD	2.20	0.71
2:D:175:ILE:HD13	2:D:192:VAL:CG2	2.20	0.71
2:D:188:TRP:HH2	2:D:190:THR:O	1.73	0.71
1:A:46:ILE:HD11	1:A:59:LEU:HD13	1.72	0.71
2:D:156:PHE:HE1	2:D:221:LEU:CD2	2.02	0.71
2:D:182:VAL:O	2:D:188:TRP:CZ3	2.43	0.71
2:D:239:ARG:CZ	2:D:239:ARG:HB3	2.19	0.71
1:A:79:VAL:HA	1:A:84:GLN:CD	2.14	0.71
1:A:111:LYS:HZ2	1:A:116:LEU:CD1	2.01	0.71
2:B:245:GLU:OE2	2:B:262:ARG:HD2	1.90	0.71
2:B:356:VAL:HG23	2:B:357:LEU:H	1.55	0.71
2:D:182:VAL:O	2:D:188:TRP:CE3	2.44	0.71
1:C:61:LYS:NZ	1:C:68:HIS:CE1	2.58	0.71
1:C:90:ASN:ND2	1:C:189:LYS:HA	2.06	0.71
2:D:181:ASP:OD1	2:D:182:VAL:N	2.23	0.71
1:A:100:PHE:HB3	1:A:103:LEU:HD13	1.70	0.71
1:A:27:LEU:HD12	1:A:27:LEU:H	1.55	0.71
1:A:163:ILE:HD12	1:A:164:TYR:N	2.05	0.71
2:B:236:SER:O	2:B:239:ARG:HG3	1.90	0.71
1:C:154:PHE:HZ	1:C:167:LEU:CD1	2.04	0.71
2:B:261:GLU:O	2:B:265:VAL:HG12	1.91	0.71
2:D:272:VAL:HG13	2:D:347:LYS:HE2	1.71	0.71
1:C:169:PRO:HD3	1:C:227:LEU:CD2	2.20	0.70
2:D:273:GLN:NE2	2:D:274:PHE:O	2.24	0.70
1:A:247:TYR:N	1:A:247:TYR:HD2	1.89	0.70
1:A:148:ALA:HB1	1:A:302:TRP:HZ3	1.57	0.70
1:A:197:TPO:O	1:A:215:TYR:OH	2.10	0.70
1:A:244:ILE:CD1	2:B:201:LEU:HB2	2.21	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:29:LYS:HE2	1:C:97:ALA:CA	2.21	0.70
2:B:245:GLU:OE1	2:B:262:ARG:HB3	1.92	0.70
1:C:45:ARG:NH1	1:C:335:ILE:HG22	2.06	0.70
1:C:174:ILE:HD12	1:C:175:ASP:N	2.07	0.70
1:A:32:THR:HG23	1:A:32:THR:O	1.92	0.70
1:C:51:THR:CG2	1:C:56:ARG:HD3	2.21	0.70
2:D:167:ASP:O	2:D:208:PRO:HA	1.92	0.70
1:A:92:LYS:NZ	1:A:350:PHE:HA	2.07	0.69
1:A:208:GLU:HA	1:A:211:LEU:HG	1.74	0.69
2:B:258:ASP:O	2:B:262:ARG:HG3	1.92	0.69
2:B:275:GLU:OE1	2:B:276:ASP:O	2.10	0.69
1:C:264:ASP:OD1	1:C:295:LYS:HE3	1.92	0.69
1:A:105:LYS:H	1:A:121:GLU:CD	2.00	0.69
2:B:182:VAL:HG12	2:B:190:THR:H	1.57	0.69
2:D:274:PHE:HD2	2:D:278:GLN:OE1	1.75	0.69
1:C:51:THR:HG23	1:C:56:ARG:NE	2.07	0.69
1:C:60:VAL:O	1:C:61:LYS:HD3	1.92	0.69
1:A:76:LYS:HD3	1:A:343:CYS:HB2	1.74	0.69
1:C:51:THR:HG23	1:C:56:ARG:CD	2.22	0.69
1:C:202:PRO:HA	1:C:205:LEU:HD22	1.73	0.69
2:D:156:PHE:CE1	2:D:221:LEU:HD23	2.27	0.69
1:A:104:VAL:HA	1:A:121:GLU:OE2	1.92	0.69
2:D:156:PHE:HE1	2:D:221:LEU:HD23	1.58	0.69
1:A:111:LYS:HZ2	1:A:116:LEU:CD2	2.05	0.68
1:C:258:PRO:HD2	1:C:261:PHE:CD1	2.27	0.68
2:D:249:SER:HA	2:D:262:ARG:NH1	2.08	0.68
2:D:288:ASP:OD2	2:D:289:GLU:HG3	1.92	0.68
1:A:39:GLN:O	1:A:42:GLN:OE1	2.11	0.68
1:A:166:ASP:HB3	1:A:187:PHE:HD2	1.57	0.68
1:A:129:PHE:HE1	1:A:133:ARG:NE	1.91	0.68
2:D:346:VAL:O	2:D:347:LYS:HD3	1.93	0.68
1:A:40:LEU:HA	1:A:43:PHE:HE1	1.57	0.68
1:C:263:SER:HA	1:C:266:LYS:HE3	1.76	0.68
1:C:204:TYR:CE2	1:C:227:LEU:CD2	2.76	0.68
1:A:328:ASP:CG	2:B:92:ARG:HH22	2.00	0.68
1:C:266:LYS:O	1:C:267:ASP:C	2.37	0.68
1:C:297:PHE:HD2	1:C:300:THR:HG21	1.59	0.68
1:A:135:ILE:HD11	1:A:138:PHE:CE1	2.29	0.67
1:A:247:TYR:N	1:A:247:TYR:CD2	2.61	0.67
1:C:204:TYR:HE2	1:C:227:LEU:HD23	1.59	0.67
1:C:243:PRO:O	1:C:246:ILE:N	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:ILE:HD12	1:A:86:GLU:N	2.09	0.67
1:A:133:ARG:HH21	2:B:95:ARG:HH22	1.42	0.67
2:D:316:LEU:HD23	2:D:320:ASP:HB3	1.75	0.67
1:C:87:HIS:O	1:C:90:ASN:CB	2.42	0.67
2:D:94:ARG:HG2	2:D:94:ARG:HH11	1.60	0.67
1:C:29:LYS:HE2	1:C:96:GLN:O	1.94	0.67
2:B:116:ILE:HG12	2:B:118:LYS:NZ	2.10	0.67
1:A:69:TYR:HB3	1:A:119:VAL:HG23	1.75	0.67
1:A:92:LYS:HE2	1:A:350:PHE:CD2	2.30	0.67
1:A:115:ASN:HB2	1:A:117:TYR:CZ	2.30	0.67
2:B:325:ILE:CD1	2:B:331:ARG:CD	2.67	0.67
2:D:257:LEU:CD1	2:D:257:LEU:C	2.64	0.67
2:D:302:GLN:OE1	2:D:313:VAL:HG11	1.95	0.67
2:B:245:GLU:OE1	2:B:262:ARG:CB	2.42	0.67
2:D:188:TRP:HH2	2:D:190:THR:C	2.00	0.67
1:C:23:LYS:O	1:C:27:LEU:HG	1.95	0.66
1:A:129:PHE:HE1	1:A:133:ARG:CZ	2.08	0.66
1:C:68:HIS:O	1:C:69:TYR:CD2	2.48	0.66
2:D:301:LEU:CD2	2:D:312:GLU:HA	2.26	0.66
2:B:308:GLU:N	2:B:308:GLU:OE1	2.28	0.66
1:A:334:GLU:CB	2:D:260:TRP:HZ2	2.08	0.66
1:C:61:LYS:NZ	1:C:68:HIS:ND1	2.44	0.66
1:A:77:GLN:HE22	1:A:342:LYS:HZ3	1.42	0.66
2:D:175:ILE:CD1	2:D:192:VAL:HG21	2.25	0.66
1:A:247:TYR:HD2	1:A:247:TYR:H	1.41	0.66
2:B:236:SER:O	2:B:239:ARG:CG	2.44	0.66
1:C:50:GLY:N	1:C:56:ARG:CZ	2.58	0.66
1:C:56:ARG:HH11	1:C:57:VAL:N	1.93	0.66
1:C:107:GLU:O	1:C:108:PHE:CD2	2.49	0.66
1:C:133:ARG:HD3	1:C:133:ARG:N	2.10	0.66
1:A:47:LYS:C	1:A:58:MET:HE3	2.21	0.66
1:A:57:VAL:HG21	3:A:400:ADP:C8	2.30	0.66
2:B:171:ASN:OD1	2:B:172:PHE:N	2.28	0.66
1:C:29:LYS:CE	1:C:96:GLN:O	2.44	0.66
1:C:169:PRO:CA	1:C:172:LEU:HD12	2.22	0.66
2:D:273:GLN:HE21	2:D:274:PHE:N	1.94	0.66
1:A:109:SER:OG	1:A:350:PHE:CE1	2.49	0.66
1:C:61:LYS:NZ	1:C:68:HIS:CD2	2.63	0.66
2:D:317:GLY:N	2:D:320:ASP:OD2	2.29	0.66
2:B:311:VAL:CG2	2:B:312:GLU:N	2.59	0.66
2:D:221:LEU:HD12	2:D:221:LEU:C	2.20	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:287:GLY:HA3	2:D:333:ARG:HE	1.60	0.66
1:A:201:THR:HG21	2:B:95:ARG:CD	2.26	0.65
1:A:120:MET:HE3	3:A:400:ADP:N7	2.11	0.65
1:C:265:LEU:HD13	1:C:296:TRP:CZ2	2.30	0.65
1:A:46:ILE:CD1	1:A:47:LYS:H	2.09	0.65
1:A:113:ASN:ND2	1:A:338:SEP:O	2.29	0.65
2:B:132:LYS:O	2:B:132:LYS:HG2	1.97	0.65
1:A:75:ASP:HB3	1:A:78:LYS:HG2	1.77	0.65
2:B:251:VAL:CG1	2:B:254:LEU:HD12	2.25	0.65
1:A:46:ILE:C	1:A:47:LYS:HD2	2.21	0.65
2:B:118:LYS:HZ3	2:B:149:ASP:HA	1.61	0.65
2:B:185:ASN:HB2	1:C:34:SER:HB2	1.78	0.65
2:B:188:TRP:HE3	2:B:188:TRP:O	1.80	0.65
1:A:242:GLN:NE2	1:A:245:GLN:CB	2.59	0.65
2:D:257:LEU:HD11	2:D:262:ARG:NE	2.12	0.65
1:A:243:PRO:O	1:A:247:TYR:CD2	2.49	0.64
1:A:128:MET:CE	1:A:172:LEU:HD13	2.27	0.64
1:C:204:TYR:HE2	1:C:227:LEU:CD2	2.10	0.64
1:A:59:LEU:HD23	1:A:60:VAL:N	2.12	0.64
2:D:169:GLY:HA2	2:D:209:ARG:NE	2.13	0.64
1:A:32:THR:O	1:A:32:THR:CG2	2.45	0.64
1:A:46:ILE:HD11	1:A:59:LEU:CB	2.22	0.64
2:B:166:GLY:HA2	2:B:208:PRO:HB3	1.79	0.64
2:D:251:VAL:HG11	2:D:254:LEU:HG	1.79	0.64
1:A:92:LYS:CD	1:A:350:PHE:CD2	2.79	0.64
2:B:115:VAL:HG13	2:B:149:ASP:CG	2.22	0.64
1:A:148:ALA:HB1	1:A:302:TRP:CZ3	2.32	0.64
1:C:30:TRP:HE1	1:C:190:ARG:HH12	1.43	0.64
1:A:23:LYS:HE3	1:A:27:LEU:HD11	1.80	0.64
1:C:250:ILE:HG22	1:C:251:VAL:N	2.12	0.64
1:A:111:LYS:CE	1:A:350:PHE:HB3	2.28	0.64
2:B:166:GLY:C	2:B:208:PRO:HB3	2.22	0.64
2:B:305:SER:O	2:B:308:GLU:OE1	2.16	0.64
1:C:48:THR:C	1:C:56:ARG:HH22	2.05	0.64
1:C:49:LEU:C	1:C:56:ARG:HH22	2.06	0.64
2:D:249:SER:HA	2:D:262:ARG:CZ	2.28	0.64
1:A:92:LYS:HD3	1:A:350:PHE:CZ	2.34	0.64
1:A:92:LYS:HZ1	1:A:350:PHE:HA	1.63	0.64
1:A:106:LEU:HD11	1:A:118:MET:HG3	1.79	0.64
2:B:166:GLY:O	2:B:208:PRO:HB3	1.97	0.64
1:A:46:ILE:CG1	1:A:59:LEU:HD22	2.21	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:PHE:HE1	1:A:179:TYR:HD1	1.46	0.63
1:C:56:ARG:CD	1:C:57:VAL:H	1.91	0.63
1:C:195:THR:C	1:C:196:TRP:CD1	2.77	0.63
1:A:77:GLN:NE2	1:A:342:LYS:CD	2.61	0.63
2:B:264:THR:O	2:B:267:ASP:OD1	2.15	0.63
1:C:132:LEU:HD13	1:C:138:PHE:HE2	1.63	0.63
2:D:172:PHE:C	2:D:173:TYR:CD1	2.76	0.63
2:D:182:VAL:N	2:D:188:TRP:HZ3	1.96	0.63
1:A:242:GLN:HE22	1:A:245:GLN:CB	2.10	0.63
2:B:308:GLU:HB2	2:B:309:GLU:OE1	1.98	0.63
2:D:272:VAL:HG11	2:D:347:LYS:CE	2.28	0.63
2:D:345:CYS:HB2	2:D:347:LYS:NZ	2.13	0.63
1:A:131:HIS:CD2	1:A:134:ARG:NH1	2.50	0.63
2:B:283:GLN:HG2	2:B:335:ALA:HA	1.79	0.63
1:C:140:GLU:O	1:C:143:ALA:N	2.32	0.63
1:C:297:PHE:CD2	1:C:300:THR:HG21	2.34	0.63
2:D:275:GLU:OE1	2:D:278:GLN:OE1	2.16	0.63
1:A:111:LYS:NZ	1:A:116:LEU:HD11	2.13	0.63
2:B:293:ILE:CD1	2:B:317:GLY:O	2.47	0.63
2:D:181:ASP:CG	2:D:188:TRP:CH2	2.77	0.63
1:A:244:ILE:O	1:A:248:GLU:HG3	1.99	0.63
2:D:216:LYS:HG3	2:D:217:THR:HG23	1.81	0.63
2:B:164:GLN:HB3	2:B:167:ASP:OD2	1.98	0.63
2:B:356:VAL:HG23	2:B:357:LEU:N	2.14	0.63
1:C:238:PHE:HD1	1:C:249:LYS:HG3	1.63	0.63
1:A:45:ARG:NH1	1:A:45:ARG:HG3	2.14	0.62
1:A:195:THR:CG2	1:A:197:TPO:O2P	2.47	0.62
1:C:133:ARG:NH2	2:D:95:ARG:HH22	1.97	0.62
2:D:321:TYR:HE1	2:D:324:GLU:CD	2.06	0.62
2:B:330:ASN:OD1	2:B:330:ASN:N	2.30	0.62
1:C:62:HIS:HB2	1:C:69:TYR:HE1	1.65	0.62
1:A:174:ILE:HD13	1:A:174:ILE:N	2.14	0.62
2:D:221:LEU:HD12	2:D:222:TRP:N	2.13	0.62
2:D:294:LEU:CD1	2:D:346:VAL:HG13	2.30	0.62
1:A:102:PHE:C	1:A:103:LEU:HD12	2.24	0.62
2:D:151:MET:CE	2:D:222:TRP:HB3	2.19	0.62
1:C:168:LYS:HA	1:C:227:LEU:HD21	1.81	0.62
2:D:281:VAL:HG11	2:D:333:ARG:CZ	2.28	0.62
1:C:163:ILE:HG12	1:C:165:ARG:HG3	1.81	0.62
2:D:120:TYR:CZ	2:D:124:ALA:HB2	2.32	0.62
1:A:40:LEU:CD1	1:A:45:ARG:HH21	2.11	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:229:TYR:O	2:B:233:LEU:HD11	2.00	0.62
2:B:298:ALA:HB2	2:B:343:LEU:HD21	1.82	0.62
2:D:290:PHE:CD2	2:D:327:LEU:HD11	2.34	0.62
2:B:305:SER:O	2:B:308:GLU:OE2	2.17	0.62
2:D:329:MET:SD	2:D:331:ARG:NE	2.73	0.62
1:A:189:LYS:NZ	1:A:195:THR:HG21	2.15	0.61
2:B:293:ILE:HD11	2:B:320:ASP:N	2.14	0.61
2:D:113:ARG:HG2	2:D:114:LYS:N	2.15	0.61
2:D:126:LEU:HB3	2:D:148:PHE:CE2	2.35	0.61
2:D:182:VAL:H	2:D:188:TRP:HZ3	1.47	0.61
1:A:41:ASP:OD1	1:A:41:ASP:N	2.31	0.61
1:A:125:GLY:O	1:A:131:HIS:CE1	2.53	0.61
2:B:116:ILE:HG12	2:B:118:LYS:HZ2	1.64	0.61
1:C:55:GLY:HA3	1:C:74:LEU:CD2	2.29	0.61
1:A:50:GLY:HA3	3:A:400:ADP:H4'	1.82	0.61
1:A:77:GLN:NE2	1:A:342:LYS:NZ	2.48	0.61
2:B:245:GLU:OE2	2:B:262:ARG:CD	2.48	0.61
2:B:281:VAL:HG22	2:B:337:VAL:CG1	2.31	0.61
1:A:301:ASP:O	1:A:305:ILE:HG12	2.00	0.61
2:B:251:VAL:HG11	2:B:254:LEU:CD1	2.30	0.61
2:D:172:PHE:CE1	2:D:197:SER:HB2	2.35	0.61
1:A:142:HIS:CE1	1:A:146:TYR:CE2	2.87	0.61
2:D:348:LEU:CD2	2:D:352:ARG:HD3	2.31	0.61
2:D:260:TRP:CD1	2:D:261:GLU:HG3	2.36	0.61
2:B:275:GLU:CD	2:B:276:ASP:N	2.59	0.61
1:C:221:TRP:O	1:C:272:LEU:HD23	2.01	0.61
2:D:276:ASP:CG	2:D:341:GLY:H	2.09	0.61
1:A:106:LEU:CD1	1:A:118:MET:HG3	2.30	0.61
1:C:49:LEU:N	1:C:56:ARG:HH22	1.99	0.61
1:C:114:SER:HB2	1:C:337:VAL:HG13	1.83	0.61
2:B:297:SER:O	2:B:343:LEU:HD11	2.01	0.61
1:C:170:GLU:OE2	2:D:95:ARG:NH1	2.33	0.61
1:C:201:THR:HG21	2:D:95:ARG:HD3	1.81	0.61
1:A:111:LYS:HD3	1:A:116:LEU:HD13	1.83	0.60
1:C:48:THR:OG1	1:C:56:ARG:CZ	2.48	0.60
2:D:259:LYS:HG3	2:D:260:TRP:N	2.15	0.60
1:C:62:HIS:ND1	1:C:65:SER:OG	2.25	0.60
1:C:154:PHE:CZ	1:C:167:LEU:CD1	2.84	0.60
2:B:293:ILE:HD13	2:B:318:PRO:CA	2.31	0.60
2:B:305:SER:O	2:B:308:GLU:CD	2.45	0.60
1:A:139:SEP:OG	1:A:141:PRO:HD2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:103:LEU:HD12	1:C:103:LEU:N	2.16	0.60
1:C:311:GLU:CD	1:C:311:GLU:H	2.09	0.60
2:D:234:MET:O	2:D:238:LEU:HB2	2.01	0.60
1:A:175:ASP:CG	1:A:181:GLN:NE2	2.60	0.60
1:A:274:GLN:HG2	1:A:279:LYS:HB2	1.82	0.60
2:D:116:ILE:HD13	2:D:152:PHE:CA	2.31	0.60
2:D:177:GLN:O	2:D:219:VAL:HG12	2.01	0.60
2:B:293:ILE:CD1	2:B:319:SER:N	2.64	0.60
1:C:238:PHE:CD1	1:C:249:LYS:HG3	2.36	0.60
2:D:151:MET:HE1	2:D:223:GLY:CA	2.31	0.60
2:D:180:MET:HB2	2:D:192:VAL:HG13	1.83	0.60
2:D:290:PHE:O	2:D:291:PHE:CD1	2.55	0.60
1:C:46:ILE:C	1:C:58:MET:HE3	2.26	0.60
1:A:40:LEU:O	1:A:45:ARG:NH2	2.29	0.60
1:A:111:LYS:HE2	1:A:350:PHE:HB3	1.84	0.60
2:B:148:PHE:HD2	2:B:151:MET:HE1	1.66	0.60
1:C:48:THR:OG1	1:C:56:ARG:NE	2.35	0.60
1:C:114:SER:HB2	1:C:337:VAL:HA	1.82	0.60
2:D:169:GLY:CA	2:D:209:ARG:CZ	2.77	0.60
2:D:176:ASP:OD1	2:D:220:LYS:HG3	2.02	0.60
2:B:143:GLU:O	2:B:146:ASP:HB2	2.01	0.60
2:B:219:VAL:CG2	2:B:220:LYS:N	2.64	0.60
2:D:173:TYR:O	2:D:198:PHE:CE2	2.54	0.60
1:C:265:LEU:CD1	1:C:296:TRP:CZ2	2.85	0.60
2:D:176:ASP:OD1	2:D:176:ASP:C	2.44	0.60
2:D:356:VAL:O	2:D:357:LEU:HD22	2.02	0.60
1:A:79:VAL:CA	1:A:84:GLN:HE22	2.00	0.59
2:B:118:LYS:NZ	2:B:149:ASP:O	2.35	0.59
1:A:23:LYS:CE	1:A:27:LEU:HD11	2.32	0.59
1:A:147:ALA:O	1:A:151:VAL:HG23	2.02	0.59
1:A:338:SEP:O1P	1:A:339:ILE:HG12	2.02	0.59
1:A:23:LYS:O	1:A:27:LEU:HD12	2.01	0.59
1:A:271:ASN:HB3	1:A:281:PHE:CD2	2.36	0.59
2:D:244:TYR:O	2:D:248:LEU:HD13	2.02	0.59
1:A:92:LYS:CG	1:A:93:ARG:N	2.64	0.59
1:C:80:VAL:HA	1:C:85:ILE:CD1	2.29	0.59
1:C:108:PHE:HB2	1:C:119:VAL:CG1	2.30	0.59
2:D:152:PHE:O	2:D:222:TRP:HE3	1.84	0.59
1:A:77:GLN:CD	1:A:342:LYS:HD2	2.28	0.59
1:A:111:LYS:NZ	1:A:350:PHE:CE1	2.54	0.59
2:B:151:MET:CG	2:B:224:ILE:HD11	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:80:VAL:CA	1:C:85:ILE:HD11	2.31	0.59
1:C:328:ASP:HB2	1:C:330:TYR:OH	2.03	0.59
1:C:75:ASP:OD1	1:C:75:ASP:C	2.46	0.59
2:D:120:TYR:O	2:D:123:MET:N	2.36	0.59
2:D:136:PHE:N	2:D:136:PHE:CD2	2.70	0.59
2:D:179:GLU:N	2:D:217:THR:OG1	2.34	0.59
2:B:244:TYR:CD1	2:B:269:LEU:HD12	2.38	0.59
2:B:283:GLN:HG3	2:B:336:THR:N	2.18	0.59
1:C:50:GLY:N	1:C:56:ARG:HH12	1.92	0.59
1:C:91:GLU:HG2	1:C:185:PHE:C	2.28	0.59
1:C:100:PHE:HB3	1:C:103:LEU:CD1	2.22	0.59
2:B:151:MET:HG2	2:B:222:TRP:HB3	1.83	0.58
2:D:350:ARG:CG	2:D:351:PRO:HD3	2.33	0.58
2:D:182:VAL:N	2:D:188:TRP:CZ3	2.71	0.58
2:B:185:ASN:HB2	1:C:34:SER:CB	2.34	0.58
1:C:201:THR:CG2	2:D:95:ARG:HD3	2.33	0.58
1:C:234:GLY:C	1:C:235:TYR:HD1	2.11	0.58
2:D:290:PHE:CE1	2:D:291:PHE:O	2.57	0.58
1:C:91:GLU:HG3	1:C:186:GLY:HA2	1.85	0.58
1:C:180:ILE:CG2	1:C:181:GLN:N	2.66	0.58
2:D:149:ASP:C	2:D:151:MET:H	2.11	0.58
2:D:172:PHE:CE1	2:D:198:PHE:N	2.48	0.58
1:A:61:LYS:CE	1:A:66:GLY:HA2	2.33	0.58
1:A:173:LEU:C	1:A:174:ILE:HD13	2.28	0.58
1:C:50:GLY:O	1:C:56:ARG:CZ	2.51	0.58
2:D:172:PHE:HZ	2:D:197:SER:HB2	1.64	0.58
1:A:40:LEU:HD12	1:A:45:ARG:NH2	2.14	0.58
1:A:261:PHE:O	1:A:266:LYS:HE2	2.02	0.58
2:B:179:GLU:HB2	2:B:216:LYS:HG2	1.85	0.58
1:C:169:PRO:HD3	1:C:227:LEU:HD22	1.84	0.58
2:D:158:ALA:CB	2:D:216:LYS:O	2.51	0.58
2:D:170:ASP:HB3	2:D:171:ASN:OD1	2.03	0.58
2:D:188:TRP:CZ2	2:D:190:THR:C	2.82	0.58
2:B:276:ASP:HB2	2:B:341:GLY:CA	2.32	0.58
2:D:221:LEU:HD12	2:D:222:TRP:CA	2.33	0.58
2:D:291:PHE:HD2	2:D:347:LYS:NZ	2.01	0.58
1:A:189:LYS:NZ	1:A:195:THR:CG2	2.67	0.58
1:A:211:LEU:HD12	1:A:212:SER:N	2.17	0.58
1:C:68:HIS:CD2	1:C:322:GLY:N	2.71	0.58
1:C:75:ASP:O	1:C:79:VAL:HG23	2.04	0.58
2:D:171:ASN:HB3	2:D:173:TYR:CE1	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:345:CYS:HB2	2:D:347:LYS:CE	2.34	0.58
1:A:102:PHE:CE1	1:A:179:TYR:HD1	2.21	0.58
2:D:176:ASP:OD1	2:D:220:LYS:CG	2.52	0.58
2:B:238:LEU:HD23	2:B:238:LEU:C	2.28	0.58
1:A:339:ILE:N	1:A:339:ILE:HD13	2.19	0.57
2:B:151:MET:SD	2:B:224:ILE:CD1	2.85	0.57
1:C:96:GLN:CA	1:C:106:LEU:HD21	2.34	0.57
2:D:224:ILE:CG1	2:D:225:ASP:N	2.67	0.57
2:D:246:GLU:O	2:D:249:SER:OG	2.21	0.57
2:B:185:ASN:CB	1:C:34:SER:HB2	2.33	0.57
2:B:236:SER:HA	2:B:239:ARG:CZ	2.34	0.57
2:B:275:GLU:CD	2:B:275:GLU:C	2.72	0.57
1:A:195:THR:HG22	1:A:196:TRP:N	2.18	0.57
2:D:174:VAL:HA	2:D:197:SER:HB3	1.86	0.57
1:A:208:GLU:O	1:A:211:LEU:HD12	2.03	0.57
2:B:281:VAL:HG22	2:B:337:VAL:HG12	1.86	0.57
1:C:89:LEU:O	1:C:92:LYS:HG3	2.05	0.57
2:D:156:PHE:HB2	2:D:219:VAL:HG23	1.86	0.57
1:A:79:VAL:HG22	1:A:84:GLN:HE21	1.69	0.57
1:C:224:LEU:O	1:C:228:ILE:HG13	2.05	0.57
2:D:260:TRP:CD1	2:D:261:GLU:CG	2.87	0.57
2:B:104:THR:HG23	2:B:107:ASP:CG	2.29	0.57
2:B:152:PHE:CZ	2:B:171:ASN:ND2	2.73	0.57
1:C:86:GLU:CD	1:C:86:GLU:H	2.12	0.57
1:C:187:PHE:CD1	1:C:199:CYS:HB2	2.39	0.57
2:D:345:CYS:HB2	2:D:347:LYS:HE2	1.87	0.57
1:C:42:GLN:OE1	1:C:42:GLN:N	2.38	0.57
2:D:329:MET:SD	2:D:331:ARG:CZ	2.93	0.57
1:A:343:CYS:C	1:A:346:GLU:OE1	2.47	0.57
2:B:283:GLN:HG3	2:B:336:THR:H	1.69	0.57
1:C:77:GLN:O	1:C:80:VAL:HG23	2.04	0.57
1:C:80:VAL:HG12	1:C:85:ILE:CD1	2.32	0.57
1:C:150:ILE:CG2	1:C:154:PHE:CE2	2.64	0.57
1:C:211:LEU:CD1	1:C:213:LYS:HD2	2.35	0.57
2:D:251:VAL:HA	2:D:321:TYR:HE2	1.69	0.57
2:D:151:MET:SD	2:D:224:ILE:HG22	2.45	0.57
2:D:254:LEU:O	2:D:257:LEU:HG	2.04	0.57
1:A:173:LEU:O	1:A:181:GLN:OE1	2.22	0.57
2:B:188:TRP:CE3	2:B:188:TRP:C	2.83	0.57
1:C:86:GLU:CD	2:D:102:VAL:HG21	2.29	0.57
1:C:165:ARG:HD2	1:C:199:CYS:SG	2.44	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:257:LEU:HD13	2:D:258:ASP:O	2.05	0.57
1:A:131:HIS:HA	1:A:134:ARG:HG2	1.87	0.56
1:A:43:PHE:N	1:A:63:LYS:HE2	2.20	0.56
1:C:49:LEU:N	1:C:56:ARG:NH2	2.53	0.56
1:C:133:ARG:NH2	1:C:230:GLU:OE1	2.37	0.56
1:A:134:ARG:NH1	1:A:314:PHE:CZ	2.72	0.56
2:B:233:LEU:HD12	2:B:233:LEU:H	1.70	0.56
2:B:233:LEU:HD12	2:B:233:LEU:N	2.20	0.56
2:B:275:GLU:OE2	2:B:276:ASP:HB3	2.05	0.56
1:C:16:LYS:CG	1:C:17:GLU:H	2.18	0.56
1:C:90:ASN:CG	1:C:94:ILE:HD13	2.31	0.56
2:D:135:LEU:C	2:D:136:PHE:CD2	2.83	0.56
2:B:251:VAL:CB	2:B:254:LEU:HD12	2.34	0.56
1:C:131:HIS:O	1:C:135:ILE:HD13	2.06	0.56
2:D:181:ASP:CG	2:D:188:TRP:CZ3	2.81	0.56
1:A:134:ARG:HH12	1:A:314:PHE:HZ	1.49	0.56
2:D:257:LEU:HD21	2:D:262:ARG:NH1	2.21	0.56
1:A:47:LYS:O	1:A:58:MET:HG2	2.05	0.56
1:A:201:THR:HG21	2:B:95:ARG:HD2	1.87	0.56
2:B:310:PHE:CE1	2:B:336:THR:HG21	2.39	0.56
1:C:47:LYS:O	1:C:58:MET:HG2	2.05	0.56
2:D:116:ILE:HD13	2:D:152:PHE:HA	1.87	0.56
2:D:130:ILE:HA	2:D:133:ASN:OD1	2.06	0.56
2:D:258:ASP:CG	2:D:260:TRP:CZ2	2.83	0.56
1:A:58:MET:SD	1:A:332:GLU:OE2	2.64	0.56
1:A:111:LYS:CE	1:A:350:PHE:CB	2.84	0.56
1:A:131:HIS:O	1:A:134:ARG:HG2	2.05	0.56
1:A:111:LYS:NZ	1:A:116:LEU:HD21	2.21	0.56
1:A:126:GLY:HA2	1:A:327:PHE:CE1	2.41	0.56
1:A:195:THR:HG22	1:A:196:TRP:H	1.71	0.56
2:B:147:ILE:HD11	2:B:148:PHE:CE2	2.41	0.56
2:B:245:GLU:OE2	2:B:262:ARG:NE	2.39	0.56
2:B:295:GLU:HG3	2:B:344:LYS:HE2	1.88	0.56
1:C:26:PHE:HD1	1:C:97:ALA:O	1.88	0.56
2:D:171:ASN:ND2	2:D:224:ILE:O	2.35	0.56
2:D:272:VAL:HG12	2:D:347:LYS:HG2	1.87	0.56
2:D:282:VAL:HB	2:D:285:GLU:CG	2.35	0.56
1:A:125:GLY:O	1:A:131:HIS:HE1	1.89	0.56
1:A:150:ILE:HG22	1:A:154:PHE:CE2	2.40	0.56
2:B:267:ASP:OD1	2:B:268:ALA:N	2.39	0.56
1:A:189:LYS:HZ3	1:A:195:THR:CG2	2.19	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:107:ASP:OD2	2:B:107:ASP:N	2.39	0.55
2:B:130:ILE:C	2:B:130:ILE:CD1	2.79	0.55
2:D:182:VAL:CG1	2:D:211:ALA:HB1	2.36	0.55
2:B:179:GLU:HB3	2:B:216:LYS:HE3	1.89	0.55
1:C:174:ILE:HD12	1:C:175:ASP:O	2.05	0.55
2:D:183:TYR:HD2	2:D:187:GLU:C	2.14	0.55
1:A:142:HIS:ND1	1:A:146:TYR:HE2	2.04	0.55
2:D:353:PHE:C	2:D:353:PHE:CD2	2.85	0.55
2:B:351:PRO:O	2:B:355:ARG:HG3	2.06	0.55
1:C:62:HIS:CG	1:C:65:SER:HG	2.24	0.55
2:D:151:MET:SD	2:D:223:GLY:O	2.64	0.55
2:D:173:TYR:HB3	2:D:221:LEU:HD13	1.87	0.55
1:A:46:ILE:HD13	1:A:59:LEU:HD13	1.87	0.55
1:C:238:PHE:CD2	1:C:250:ILE:HG13	2.42	0.55
2:D:292:ILE:O	2:D:345:CYS:HB3	2.07	0.55
2:B:166:GLY:CA	2:B:208:PRO:HB3	2.37	0.55
2:D:251:VAL:HA	2:D:321:TYR:CE2	2.42	0.55
1:A:89:LEU:O	1:A:93:ARG:HG3	2.06	0.55
2:B:148:PHE:CD2	2:B:151:MET:HE1	2.40	0.55
1:A:91:GLU:HG3	1:A:185:PHE:HB2	1.88	0.55
2:B:188:TRP:O	2:B:188:TRP:CE3	2.59	0.55
2:B:257:LEU:HG	2:B:261:GLU:HB2	1.89	0.55
1:C:287:GLY:O	1:C:290:ASP:OD2	2.25	0.55
1:A:95:LEU:CD1	1:A:185:PHE:HB2	2.28	0.54
1:A:100:PHE:CG	1:A:101:PRO:HD2	2.41	0.54
2:B:325:ILE:HD11	2:B:331:ARG:HD3	1.82	0.54
1:C:170:GLU:OE2	2:D:95:ARG:HG2	2.07	0.54
1:C:243:PRO:HA	1:C:246:ILE:CD1	2.30	0.54
2:D:317:GLY:O	2:D:320:ASP:OD2	2.24	0.54
2:B:173:TYR:HB2	2:B:198:PHE:CZ	2.42	0.54
1:C:289:ASN:OD1	1:C:292:LYS:HE3	2.08	0.54
1:C:154:PHE:HZ	1:C:167:LEU:HD13	1.72	0.54
1:A:268:LEU:HB2	1:A:294:HIS:NE2	2.23	0.54
2:B:152:PHE:HZ	2:B:171:ASN:ND2	2.04	0.54
1:A:103:LEU:HD12	1:A:103:LEU:N	2.23	0.54
2:B:230:ARG:O	2:B:233:LEU:CD1	2.56	0.54
1:C:40:LEU:CD2	1:C:112:ASP:OD2	2.56	0.54
2:B:182:VAL:HG23	2:B:213:VAL:HG22	1.88	0.54
1:C:258:PRO:HD2	1:C:261:PHE:CE1	2.43	0.54
1:A:111:LYS:NZ	1:A:350:PHE:CE2	2.76	0.54
2:B:353:PHE:O	2:B:356:VAL:HG23	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:87:HIS:O	1:C:88:THR:C	2.50	0.54
2:D:154:VAL:O	2:D:221:LEU:CG	2.45	0.54
1:A:40:LEU:O	1:A:43:PHE:CE1	2.60	0.54
1:A:189:LYS:NZ	1:A:197:TPO:O1P	2.40	0.54
1:C:268:LEU:HB2	1:C:294:HIS:CE1	2.43	0.54
2:D:188:TRP:CZ3	2:D:190:THR:O	2.60	0.54
2:D:255:GLU:HA	2:D:255:GLU:OE1	2.07	0.54
1:A:166:ASP:HB3	1:A:187:PHE:CD2	2.42	0.54
1:C:90:ASN:OD1	1:C:90:ASN:C	2.51	0.54
2:D:288:ASP:HB2	2:D:350:ARG:HG2	1.90	0.54
1:A:146:TYR:HB2	1:A:231:MET:HE1	1.90	0.53
1:C:153:THR:O	1:C:156:TYR:HB3	2.08	0.53
1:C:163:ILE:O	1:C:188:ALA:HA	2.08	0.53
1:C:195:THR:OG1	1:C:196:TRP:N	2.37	0.53
1:C:245:GLN:O	1:C:249:LYS:HB2	2.07	0.53
2:D:172:PHE:O	2:D:173:TYR:HD1	1.90	0.53
1:A:307:GLN:NE2	1:A:309:LYS:CD	2.71	0.53
1:C:75:ASP:HB3	1:C:78:LYS:HE2	1.90	0.53
2:D:158:ALA:HB1	2:D:216:LYS:O	2.09	0.53
2:D:258:ASP:OD2	2:D:260:TRP:CZ2	2.61	0.53
2:D:345:CYS:CB	2:D:347:LYS:NZ	2.71	0.53
1:A:84:GLN:N	1:A:84:GLN:OE1	2.41	0.53
1:A:103:LEU:N	1:A:103:LEU:CD1	2.71	0.53
2:B:116:ILE:CG1	2:B:118:LYS:HZ2	2.22	0.53
1:C:154:PHE:CZ	1:C:167:LEU:HD13	2.43	0.53
2:D:273:GLN:NE2	2:D:274:PHE:N	2.56	0.53
1:A:133:ARG:NH2	2:B:95:ARG:NH2	2.53	0.53
2:B:103:TYR:HB3	2:B:234:MET:HE1	1.89	0.53
2:B:325:ILE:CD1	2:B:331:ARG:HH21	2.20	0.53
2:D:135:LEU:HB2	2:D:136:PHE:CE2	2.44	0.53
1:A:61:LYS:HE2	1:A:66:GLY:O	2.09	0.53
2:D:149:ASP:C	2:D:151:MET:N	2.64	0.53
1:A:86:GLU:O	1:A:89:LEU:HG	2.08	0.53
2:D:104:THR:O	2:D:105:GLU:C	2.51	0.53
1:C:92:LYS:HD2	1:C:93:ARG:N	2.24	0.53
2:D:151:MET:HE2	2:D:222:TRP:C	2.32	0.53
1:A:189:LYS:HZ2	1:A:195:THR:HG21	1.72	0.53
2:B:93:ARG:HA	2:B:93:ARG:NE	2.24	0.53
2:D:183:TYR:HD2	2:D:188:TRP:N	2.07	0.53
2:D:261:GLU:O	2:D:265:VAL:HG12	2.09	0.53
2:D:272:VAL:HG11	2:D:347:LYS:HE3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:HIS:CA	1:A:134:ARG:HE	2.18	0.52
1:A:215:TYR:CD2	1:A:215:TYR:N	2.77	0.52
1:A:133:ARG:HH21	2:B:95:ARG:NH2	2.07	0.52
2:D:321:TYR:CD1	2:D:321:TYR:C	2.86	0.52
2:B:330:ASN:HA	2:B:350:ARG:HH22	1.74	0.52
1:C:150:ILE:O	1:C:154:PHE:CD2	2.55	0.52
1:C:174:ILE:CD1	1:C:175:ASP:O	2.58	0.52
1:C:329:ASP:C	1:C:330:TYR:CD2	2.88	0.52
2:D:173:TYR:O	2:D:198:PHE:HE2	1.92	0.52
2:D:257:LEU:HD11	2:D:262:ARG:CG	2.39	0.52
2:D:290:PHE:O	2:D:291:PHE:CG	2.63	0.52
2:D:349:ASP:OD2	2:D:351:PRO:HD2	2.10	0.52
1:A:61:LYS:HD3	1:A:67:ASN:O	2.08	0.52
1:A:79:VAL:HG11	1:A:347:PHE:HZ	1.74	0.52
1:A:111:LYS:HD3	1:A:116:LEU:CD1	2.38	0.52
1:A:43:PHE:C	1:A:63:LYS:NZ	2.67	0.52
1:A:208:GLU:O	1:A:211:LEU:CD1	2.57	0.52
2:B:300:VAL:HG23	2:B:314:GLY:N	2.25	0.52
1:C:68:HIS:NE2	1:C:321:PRO:HB2	2.24	0.52
1:C:90:ASN:O	1:C:91:GLU:C	2.53	0.52
1:A:238:PHE:HD1	1:A:249:LYS:HD2	1.74	0.52
2:B:337:VAL:HG22	2:B:338:VAL:N	2.25	0.52
1:C:103:LEU:N	1:C:103:LEU:CD1	2.72	0.52
1:C:234:GLY:C	1:C:235:TYR:CD1	2.88	0.52
2:D:136:PHE:O	2:D:139:LEU:HG	2.09	0.52
2:D:272:VAL:CG1	2:D:347:LYS:HG2	2.40	0.52
1:C:89:LEU:O	1:C:92:LYS:NZ	2.35	0.52
1:C:154:PHE:HZ	1:C:167:LEU:HD11	1.75	0.52
2:B:246:GLU:O	2:B:249:SER:OG	2.28	0.52
1:C:68:HIS:CD2	1:C:322:GLY:H	2.27	0.52
1:C:139:SEP:O	1:C:142:HIS:HB3	2.10	0.52
1:C:224:LEU:HG	1:C:228:ILE:HD11	1.92	0.52
2:D:272:VAL:HG11	2:D:347:LYS:CG	2.39	0.52
1:A:46:ILE:CD1	1:A:47:LYS:N	2.68	0.52
1:A:75:ASP:HB3	1:A:78:LYS:NZ	2.24	0.52
2:B:147:ILE:HD11	2:B:148:PHE:CD2	2.44	0.52
1:C:23:LYS:HG3	1:C:27:LEU:HD11	1.92	0.52
1:C:242:GLN:O	1:C:243:PRO:C	2.52	0.52
2:D:154:VAL:HB	2:D:221:LEU:CD2	2.32	0.52
1:A:59:LEU:HD23	1:A:59:LEU:C	2.35	0.52
1:A:201:THR:HG21	2:B:95:ARG:HD3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:129:PHE:HE1	1:C:133:ARG:NH2	2.08	0.52
1:C:174:ILE:HD13	1:C:178:GLY:CA	2.39	0.52
2:D:162:VAL:HG12	2:D:163:ILE:HG12	1.91	0.52
2:D:293:ILE:HG22	2:D:318:PRO:HA	1.92	0.52
1:A:29:LYS:HD2	1:A:97:ALA:O	2.10	0.51
1:A:201:THR:CG2	2:B:95:ARG:HD3	2.40	0.51
1:A:328:ASP:OD1	2:B:92:ARG:NH2	2.41	0.51
2:B:240:LYS:HA	2:B:243:MET:CG	2.39	0.51
1:C:56:ARG:CD	1:C:57:VAL:N	2.57	0.51
2:D:262:ARG:O	2:D:265:VAL:HG13	2.10	0.51
2:D:245:GLU:HA	2:D:248:LEU:HD22	1.93	0.51
1:A:56:ARG:HH22	1:A:333:GLU:CB	2.24	0.51
1:A:85:ILE:CD1	1:A:86:GLU:H	2.22	0.51
1:A:266:LYS:O	1:A:270:ARG:CG	2.55	0.51
2:D:288:ASP:HB3	2:D:350:ARG:CZ	2.40	0.51
1:A:29:LYS:HD3	1:A:97:ALA:HA	1.92	0.51
1:A:164:TYR:C	1:A:164:TYR:CD2	2.87	0.51
1:C:61:LYS:HZ1	1:C:68:HIS:CD2	2.27	0.51
2:D:300:VAL:C	2:D:301:LEU:HD23	2.36	0.51
1:A:211:LEU:CD1	1:A:213:LYS:H	2.24	0.51
2:D:113:ARG:NH1	2:D:149:ASP:OD2	2.36	0.51
1:A:46:ILE:HD12	1:A:47:LYS:CB	2.39	0.51
1:A:79:VAL:O	1:A:84:GLN:OE1	2.29	0.51
1:A:92:LYS:CE	1:A:350:PHE:CD2	2.94	0.51
1:A:197:TPO:O2P	1:A:197:TPO:N	2.43	0.51
1:A:294:HIS:ND1	1:A:295:LYS:N	2.59	0.51
2:B:236:SER:HA	2:B:239:ARG:HG2	1.92	0.51
1:C:315:ILE:O	1:C:315:ILE:HD12	2.10	0.51
2:D:113:ARG:NH1	2:D:149:ASP:CB	2.74	0.51
1:A:111:LYS:NZ	1:A:116:LEU:CD2	2.74	0.51
1:A:131:HIS:O	1:A:135:ILE:CD1	2.56	0.51
2:B:353:PHE:C	2:B:353:PHE:CD2	2.88	0.51
2:D:182:VAL:HG23	2:D:190:THR:O	2.11	0.51
1:A:128:MET:HE2	1:A:172:LEU:HB2	1.91	0.51
1:A:243:PRO:O	1:A:247:TYR:CE2	2.64	0.51
2:B:275:GLU:OE1	2:B:275:GLU:C	2.53	0.51
2:B:295:GLU:HG3	2:B:344:LYS:CE	2.41	0.51
2:D:116:ILE:HD12	2:D:151:MET:O	2.11	0.51
2:D:233:LEU:CD1	2:D:233:LEU:N	2.74	0.51
1:A:48:THR:HG23	1:A:48:THR:O	2.09	0.51
1:C:146:TYR:O	1:C:150:ILE:HG12	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:174:ILE:HD12	1:C:174:ILE:C	2.36	0.51
2:D:182:VAL:O	2:D:188:TRP:HZ3	1.93	0.51
2:D:252:SER:OG	2:D:253:ILE:N	2.44	0.51
1:A:158:HIS:HE1	1:A:220:ASP:OD2	1.94	0.51
2:D:282:VAL:HB	2:D:285:GLU:HG3	1.92	0.51
2:B:179:GLU:HB3	2:B:216:LYS:CD	2.41	0.50
1:C:92:LYS:HG3	1:C:93:ARG:H	1.75	0.50
1:C:124:ALA:O	1:C:327:PHE:HE2	1.95	0.50
2:D:151:MET:HE1	2:D:223:GLY:C	2.35	0.50
2:D:153:PRO:HG3	2:D:222:TRP:CZ3	2.46	0.50
2:D:258:ASP:HB2	2:D:261:GLU:HG3	1.94	0.50
1:A:46:ILE:CG1	1:A:47:LYS:H	2.23	0.50
1:A:61:LYS:NZ	1:A:66:GLY:CA	2.64	0.50
2:B:151:MET:HA	2:B:224:ILE:HG13	1.93	0.50
2:B:300:VAL:HG22	2:B:314:GLY:O	2.11	0.50
2:B:330:ASN:HA	2:B:350:ARG:NH2	2.25	0.50
1:C:140:GLU:O	1:C:141:PRO:C	2.52	0.50
2:D:133:ASN:ND2	2:D:200:GLU:OE1	2.43	0.50
2:D:140:ASP:OD2	2:D:140:ASP:C	2.53	0.50
2:D:172:PHE:C	2:D:173:TYR:HD1	2.18	0.50
2:D:295:GLU:HB2	2:D:344:LYS:HB2	1.92	0.50
1:A:102:PHE:HE1	1:A:179:TYR:CD1	2.28	0.50
2:B:93:ARG:HB2	2:B:93:ARG:CZ	2.42	0.50
2:D:113:ARG:CG	2:D:114:LYS:N	2.74	0.50
2:D:136:PHE:N	2:D:136:PHE:HD2	2.07	0.50
2:B:179:GLU:HB3	2:B:216:LYS:CE	2.41	0.50
1:C:264:ASP:O	1:C:267:ASP:N	2.44	0.50
2:B:161:THR:HA	2:B:214:LYS:HG2	1.93	0.50
2:B:179:GLU:HB3	2:B:216:LYS:HD2	1.94	0.50
2:B:243:MET:HE1	2:B:294:LEU:HD22	1.94	0.50
1:A:184:ASP:HB2	3:A:400:ADP:O1A	2.11	0.50
2:B:243:MET:HE1	2:B:294:LEU:CD2	2.42	0.50
1:C:86:GLU:OE2	1:C:87:HIS:CD2	2.65	0.50
1:A:140:GLU:HB2	1:A:141:PRO:HD3	1.93	0.50
1:A:247:TYR:O	1:A:251:VAL:HG23	2.12	0.50
1:C:30:TRP:CZ2	1:C:190:ARG:CD	2.95	0.50
1:C:89:LEU:HD11	1:C:349:GLU:CG	2.41	0.50
1:C:264:ASP:O	1:C:265:LEU:C	2.55	0.50
2:D:112:VAL:HG12	2:D:113:ARG:O	2.12	0.50
1:A:111:LYS:NZ	1:A:350:PHE:CZ	2.80	0.50
1:A:135:ILE:CD1	1:A:138:PHE:HE1	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:ASP:HA	1:A:217:LYS:HE2	1.94	0.50
1:A:211:LEU:HD12	1:A:211:LEU:C	2.37	0.50
1:A:274:GLN:HG2	1:A:279:LYS:CB	2.42	0.50
2:B:171:ASN:OD1	2:B:172:PHE:O	2.29	0.50
2:B:245:GLU:OE1	2:B:262:ARG:HB2	2.11	0.49
2:B:281:VAL:CG2	2:B:337:VAL:HG12	2.42	0.49
2:B:311:VAL:HG23	2:B:312:GLU:H	1.77	0.49
2:B:353:PHE:O	2:B:356:VAL:CG2	2.60	0.49
2:B:151:MET:HG3	2:B:224:ILE:HD11	1.93	0.49
1:C:90:ASN:HD21	1:C:189:LYS:CA	2.19	0.49
2:D:98:ILE:HG13	2:D:98:ILE:O	2.10	0.49
2:B:179:GLU:C	2:B:216:LYS:HE3	2.37	0.49
2:B:181:ASP:OD1	2:B:214:LYS:HB2	2.11	0.49
2:B:311:VAL:HG22	2:B:312:GLU:N	2.26	0.49
2:D:126:LEU:HD13	2:D:148:PHE:CD2	2.47	0.49
2:B:148:PHE:HD2	2:B:151:MET:CE	2.26	0.49
1:C:183:THR:OG1	1:C:184:ASP:N	2.45	0.49
1:C:195:THR:OG1	1:C:197:TPO:O2P	2.29	0.49
2:B:325:ILE:HD12	2:B:331:ARG:HH21	1.77	0.49
2:D:173:TYR:CA	2:D:222:TRP:O	2.60	0.49
2:D:183:TYR:CD2	2:D:188:TRP:HA	2.47	0.49
2:D:250:LYS:O	2:D:250:LYS:HG2	2.08	0.49
1:A:334:GLU:CB	2:D:260:TRP:CH2	2.96	0.49
2:B:201:LEU:HD21	2:B:205:TYR:CZ	2.48	0.49
1:C:215:TYR:CD1	1:C:219:VAL:HG11	2.48	0.49
1:C:235:TYR:CD1	1:C:235:TYR:N	2.81	0.49
2:D:162:VAL:HG21	2:D:180:MET:SD	2.53	0.49
1:A:39:GLN:HG3	1:A:40:LEU:N	2.28	0.49
1:A:46:ILE:HD11	1:A:59:LEU:CD1	2.39	0.49
1:A:176:GLN:NE2	1:A:177:GLN:OE1	2.38	0.49
1:A:211:LEU:CD1	1:A:211:LEU:C	2.86	0.49
1:C:201:THR:O	1:C:205:LEU:HD13	2.12	0.49
1:C:194:ARG:HE	2:D:241:ARG:NH2	2.10	0.49
2:B:173:TYR:HA	2:B:222:TRP:O	2.13	0.49
2:B:180:MET:N	2:B:216:LYS:HE3	2.27	0.49
1:C:115:ASN:ND2	1:C:337:VAL:HG22	2.28	0.48
1:A:59:LEU:C	1:A:59:LEU:CD2	2.86	0.48
1:A:111:LYS:NZ	1:A:116:LEU:CD1	2.71	0.48
2:B:153:PRO:HB3	2:B:222:TRP:CZ3	2.48	0.48
2:B:161:THR:CA	2:B:214:LYS:HG2	2.43	0.48
2:B:190:THR:OG1	2:B:191:SER:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:23:LYS:HD2	1:C:160:LEU:HD23	1.94	0.48
1:C:48:THR:O	1:C:56:ARG:NH2	2.46	0.48
1:C:163:ILE:HD11	1:C:219:VAL:CG2	2.43	0.48
1:C:60:VAL:O	1:C:61:LYS:CD	2.62	0.48
2:D:136:PHE:HA	2:D:139:LEU:CD1	2.43	0.48
2:D:282:VAL:HB	2:D:285:GLU:HG2	1.96	0.48
1:A:148:ALA:CB	1:A:302:TRP:HZ3	2.24	0.48
1:C:285:LYS:HD3	2:D:357:LEU:HD13	1.96	0.48
2:D:176:ASP:OD2	2:D:220:LYS:HE2	2.14	0.48
2:D:180:MET:HB2	2:D:192:VAL:CG1	2.42	0.48
1:A:135:ILE:CD1	1:A:138:PHE:CE1	2.96	0.48
2:B:180:MET:SD	2:B:213:VAL:HG12	2.53	0.48
1:C:115:ASN:HD22	1:C:337:VAL:HG22	1.78	0.48
1:C:204:TYR:CZ	1:C:227:LEU:HD23	2.48	0.48
1:A:105:LYS:N	1:A:121:GLU:OE1	2.47	0.48
1:C:111:LYS:HB3	1:C:116:LEU:HD23	1.95	0.48
1:A:172:LEU:HD11	1:A:227:LEU:HD11	1.95	0.48
2:D:105:GLU:O	2:D:107:ASP:N	2.47	0.48
2:D:281:VAL:CG1	2:D:333:ARG:CZ	2.92	0.48
1:A:105:LYS:O	1:A:121:GLU:OE1	2.31	0.48
1:C:185:PHE:N	1:C:185:PHE:CD2	2.81	0.48
2:D:309:GLU:C	2:D:310:PHE:HD1	2.21	0.48
1:A:105:LYS:N	1:A:121:GLU:OE2	2.39	0.48
2:B:172:PHE:CD1	2:B:198:PHE:O	2.66	0.48
2:B:230:ARG:O	2:B:233:LEU:HD12	2.14	0.48
2:B:236:SER:HB2	2:B:239:ARG:NH2	2.29	0.48
1:C:47:LYS:N	1:C:58:MET:HE3	2.28	0.48
1:A:111:LYS:HZ2	1:A:116:LEU:CG	2.26	0.48
1:A:345:LYS:O	1:A:348:THR:HG23	2.13	0.48
1:C:93:ARG:HG3	1:C:94:ILE:HD12	1.96	0.48
1:C:135:ILE:HD11	1:C:138:PHE:CE2	2.49	0.48
2:D:94:ARG:HG2	2:D:94:ARG:NH1	2.28	0.48
2:D:136:PHE:C	2:D:138:HIS:N	2.65	0.48
2:D:280:ILE:HB	2:D:337:VAL:CG2	2.44	0.48
2:D:283:GLN:HE22	2:D:303:ARG:N	2.12	0.48
1:A:48:THR:CG2	1:A:330:TYR:CB	2.72	0.47
2:B:293:ILE:HD12	2:B:293:ILE:O	2.13	0.47
2:B:305:SER:C	2:B:308:GLU:OE1	2.57	0.47
1:C:30:TRP:CZ2	1:C:190:ARG:HD3	2.48	0.47
1:C:55:GLY:CA	1:C:74:LEU:HD23	2.40	0.47
2:D:269:LEU:HD23	2:D:348:LEU:HG	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:LEU:HD12	1:A:209:ILE:HG22	1.96	0.47
1:A:142:HIS:HE1	1:A:146:TYR:CE2	2.33	0.47
1:C:195:THR:C	1:C:196:TRP:CG	2.92	0.47
2:D:111:TYR:HD1	2:D:231:ARG:NH2	2.12	0.47
2:D:151:MET:CE	2:D:222:TRP:CA	2.92	0.47
2:D:354:GLU:HA	2:D:357:LEU:C	2.39	0.47
1:A:172:LEU:CD1	1:A:227:LEU:HD11	2.43	0.47
1:A:189:LYS:HZ3	1:A:195:THR:HG23	1.79	0.47
2:B:172:PHE:CE1	2:B:200:GLU:HG3	2.50	0.47
2:B:297:SER:N	2:B:343:LEU:HD11	2.30	0.47
1:A:104:VAL:HG13	1:A:182:VAL:O	2.14	0.47
2:B:308:GLU:HG3	2:B:309:GLU:OE2	2.14	0.47
1:C:46:ILE:N	1:C:58:MET:CE	2.78	0.47
2:D:272:VAL:CG1	2:D:347:LYS:CG	2.92	0.47
1:C:230:GLU:HA	1:C:235:TYR:O	2.15	0.47
1:C:244:ILE:O	1:C:248:GLU:HG2	2.14	0.47
2:D:93:ARG:O	2:D:93:ARG:CG	2.60	0.47
2:D:163:ILE:HD11	2:D:198:PHE:HE1	1.79	0.47
2:D:241:ARG:HH21	2:D:267:ASP:CG	2.23	0.47
2:D:260:TRP:CD1	2:D:261:GLU:HG2	2.49	0.47
1:A:39:GLN:HG3	1:A:40:LEU:H	1.79	0.47
1:A:92:LYS:HG3	1:A:93:ARG:H	1.77	0.47
1:A:311:GLU:HG2	1:A:311:GLU:O	2.14	0.47
2:B:274:PHE:CG	2:B:280:ILE:HD11	2.50	0.47
1:C:185:PHE:O	1:C:186:GLY:C	2.57	0.47
1:C:235:TYR:HB2	1:C:236:PRO:HD2	1.95	0.47
1:C:265:LEU:CD1	1:C:296:TRP:CE2	2.98	0.47
1:C:271:ASN:HB3	1:C:281:PHE:CD2	2.49	0.47
1:C:329:ASP:C	1:C:330:TYR:CG	2.93	0.47
2:D:115:VAL:HG22	2:D:149:ASP:HB3	1.96	0.47
2:D:147:ILE:C	2:D:149:ASP:N	2.71	0.47
2:D:173:TYR:CD1	2:D:223:GLY:HA2	2.50	0.47
2:D:221:LEU:CD1	2:D:223:GLY:N	2.78	0.47
2:D:301:LEU:HD23	2:D:312:GLU:HA	1.96	0.47
2:D:357:LEU:HD13	2:D:357:LEU:HA	1.73	0.47
1:A:131:HIS:HA	1:A:134:ARG:CD	2.45	0.47
1:A:271:ASN:HB3	1:A:281:PHE:CE2	2.49	0.47
2:B:236:SER:O	2:B:239:ARG:HG2	2.14	0.47
1:C:26:PHE:CE1	1:C:97:ALA:HB1	2.50	0.47
1:C:65:SER:OG	1:C:67:ASN:OD1	2.33	0.47
1:A:91:GLU:HG3	1:A:95:LEU:HD11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:PHE:CE1	1:A:133:ARG:NE	2.79	0.47
2:B:253:ILE:N	2:B:253:ILE:HD12	2.29	0.47
1:C:48:THR:CG2	1:C:332:GLU:HG2	2.42	0.47
2:D:344:LYS:C	2:D:345:CYS:SG	2.98	0.47
1:C:91:GLU:CG	1:C:186:GLY:HA2	2.45	0.47
1:C:119:VAL:O	1:C:119:VAL:HG22	2.13	0.47
2:D:294:LEU:HG	2:D:345:CYS:HA	1.97	0.47
1:A:48:THR:CG2	1:A:48:THR:O	2.62	0.46
1:A:92:LYS:CG	1:A:93:ARG:H	2.28	0.46
2:B:141:ASP:OD1	2:B:144:ARG:NH2	2.48	0.46
2:B:352:ARG:HA	2:B:355:ARG:NH2	2.30	0.46
1:C:287:GLY:O	1:C:290:ASP:CG	2.57	0.46
2:D:176:ASP:OD1	2:D:220:LYS:O	2.33	0.46
2:B:202:ALA:O	2:B:226:ARG:HD3	2.15	0.46
1:C:16:LYS:HA	1:C:19:LEU:HD23	1.98	0.46
1:C:40:LEU:HD23	1:C:112:ASP:OD2	2.15	0.46
1:C:61:LYS:HD2	1:C:67:ASN:O	2.15	0.46
1:C:167:LEU:CD2	1:C:227:LEU:CD1	2.83	0.46
1:C:179:TYR:CZ	1:C:308:ARG:HA	2.50	0.46
1:C:185:PHE:O	1:C:188:ALA:N	2.40	0.46
2:D:244:TYR:CZ	2:D:346:VAL:HG11	2.50	0.46
2:D:272:VAL:HG22	2:D:273:GLN:N	2.29	0.46
2:D:321:TYR:CE1	2:D:324:GLU:CG	2.99	0.46
2:B:156:PHE:HD1	2:B:160:GLU:OE2	1.98	0.46
1:C:32:THR:HG23	1:C:32:THR:O	2.16	0.46
1:C:50:GLY:C	1:C:56:ARG:CZ	2.88	0.46
1:C:164:TYR:CE2	1:C:166:ASP:C	2.91	0.46
1:C:307:GLN:HG3	1:C:307:GLN:O	2.15	0.46
2:D:220:LYS:HG3	2:D:220:LYS:O	2.14	0.46
2:D:238:LEU:HD23	2:D:238:LEU:HA	1.68	0.46
2:D:282:VAL:O	2:D:285:GLU:HB2	2.15	0.46
2:B:261:GLU:O	2:B:265:VAL:CG1	2.61	0.46
1:C:41:ASP:HB2	1:C:42:GLN:OE1	2.15	0.46
1:C:46:ILE:HG21	1:C:59:LEU:HD23	1.98	0.46
2:B:219:VAL:HG22	2:B:220:LYS:H	1.79	0.46
1:C:189:LYS:HE2	1:C:191:VAL:HG22	1.98	0.46
2:B:300:VAL:HG22	2:B:314:GLY:C	2.41	0.46
1:A:51:THR:HG22	1:A:52:GLY:N	2.30	0.46
1:A:118:MET:HE2	1:A:118:MET:HB2	1.83	0.46
2:B:308:GLU:CG	2:B:309:GLU:OE2	2.64	0.46
2:D:94:ARG:HG2	2:D:94:ARG:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:350:ARG:HG3	2:D:351:PRO:CD	2.38	0.46
1:C:111:LYS:O	1:C:112:ASP:OD1	2.34	0.46
2:B:157:ILE:HG12	2:B:160:GLU:OE1	2.16	0.46
2:B:243:MET:CE	2:B:244:TYR:HD2	2.26	0.46
1:C:23:LYS:HE3	1:C:160:LEU:HA	1.98	0.46
1:C:80:VAL:CG1	1:C:85:ILE:CD1	2.89	0.46
1:A:249:LYS:O	1:A:252:SER:OG	2.33	0.45
1:C:30:TRP:CE2	1:C:190:ARG:NH1	2.83	0.45
1:C:300:THR:HG23	1:C:300:THR:O	2.16	0.45
2:D:188:TRP:CH2	2:D:190:THR:CA	3.00	0.45
1:A:103:LEU:HA	1:A:182:VAL:HG22	1.97	0.45
1:A:111:LYS:HE2	1:A:350:PHE:CG	2.40	0.45
2:B:185:ASN:N	2:B:185:ASN:HD22	2.14	0.45
2:B:337:VAL:CG2	2:B:338:VAL:N	2.79	0.45
1:C:138:PHE:O	1:C:139:SEP:C	2.62	0.45
1:C:196:TRP:O	1:C:197:TPO:C	2.64	0.45
2:D:126:LEU:HD23	2:D:174:VAL:HG11	1.98	0.45
2:D:173:TYR:HB3	2:D:222:TRP:C	2.41	0.45
2:D:237:THR:O	2:D:238:LEU:C	2.58	0.45
1:A:116:LEU:HD13	1:A:116:LEU:HA	1.09	0.45
2:B:147:ILE:CD1	2:B:148:PHE:CD2	2.99	0.45
1:C:267:ASP:OD2	1:C:294:HIS:NE2	2.36	0.45
2:D:135:LEU:C	2:D:136:PHE:HD2	2.23	0.45
2:D:188:TRP:CE3	2:D:189:ALA:N	2.84	0.45
1:C:36:ASN:CG	1:C:36:ASN:O	2.58	0.45
2:D:290:PHE:C	2:D:291:PHE:CD1	2.95	0.45
2:D:321:TYR:CE1	2:D:324:GLU:HG2	2.51	0.45
1:A:54:PHE:O	1:A:78:LYS:HE2	2.16	0.45
1:A:96:GLN:HB3	1:A:106:LEU:HD23	1.98	0.45
1:A:111:LYS:HE2	1:A:350:PHE:CB	2.47	0.45
1:A:175:ASP:C	1:A:175:ASP:OD2	2.60	0.45
2:B:104:THR:OG1	2:B:105:GLU:N	2.50	0.45
2:D:247:PHE:CD1	2:D:247:PHE:N	2.84	0.45
2:B:243:MET:HE3	2:B:247:PHE:CE2	2.52	0.45
2:B:333:ARG:HD2	2:B:333:ARG:HA	1.72	0.45
1:C:67:ASN:CB	1:C:69:TYR:OH	2.64	0.45
1:C:91:GLU:OE2	1:C:185:PHE:N	2.49	0.45
1:C:349:GLU:CD	1:C:349:GLU:H	2.24	0.45
2:B:116:ILE:HG12	2:B:149:ASP:O	2.17	0.45
2:B:248:LEU:HD21	2:B:265:VAL:HG22	1.97	0.45
2:B:303:ARG:C	2:B:308:GLU:OE2	2.60	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:23:LYS:HG3	1:C:27:LEU:CD1	2.46	0.45
1:C:125:GLY:HA3	1:C:174:ILE:O	2.17	0.45
2:D:95:ARG:O	2:D:95:ARG:HG3	2.16	0.45
2:D:302:GLN:O	2:D:310:PHE:HA	2.17	0.45
1:A:160:LEU:HB2	1:A:162:LEU:HD11	1.95	0.45
1:A:344:GLY:O	1:A:348:THR:HG22	2.16	0.45
1:A:170:GLU:OE2	2:B:95:ARG:HG2	2.17	0.45
1:A:326:ASN:H	1:A:326:ASN:HD22	1.65	0.45
1:A:111:LYS:CD	1:A:116:LEU:HD13	2.47	0.45
2:B:305:SER:N	2:B:308:GLU:OE2	2.50	0.45
1:C:107:GLU:N	1:C:119:VAL:O	2.45	0.45
2:B:243:MET:HE2	2:B:244:TYR:CD2	2.42	0.44
1:C:68:HIS:CE1	1:C:321:PRO:CB	2.94	0.44
1:C:140:GLU:HB2	1:C:141:PRO:HD3	1.99	0.44
1:C:182:VAL:CG1	1:C:183:THR:N	2.80	0.44
2:D:111:TYR:HD1	2:D:231:ARG:HD2	1.72	0.44
2:D:148:PHE:O	2:D:151:MET:HB3	2.16	0.44
2:D:258:ASP:OD2	2:D:260:TRP:CE2	2.70	0.44
2:B:281:VAL:H	2:B:337:VAL:HG13	1.81	0.44
1:C:194:ARG:HG3	2:D:241:ARG:NH1	2.32	0.44
2:D:136:PHE:O	2:D:138:HIS:N	2.50	0.44
2:D:201:LEU:O	2:D:201:LEU:HG	2.17	0.44
1:A:75:ASP:HB3	1:A:78:LYS:CG	2.44	0.44
1:A:195:THR:O	1:A:215:TYR:CD2	2.71	0.44
2:B:116:ILE:CG1	2:B:118:LYS:NZ	2.78	0.44
2:B:348:LEU:HD23	2:B:352:ARG:HD3	1.99	0.44
1:C:16:LYS:CG	1:C:17:GLU:N	2.78	0.44
1:A:129:PHE:CE1	1:A:133:ARG:HG3	2.53	0.44
1:A:307:GLN:HE21	1:A:309:LYS:CD	2.31	0.44
2:B:182:VAL:HG22	2:B:211:ALA:HB1	2.00	0.44
2:B:269:LEU:HB3	2:B:346:VAL:HB	1.99	0.44
1:C:62:HIS:O	1:C:66:GLY:N	2.50	0.44
1:C:91:GLU:O	1:C:95:LEU:HB2	2.18	0.44
2:D:105:GLU:OE1	2:D:105:GLU:N	2.36	0.44
2:D:248:LEU:HD13	2:D:248:LEU:H	1.82	0.44
2:D:285:GLU:O	2:D:333:ARG:HG2	2.16	0.44
2:D:295:GLU:O	2:D:343:LEU:HD12	2.17	0.44
1:A:47:LYS:C	1:A:58:MET:HG2	2.43	0.44
2:B:182:VAL:HG12	2:B:190:THR:N	2.29	0.44
2:B:248:LEU:CD2	2:B:265:VAL:HG22	2.47	0.44
2:B:298:ALA:HB3	2:B:316:LEU:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:19:LEU:HG	1:C:20:ALA:H	1.81	0.44
1:C:75:ASP:CG	1:C:78:LYS:HG3	2.42	0.44
2:D:173:TYR:CD1	2:D:173:TYR:N	2.83	0.44
2:D:176:ASP:OD2	2:D:222:TRP:NE1	2.50	0.44
1:A:77:GLN:NE2	1:A:342:LYS:CE	2.81	0.44
1:A:133:ARG:NH2	1:A:230:GLU:OE1	2.35	0.44
1:A:280:ARG:O	1:A:284:LEU:HD13	2.18	0.44
2:B:255:GLU:C	2:B:257:LEU:H	2.25	0.44
2:D:174:VAL:HG22	2:D:197:SER:HB3	1.98	0.44
2:D:316:LEU:HB3	2:D:320:ASP:HB2	2.00	0.44
2:B:173:TYR:HD2	2:B:198:PHE:CE1	2.36	0.44
2:B:287:GLY:HA3	2:B:333:ARG:CZ	2.48	0.44
1:C:169:PRO:HA	1:C:172:LEU:CD1	2.33	0.44
2:D:116:ILE:HB	2:D:118:LYS:NZ	2.32	0.44
2:D:152:PHE:CE1	2:D:223:GLY:O	2.71	0.44
1:A:23:LYS:O	1:A:27:LEU:HD13	2.15	0.44
1:A:195:THR:CG2	1:A:196:TRP:N	2.81	0.44
2:B:259:LYS:HG3	2:B:262:ARG:NH2	2.30	0.44
1:C:48:THR:CA	1:C:58:MET:HG3	2.41	0.44
1:C:88:THR:OG1	1:C:89:LEU:N	2.51	0.44
2:D:274:PHE:HD2	2:D:278:GLN:CD	2.26	0.44
1:A:44:ASP:N	1:A:63:LYS:HZ3	2.15	0.44
1:A:62:HIS:HB2	1:A:69:TYR:HE1	1.82	0.44
1:A:75:ASP:HB3	1:A:78:LYS:HZ3	1.82	0.44
2:B:251:VAL:HG21	2:B:254:LEU:HD12	2.00	0.44
2:B:275:GLU:HA	2:B:342:PRO:HA	1.99	0.44
1:C:175:ASP:OD2	1:C:175:ASP:C	2.61	0.44
2:D:136:PHE:HA	2:D:139:LEU:HG	2.00	0.44
2:D:151:MET:HE2	2:D:222:TRP:CA	2.48	0.44
2:D:155:SER:OG	2:D:220:LYS:HA	2.18	0.44
2:D:176:ASP:CG	2:D:220:LYS:HG3	2.43	0.44
1:A:23:LYS:NZ	1:A:190:ARG:HH12	2.16	0.43
1:A:43:PHE:C	1:A:63:LYS:HZ1	2.25	0.43
1:C:165:ARG:HH21	1:C:189:LYS:HB2	1.82	0.43
1:C:230:GLU:HG3	1:C:235:TYR:HA	1.99	0.43
2:D:176:ASP:C	2:D:194:GLU:OE1	2.61	0.43
2:D:321:TYR:CE1	2:D:324:GLU:CD	2.92	0.43
2:D:350:ARG:O	2:D:353:PHE:HB3	2.18	0.43
1:A:138:PHE:CE2	1:A:231:MET:HE3	2.53	0.43
1:A:315:ILE:O	1:A:315:ILE:CD1	2.60	0.43
1:C:262:SER:O	1:C:266:LYS:HE2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:258:ASP:CG	2:D:260:TRP:CE2	2.96	0.43
1:A:79:VAL:HG22	1:A:84:GLN:NE2	2.32	0.43
1:A:131:HIS:CA	1:A:134:ARG:HG2	2.48	0.43
1:C:89:LEU:CD2	1:C:93:ARG:HD3	2.42	0.43
2:D:188:TRP:CZ2	2:D:191:SER:HB3	2.53	0.43
1:C:107:GLU:C	1:C:108:PHE:CG	2.96	0.43
1:C:327:PHE:N	1:C:327:PHE:CD2	2.86	0.43
2:D:166:GLY:O	2:D:208:PRO:HB3	2.17	0.43
1:A:48:THR:HA	1:A:58:MET:HG3	1.96	0.43
2:B:153:PRO:HA	2:B:221:LEU:O	2.19	0.43
1:C:180:ILE:HD13	1:C:180:ILE:HA	1.88	0.43
1:C:229:TYR:O	1:C:230:GLU:C	2.61	0.43
2:D:111:TYR:CE2	2:D:113:ARG:HA	2.53	0.43
2:B:164:GLN:O	2:B:167:ASP:HB2	2.18	0.43
2:B:254:LEU:O	2:B:257:LEU:HB2	2.19	0.43
2:D:204:ILE:H	2:D:204:ILE:HG12	1.60	0.43
1:A:75:ASP:H	1:A:78:LYS:NZ	2.17	0.43
1:C:92:LYS:CG	1:C:93:ARG:N	2.82	0.43
1:C:245:GLN:O	1:C:249:LYS:CB	2.66	0.43
1:A:46:ILE:HD12	1:A:47:LYS:CA	2.48	0.43
1:A:47:LYS:N	1:A:58:MET:CE	2.74	0.43
1:A:113:ASN:CG	1:A:338:SEP:O	2.62	0.43
1:A:131:HIS:C	1:A:134:ARG:HG2	2.44	0.43
1:C:211:LEU:HD13	1:C:213:LYS:HD2	2.00	0.43
1:A:61:LYS:HE2	1:A:66:GLY:CA	2.49	0.43
1:A:148:ALA:CB	1:A:302:TRP:CZ3	3.01	0.43
1:A:244:ILE:HD12	2:B:201:LEU:HB2	2.01	0.43
2:B:171:ASN:H	2:B:209:ARG:NH1	2.17	0.43
1:C:47:LYS:O	1:C:58:MET:CG	2.67	0.43
2:D:179:GLU:HA	2:D:192:VAL:O	2.18	0.43
2:D:240:LYS:O	2:D:244:TYR:CG	2.71	0.43
1:C:261:PHE:HB3	1:C:266:LYS:HG3	2.01	0.43
2:D:130:ILE:C	2:D:130:ILE:HD12	2.43	0.43
2:D:283:GLN:HG3	2:D:336:THR:N	2.34	0.43
2:B:225:ASP:OD1	2:B:227:ASP:HB3	2.19	0.42
2:B:233:LEU:O	2:B:237:THR:HG23	2.19	0.42
1:C:265:LEU:HD12	1:C:296:TRP:CE2	2.53	0.42
2:D:165:GLN:HB3	2:D:212:THR:OG1	2.18	0.42
2:D:259:LYS:CG	2:D:260:TRP:N	2.82	0.42
2:D:322:PHE:CE1	2:D:337:VAL:HG11	2.53	0.42
1:A:57:VAL:HG11	3:A:400:ADP:C8	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:LEU:HD11	1:A:185:PHE:CB	2.36	0.42
1:A:137:ARG:NH2	1:A:260:HIS:CD2	2.86	0.42
1:C:28:LYS:O	1:C:29:LYS:C	2.61	0.42
1:C:264:ASP:C	1:C:266:LYS:N	2.76	0.42
1:C:292:LYS:HA	1:C:302:TRP:CZ2	2.53	0.42
2:D:113:ARG:CG	2:D:114:LYS:H	2.32	0.42
2:D:272:VAL:HG12	2:D:347:LYS:HE2	1.91	0.42
1:A:111:LYS:HE3	1:A:350:PHE:HB3	2.01	0.42
1:A:131:HIS:HA	1:A:134:ARG:CG	2.49	0.42
1:C:51:THR:HG22	1:C:56:ARG:HD3	1.98	0.42
1:C:88:THR:C	1:C:90:ASN:N	2.77	0.42
1:C:96:GLN:N	1:C:106:LEU:CD2	2.75	0.42
1:C:96:GLN:HB2	1:C:106:LEU:HD11	2.01	0.42
2:D:135:LEU:HB2	2:D:136:PHE:HE2	1.83	0.42
2:D:221:LEU:C	2:D:221:LEU:CD1	2.88	0.42
1:A:215:TYR:N	1:A:215:TYR:HD2	2.18	0.42
1:A:335:ILE:HG23	1:A:335:ILE:O	2.19	0.42
2:B:167:ASP:O	2:B:209:ARG:HG2	2.19	0.42
1:C:131:HIS:O	1:C:132:LEU:C	2.63	0.42
1:C:230:GLU:HG3	1:C:235:TYR:CA	2.50	0.42
1:C:349:GLU:OE1	1:C:349:GLU:N	2.49	0.42
2:D:183:TYR:CD2	2:D:188:TRP:N	2.87	0.42
2:D:262:ARG:HH11	2:D:262:ARG:HG2	1.85	0.42
1:A:40:LEU:CA	1:A:43:PHE:HE1	2.30	0.42
1:C:185:PHE:O	1:C:187:PHE:N	2.52	0.42
2:D:288:ASP:CA	2:D:350:ARG:NH1	2.80	0.42
2:D:302:GLN:O	2:D:311:VAL:HG12	2.19	0.42
1:A:117:TYR:N	1:A:117:TYR:CD1	2.86	0.42
2:B:323:GLY:O	2:B:326:ALA:HB3	2.19	0.42
1:C:56:ARG:HH11	1:C:57:VAL:CA	2.33	0.42
1:C:75:ASP:OD1	1:C:77:GLN:N	2.53	0.42
2:D:252:SER:HG	2:D:253:ILE:HD12	1.73	0.42
2:D:272:VAL:CG2	2:D:273:GLN:N	2.82	0.42
1:A:286:ASN:HB2	1:A:290:ASP:OD1	2.19	0.42
1:C:94:ILE:HD12	1:C:94:ILE:N	2.34	0.42
2:D:147:ILE:O	2:D:151:MET:HB2	2.19	0.42
2:B:229:TYR:O	2:B:233:LEU:CD1	2.66	0.42
2:B:258:ASP:HA	2:B:262:ARG:HH12	1.83	0.42
2:B:301:LEU:HA	2:B:311:VAL:O	2.19	0.42
2:B:321:TYR:CD2	2:B:321:TYR:N	2.88	0.42
1:C:68:HIS:NE2	1:C:321:PRO:C	2.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:76:LYS:O	1:C:80:VAL:HG22	2.20	0.42
1:C:91:GLU:HG2	1:C:185:PHE:HB2	2.02	0.42
2:D:183:TYR:HE1	2:D:214:LYS:NZ	2.16	0.42
2:B:140:ASP:CG	2:B:141:ASP:H	2.27	0.42
2:B:248:LEU:N	2:B:248:LEU:CD1	2.82	0.42
1:C:179:TYR:CE1	1:C:308:ARG:HA	2.55	0.42
2:D:113:ARG:HG2	2:D:114:LYS:H	1.83	0.42
2:D:283:GLN:NE2	2:D:302:GLN:HA	2.35	0.42
2:D:301:LEU:HD22	2:D:312:GLU:HA	2.00	0.42
1:A:156:TYR:O	1:A:159:SER:OG	2.21	0.42
2:B:258:ASP:C	2:B:262:ARG:NH1	2.78	0.42
1:C:44:ASP:OD1	1:C:44:ASP:C	2.63	0.42
1:C:50:GLY:N	1:C:56:ARG:NH1	2.37	0.42
1:C:175:ASP:OD2	1:C:178:GLY:N	2.53	0.42
1:C:228:ILE:HG13	1:C:228:ILE:H	1.62	0.42
1:C:264:ASP:O	1:C:266:LYS:N	2.52	0.42
1:A:19:LEU:O	1:A:22:ALA:HB3	2.21	0.41
1:A:43:PHE:N	1:A:43:PHE:CD1	2.87	0.41
1:A:187:PHE:CZ	2:B:99:SER:OG	2.72	0.41
2:B:133:ASN:HB3	2:B:136:PHE:CD2	2.55	0.41
2:B:182:VAL:CG1	2:B:189:ALA:HB3	2.46	0.41
1:A:116:LEU:HD21	1:A:350:PHE:CE2	2.55	0.41
1:A:185:PHE:N	1:A:185:PHE:CD2	2.89	0.41
1:C:150:ILE:O	1:C:151:VAL:C	2.63	0.41
2:D:167:ASP:O	2:D:209:ARG:HG2	2.19	0.41
2:D:243:MET:O	2:D:244:TYR:C	2.63	0.41
1:A:113:ASN:HB2	1:A:340:ASN:O	2.20	0.41
1:A:176:GLN:HG3	1:A:177:GLN:CD	2.45	0.41
1:A:195:THR:CG2	1:A:196:TRP:H	2.31	0.41
1:C:82:LEU:O	1:C:83:LYS:HD3	2.20	0.41
1:C:196:TRP:CD1	1:C:196:TRP:N	2.88	0.41
2:D:316:LEU:HB3	2:D:320:ASP:CB	2.50	0.41
2:D:336:THR:CG2	2:D:337:VAL:N	2.83	0.41
2:B:236:SER:CA	2:B:239:ARG:NH1	2.78	0.41
1:C:75:ASP:OD1	1:C:76:LYS:N	2.54	0.41
1:C:89:LEU:HD11	1:C:349:GLU:HG2	2.01	0.41
1:C:91:GLU:CD	1:C:186:GLY:N	2.78	0.41
1:C:180:ILE:HG22	1:C:181:GLN:N	2.34	0.41
1:A:61:LYS:CE	1:A:66:GLY:C	2.84	0.41
1:A:142:HIS:CE1	1:A:313:PRO:HG2	2.56	0.41
1:A:160:LEU:CB	1:A:162:LEU:HD12	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:329:MET:O	2:B:350:ARG:NH2	2.53	0.41
1:C:16:LYS:HA	1:C:19:LEU:CD2	2.50	0.41
1:C:49:LEU:CA	1:C:56:ARG:HH22	2.33	0.41
1:C:146:TYR:HA	1:C:149:GLN:NE2	2.36	0.41
1:C:165:ARG:NH2	1:C:189:LYS:HB2	2.34	0.41
1:C:267:ASP:O	1:C:268:LEU:C	2.63	0.41
1:A:167:LEU:HG	1:A:227:LEU:HD13	2.02	0.41
1:C:79:VAL:HG13	1:C:88:THR:HG21	2.01	0.41
2:D:111:TYR:HD1	2:D:231:ARG:HH21	1.69	0.41
1:A:80:VAL:H	1:A:80:VAL:HG22	1.68	0.41
1:A:86:GLU:O	1:A:90:ASN:ND2	2.53	0.41
1:C:204:TYR:OH	1:C:227:LEU:HD23	2.21	0.41
1:C:210:ILE:HD13	1:C:250:ILE:HG21	2.02	0.41
2:D:152:PHE:O	2:D:222:TRP:CE3	2.70	0.41
1:A:129:PHE:CE1	1:A:133:ARG:CZ	2.97	0.41
1:A:222:TRP:CD1	1:A:222:TRP:C	2.98	0.41
2:B:161:THR:HA	2:B:214:LYS:HA	2.03	0.41
2:B:185:ASN:HB3	1:C:96:GLN:HG2	2.03	0.41
2:B:350:ARG:HG3	2:B:351:PRO:HD3	2.03	0.41
1:C:91:GLU:HG2	1:C:185:PHE:CB	2.51	0.41
1:A:146:TYR:O	1:A:150:ILE:HG12	2.21	0.41
1:A:154:PHE:CD1	1:A:220:ASP:OD2	2.74	0.41
1:A:170:GLU:OE2	2:B:95:ARG:NH1	2.54	0.41
1:A:189:LYS:NZ	1:A:195:THR:HG23	2.36	0.41
1:A:207:PRO:HG2	1:A:275:VAL:HG22	2.03	0.41
2:B:126:LEU:HA	2:B:126:LEU:HD23	1.74	0.41
2:B:188:TRP:CZ3	2:B:189:ALA:C	2.98	0.41
2:B:325:ILE:HD11	2:B:331:ARG:CD	2.46	0.41
1:C:19:LEU:HG	1:C:20:ALA:N	2.35	0.41
1:C:39:GLN:HB2	1:C:42:GLN:HE22	1.86	0.41
1:C:65:SER:O	1:C:67:ASN:ND2	2.54	0.41
1:C:89:LEU:CG	1:C:92:LYS:NZ	2.71	0.41
1:C:102:PHE:HE1	1:C:179:TYR:HB3	1.86	0.41
1:C:129:PHE:CE1	1:C:133:ARG:NE	2.88	0.41
1:C:132:LEU:HA	1:C:138:PHE:HE2	1.86	0.41
1:C:150:ILE:HG23	1:C:150:ILE:HD12	1.60	0.41
1:C:167:LEU:O	1:C:168:LYS:HB3	2.20	0.41
2:D:118:LYS:NZ	2:D:151:MET:O	2.26	0.41
2:D:294:LEU:HD11	2:D:346:VAL:CG1	2.42	0.41
2:D:294:LEU:HD11	2:D:346:VAL:HG22	2.02	0.41
1:C:245:GLN:HA	1:C:248:GLU:HG2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:261:PHE:HD2	1:C:261:PHE:HA	1.70	0.41
2:D:247:PHE:N	2:D:247:PHE:HD1	2.19	0.41
2:D:275:GLU:OE2	2:D:278:GLN:HB2	2.21	0.41
1:C:330:TYR:CD2	1:C:330:TYR:N	2.88	0.40
2:D:136:PHE:O	2:D:137:SER:C	2.64	0.40
1:A:175:ASP:OD1	1:A:181:GLN:NE2	2.54	0.40
1:A:286:ASN:O	1:A:287:GLY:C	2.60	0.40
2:B:219:VAL:CG2	2:B:220:LYS:H	2.31	0.40
1:C:132:LEU:HD21	1:C:230:GLU:HG2	2.02	0.40
2:B:270:GLU:HA	2:B:271:PRO:HD3	1.89	0.40
1:C:44:ASP:O	1:C:46:ILE:HG12	2.21	0.40
1:C:129:PHE:O	1:C:130:SER:C	2.65	0.40
2:D:349:ASP:OD2	2:D:349:ASP:C	2.64	0.40
1:A:87:HIS:HB3	1:A:186:GLY:O	2.22	0.40
2:B:243:MET:HG3	2:B:244:TYR:N	2.36	0.40
2:B:291:PHE:CD2	2:B:322:PHE:CE2	3.09	0.40
2:B:340:ARG:HA	2:B:340:ARG:HD3	1.71	0.40
1:C:68:HIS:NE2	1:C:321:PRO:CB	2.85	0.40
1:C:82:LEU:O	1:C:83:LYS:CD	2.70	0.40
1:C:82:LEU:C	1:C:83:LYS:HD3	2.46	0.40
1:C:133:ARG:HH22	2:D:95:ARG:NH2	2.08	0.40
1:C:261:PHE:C	1:C:266:LYS:HE2	2.47	0.40
2:D:258:ASP:CB	2:D:260:TRP:CE2	3.05	0.40
2:D:272:VAL:HG11	2:D:347:LYS:HG3	2.03	0.40
1:A:76:LYS:HB2	1:A:114:SER:O	2.21	0.40
1:A:229:TYR:C	1:A:229:TYR:CD1	2.99	0.40
2:B:172:PHE:HD1	2:B:198:PHE:O	2.04	0.40
2:B:324:GLU:H	2:B:324:GLU:CD	2.29	0.40
1:C:61:LYS:HD3	1:C:61:LYS:HA	1.74	0.40
1:C:265:LEU:HD13	1:C:296:TRP:CE2	2.56	0.40
2:D:171:ASN:O	2:D:202:ALA:HB3	2.21	0.40
2:D:176:ASP:OD1	2:D:220:LYS:HG2	2.21	0.40
2:D:198:PHE:N	2:D:198:PHE:CD2	2.89	0.40
2:D:253:ILE:HD12	2:D:253:ILE:H	1.87	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	333/350 (95%)	323 (97%)	10 (3%)	0	100	100
1	C	333/350 (95%)	296 (89%)	36 (11%)	1 (0%)	36	65
2	B	265/275 (96%)	255 (96%)	10 (4%)	0	100	100
2	D	264/275 (96%)	234 (89%)	30 (11%)	0	100	100
All	All	1195/1250 (96%)	1108 (93%)	86 (7%)	1 (0%)	48	79

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	229	TYR

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	278/302 (92%)	249 (90%)	29 (10%)	7	29
1	C	277/302 (92%)	232 (84%)	45 (16%)	2	14
2	B	212/230 (92%)	184 (87%)	28 (13%)	4	21
2	D	210/230 (91%)	170 (81%)	40 (19%)	1	9
All	All	977/1064 (92%)	835 (86%)	142 (14%)	3	18

All (142) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	LEU
1	A	32	THR
1	A	40	LEU
1	A	41	ASP
1	A	43	PHE
1	A	45	ARG
1	A	57	VAL
1	A	59	LEU
1	A	85	ILE
1	A	103	LEU
1	A	116	LEU
1	A	119	VAL
1	A	120	MET
1	A	135	ILE
1	A	163	ILE
1	A	174	ILE
1	A	177	GLN
1	A	199	CYS
1	A	201	THR
1	A	211	LEU
1	A	215	TYR
1	A	244	ILE
1	A	247	TYR
1	A	263	SER
1	A	290	ASP
1	A	300	THR
1	A	303	ILE
1	A	323	ASP
1	A	339	ILE
2	B	102	VAL
2	B	104	THR
2	B	116	ILE
2	B	130	ILE
2	B	151	MET
2	B	154	VAL
2	B	161	THR
2	B	182	VAL
2	B	185	ASN
2	B	192	VAL
2	B	194	GLU
2	B	197	SER
2	B	201	LEU
2	B	207	THR

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Mol	Chain	Res	Type
2	B	224	ILE
2	B	233	LEU
2	B	236	SER
2	B	243	MET
2	B	248	LEU
2	B	265	VAL
2	B	282	VAL
2	B	293	ILE
2	B	311	VAL
2	B	328	LEU
2	B	330	ASN
2	B	333	ARG
2	B	336	THR
2	B	348	LEU
1	C	15	VAL
1	C	34	SER
1	C	48	THR
1	C	51	THR
1	C	53	SER
1	C	56	ARG
1	C	64	GLU
1	C	72	LYS
1	C	80	VAL
1	C	83	LYS
1	C	86	GLU
1	C	92	LYS
1	C	95	LEU
1	C	103	LEU
1	C	111	LYS
1	C	116	LEU
1	C	119	VAL
1	C	120	MET
1	C	135	ILE
1	C	150	ILE
1	C	155	GLU
1	C	162	LEU
1	C	172	LEU
1	C	174	ILE
1	C	175	ASP
1	C	180	ILE
1	C	183	THR
1	C	205	LEU

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Mol	Chain	Res	Type
1	C	211	LEU
1	C	244	ILE
1	C	250	ILE
1	C	255	VAL
1	C	265	LEU
1	C	272	LEU
1	C	273	LEU
1	C	284	LEU
1	C	286	ASN
1	C	288	VAL
1	C	295	LYS
1	C	303	ILE
1	C	310	VAL
1	C	311	GLU
1	C	324	THR
1	C	340	ASN
1	C	348	THR
2	D	93	ARG
2	D	94	ARG
2	D	104	THR
2	D	115	VAL
2	D	136	PHE
2	D	152	PHE
2	D	154	VAL
2	D	161	THR
2	D	163	ILE
2	D	173	TYR
2	D	182	VAL
2	D	192	VAL
2	D	204	ILE
2	D	207	THR
2	D	209	ARG
2	D	213	VAL
2	D	219	VAL
2	D	224	ILE
2	D	233	LEU
2	D	237	THR
2	D	239	ARG
2	D	242	LYS
2	D	248	LEU
2	D	250	LYS
2	D	255	GLU

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Mol	Chain	Res	Type
2	D	257	LEU
2	D	264	THR
2	D	265	VAL
2	D	300	VAL
2	D	302	GLN
2	D	319	SER
2	D	324	GLU
2	D	325	ILE
2	D	330	ASN
2	D	336	THR
2	D	337	VAL
2	D	345	CYS
2	D	348	LEU
2	D	356	VAL
2	D	357	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	GLN
1	A	36	ASN
1	A	77	GLN
1	A	131	HIS
1	A	158	HIS
1	A	271	ASN
1	A	307	GLN
1	A	326	ASN
2	B	138	HIS
2	B	165	GLN
2	B	185	ASN
2	B	186	ASN
1	C	39	GLN
1	C	87	HIS
1	C	271	ASN
2	D	273	GLN
2	D	283	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues are modelled in this entry.

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
1	SEP	A	338	1	8,9,10	1.61	1 (12%)	7,12,14	1.29	1 (14%)
1	SEP	C	139	1	8,9,10	1.68	1 (12%)	7,12,14	1.21	1 (14%)
1	TPO	C	197	1	8,10,11	1.58	1 (12%)	10,14,16	2.41	1 (10%)
1	TPO	A	197	1	8,10,11	1.58	1 (12%)	10,14,16	2.35	1 (10%)
1	SEP	C	338	1	8,9,10	1.62	1 (12%)	7,12,14	1.62	1 (14%)
1	SEP	A	139	1	8,9,10	1.60	1 (12%)	7,12,14	1.61	1 (14%)

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
1	SEP	A	338	1	-	6/6/8/10	-
1	SEP	C	139	1	-	1/6/8/10	-
1	TPO	C	197	1	-	0/9/11/13	-
1	TPO	A	197	1	-	0/9/11/13	-
1	SEP	C	338	1	-	5/6/8/10	-
1	SEP	A	139	1	-	5/6/8/10	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	139	SEP	P-O1P	3.68	1.61	1.50
1	C	338	SEP	P-O1P	3.54	1.61	1.50
1	A	197	TPO	P-O1P	3.52	1.61	1.50
1	A	139	SEP	P-O1P	3.52	1.61	1.50
1	C	197	TPO	P-O1P	3.47	1.61	1.50
1	A	338	SEP	P-O1P	3.46	1.61	1.50

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	197	TPO	P-OG1-CB	-7.17	103.86	123.33
1	A	197	TPO	P-OG1-CB	-7.00	104.32	123.33
1	A	139	SEP	OG-CB-CA	3.88	111.92	108.14
1	C	338	SEP	OG-CB-CA	3.75	111.80	108.14
1	A	338	SEP	OG-CB-CA	2.77	110.84	108.14
1	C	139	SEP	OG-CB-CA	2.58	110.65	108.14

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	139	SEP	N-CA-CB-OG
1	A	139	SEP	C-CA-CB-OG
1	A	139	SEP	CB-OG-P-O1P
1	A	139	SEP	CB-OG-P-O2P
1	A	139	SEP	CB-OG-P-O3P
1	A	338	SEP	C-CA-CB-OG
1	A	338	SEP	CB-OG-P-O2P
1	A	338	SEP	CB-OG-P-O3P
1	C	139	SEP	C-CA-CB-OG
1	C	338	SEP	N-CA-CB-OG
1	C	338	SEP	CB-OG-P-O2P
1	C	338	SEP	CB-OG-P-O3P
1	A	338	SEP	CB-OG-P-O1P
1	C	338	SEP	CB-OG-P-O1P
1	A	338	SEP	CA-CB-OG-P
1	A	338	SEP	N-CA-CB-OG
1	C	338	SEP	CA-CB-OG-P

There are no ring outliers.

5 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	338	SEP	3	0
1	C	139	SEP	2	0
1	C	197	TPO	2	0
1	A	197	TPO	5	0
1	A	139	SEP	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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	ADP	C	400	-	28,29,29	1.44	5 (17%)	43,45,45	1.85	8 (18%)
3	ADP	A	400	-	28,29,29	1.43	5 (17%)	43,45,45	1.84	9 (20%)

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
3	ADP	C	400	-	-	6/16/32/32	0/3/3/3
3	ADP	A	400	-	-	3/16/32/32	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	400	ADP	C5-C4	4.79	1.47	1.39
3	C	400	ADP	C5-C4	4.79	1.47	1.39
3	A	400	ADP	C5-C6	2.76	1.48	1.41
3	C	400	ADP	C5-C6	2.73	1.48	1.41
3	A	400	ADP	C5-N7	-2.30	1.34	1.39
3	C	400	ADP	C8-N7	2.30	1.36	1.31
3	A	400	ADP	C8-N7	2.26	1.36	1.31
3	C	400	ADP	C5-N7	-2.24	1.35	1.39
3	C	400	ADP	PA-O3A	2.22	1.61	1.59
3	A	400	ADP	PA-O3A	2.05	1.61	1.59

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	400	ADP	C5-C4-N3	-6.14	118.26	126.72
3	A	400	ADP	C5-C4-N3	-6.03	118.41	126.72
3	C	400	ADP	N3-C4-N9	4.94	135.56	127.17
3	A	400	ADP	N3-C4-N9	4.80	135.33	127.17
3	A	400	ADP	C2-N3-C4	3.74	120.97	111.83
3	C	400	ADP	C2-N3-C4	3.74	120.97	111.83
3	A	400	ADP	C4-C5-N7	-3.51	106.57	110.58
3	C	400	ADP	C4-C5-N7	-3.35	106.75	110.58
3	A	400	ADP	N3-C2-N1	-3.13	123.85	128.58
3	C	400	ADP	N3-C2-N1	-3.12	123.87	128.58
3	A	400	ADP	C5-N7-C8	2.60	107.53	103.45
3	A	400	ADP	C4-N9-C8	2.50	108.36	105.74
3	C	400	ADP	C4-N9-C8	2.49	108.35	105.74
3	C	400	ADP	C5-N7-C8	2.45	107.31	103.45
3	A	400	ADP	C3'-C2'-C1'	2.28	105.78	101.46
3	C	400	ADP	C3'-C2'-C1'	2.11	105.46	101.46
3	A	400	ADP	C6-C5-N7	2.03	136.01	132.09

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	400	ADP	PA-O3A-PB-O2B
3	C	400	ADP	PA-O3A-PB-O3B
3	C	400	ADP	C5'-O5'-PA-O2A
3	A	400	ADP	PA-O3A-PB-O3B
3	C	400	ADP	C5'-O5'-PA-O1A
3	C	400	ADP	C5'-O5'-PA-O3A
3	A	400	ADP	PB-O3A-PA-O1A
3	A	400	ADP	PA-O3A-PB-O2B
3	C	400	ADP	PB-O3A-PA-O1A

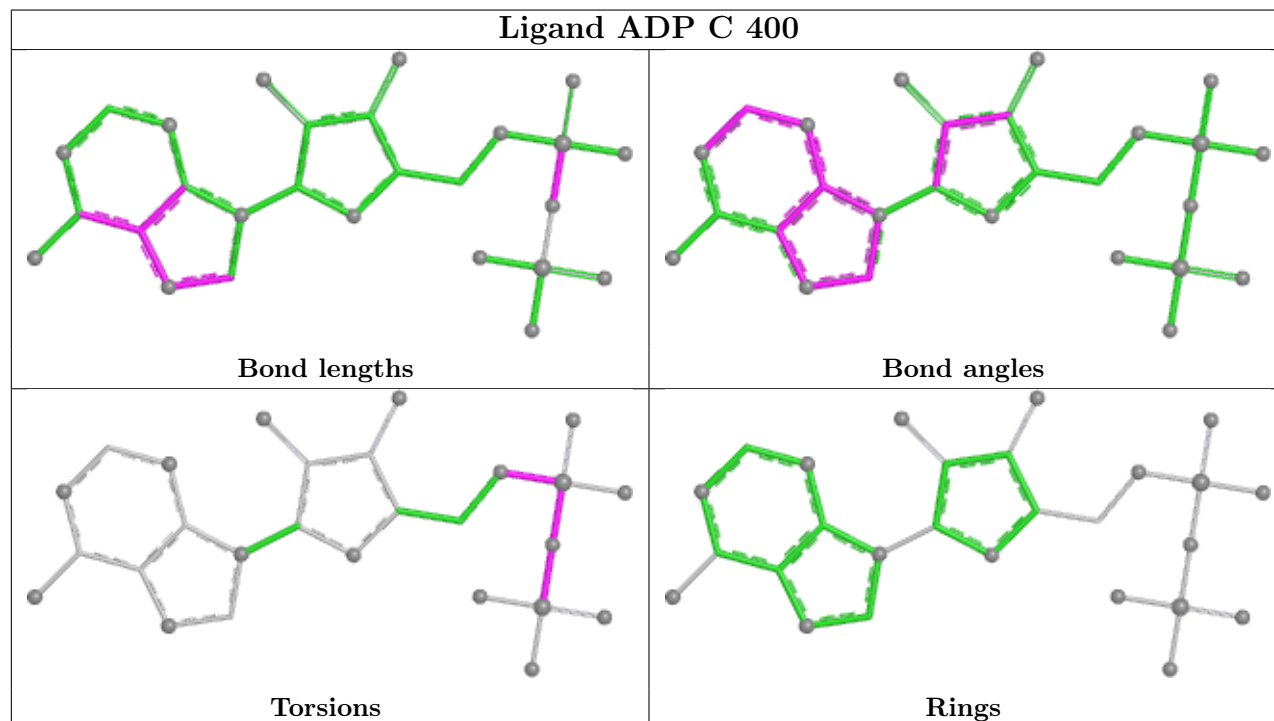
There are no ring outliers.

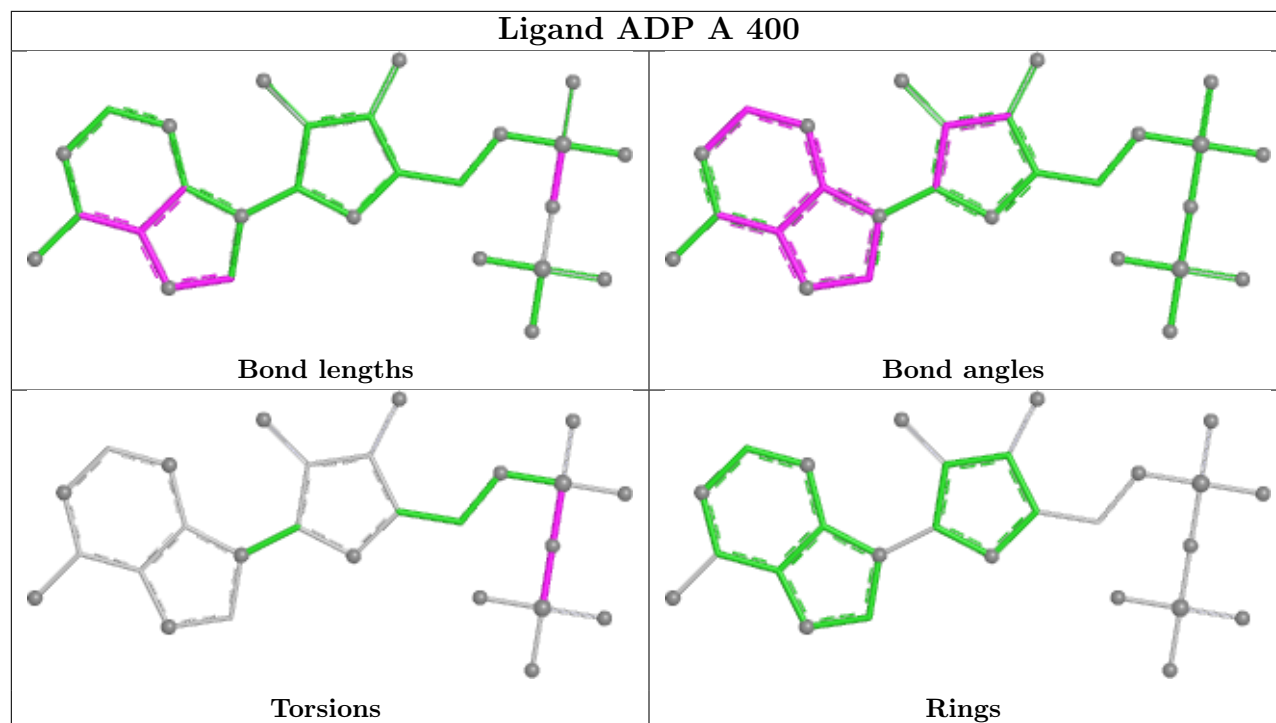
2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	400	ADP	1	0
3	A	400	ADP	5	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	335/350 (95%)	0.02	0 100 100	33, 84, 183, 220	1 (0%)
1	C	335/350 (95%)	0.03	3 (0%) 81 56	29, 101, 194, 292	0
2	B	267/275 (97%)	0.15	0 100 100	54, 100, 185, 222	1 (0%)
2	D	266/275 (96%)	0.09	0 100 100	47, 119, 214, 254	2 (0%)
All	All	1203/1250 (96%)	0.07	3 (0%) 91 80	29, 100, 196, 292	4 (0%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	334	GLU	2.1
1	C	322	GLY	2.0
1	C	71	MET	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	SEP	C	338	10/11	0.52	0.13	214,238,337,355	0
1	SEP	A	338	10/11	0.69	0.10	153,180,183,187	0
1	SEP	C	139	10/11	0.87	0.07	43,85,92,195	0
1	SEP	A	139	10/11	0.87	0.10	50,70,84,155	0
1	TPO	C	197	11/12	0.93	0.10	51,90,107,164	0
1	TPO	A	197	11/12	0.96	0.08	35,83,96,186	0

6.3 Carbohydrates [i](#)

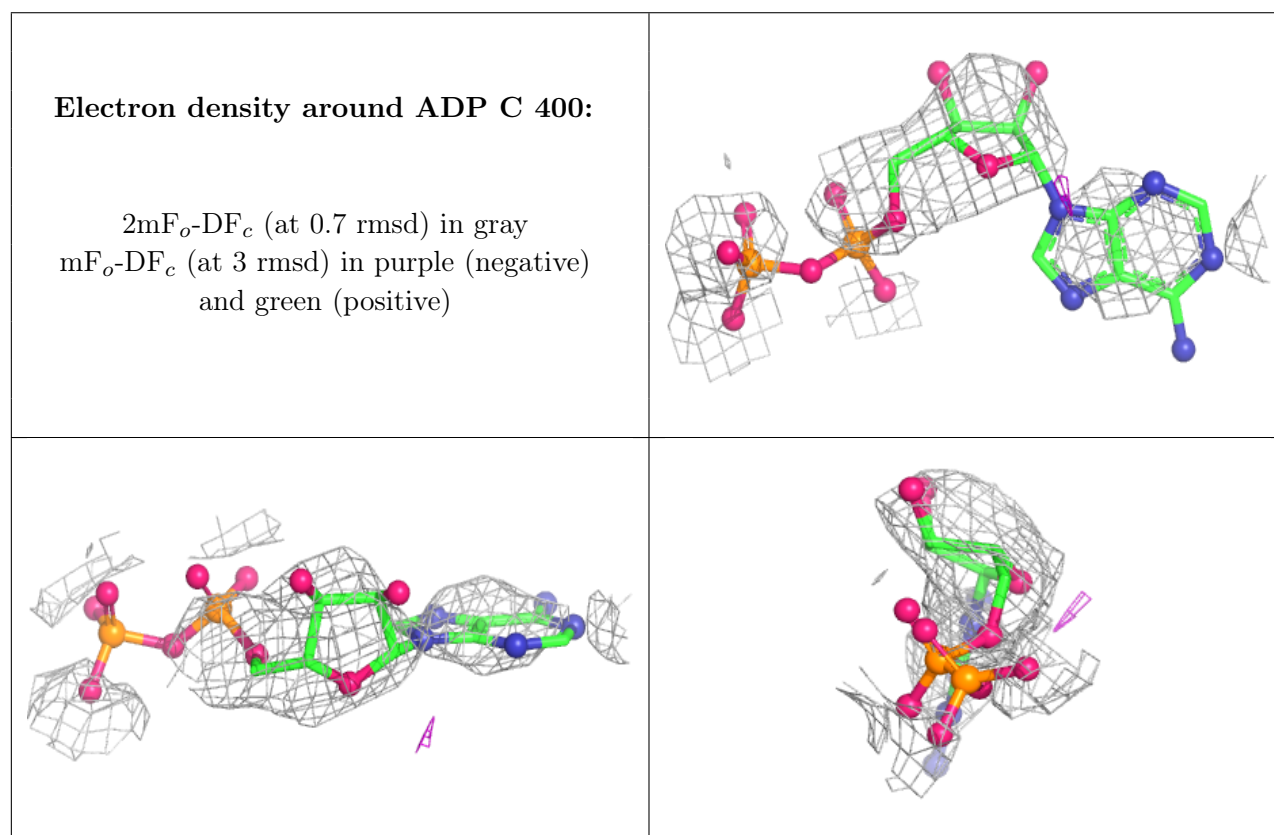
There are no oligosaccharides in this entry.

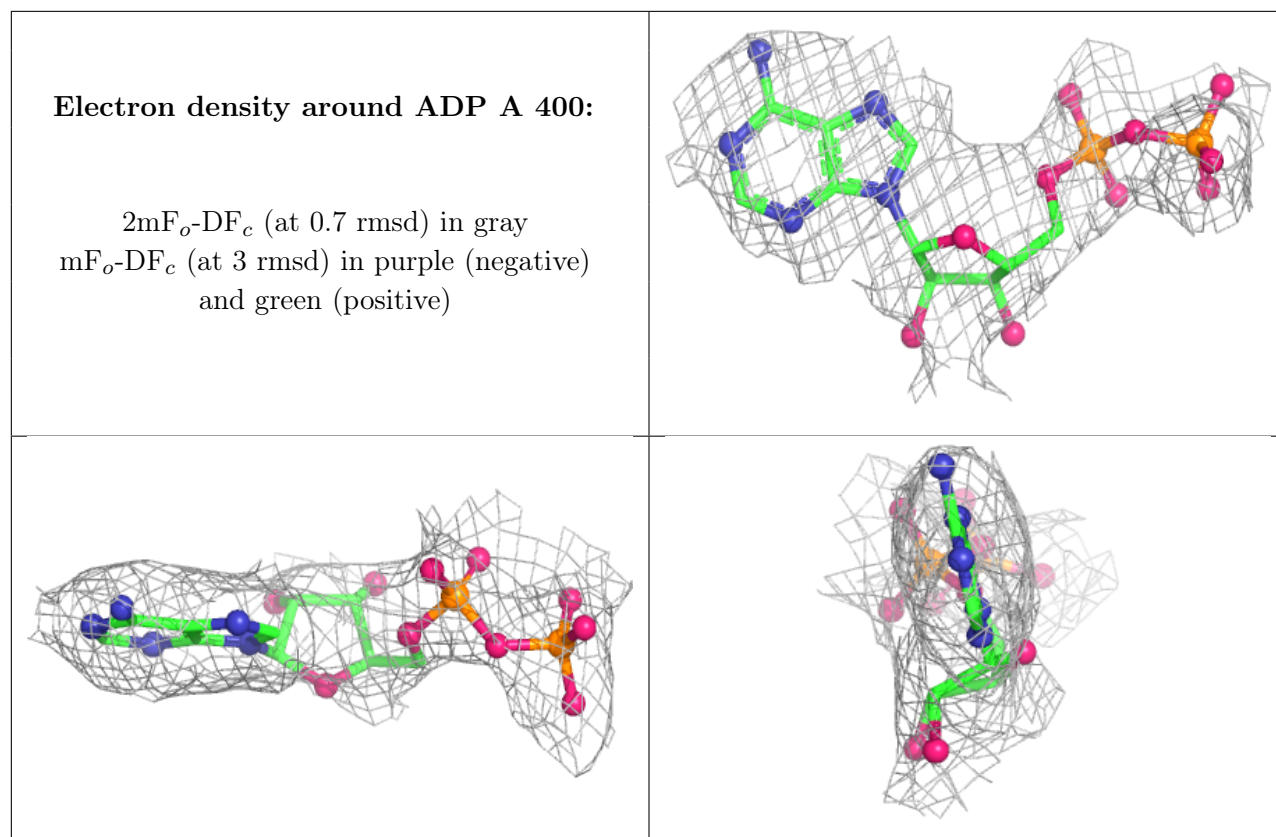
6.4 Ligands [i](#)

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	ADP	C	400	27/27	0.75	0.13	101,118,305,311	0
3	ADP	A	400	27/27	0.86	0.10	57,103,213,304	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.