



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:54 AM GMT

PDB ID : 2J7N
Title : STRUCTURE OF THE RNAI POLYMERASE FROM NEUROSPORA CRASSA
Authors : Salgado, P.S.; Koivunen, M.R.L.; Makeyev, E.V.; Bamford, D.H.; Stuart, D.I.; Grimes, J.M.
Deposited on : 2006-10-13
Resolution : 2.30 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

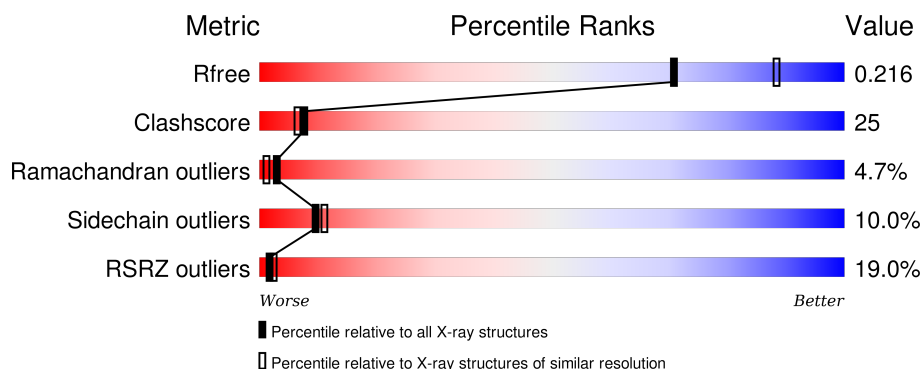
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	1022	<div> <div>15%</div> <div>62%</div> <div>23%</div> <div>6%</div> <div>•</div> <div>9%</div> </div>
1	B	1022	<div> <div>19%</div> <div>57%</div> <div>24%</div> <div>8%</div> <div>•</div> <div>9%</div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	B	3375	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15945 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called RNA-DEPENDENT RNA POLYMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	935	Total	C	N	O	S	0	0	1
			7520	4814	1304	1368	34			
1	B	932	Total	C	N	O	S	0	0	1
			7498	4798	1300	1366	34			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	559	ALA	GLY	CONFLICT	UNP Q9Y7G6
B	559	ALA	GLY	CONFLICT	UNP Q9Y7G6

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		

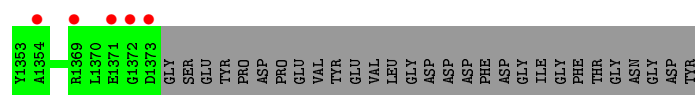
- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



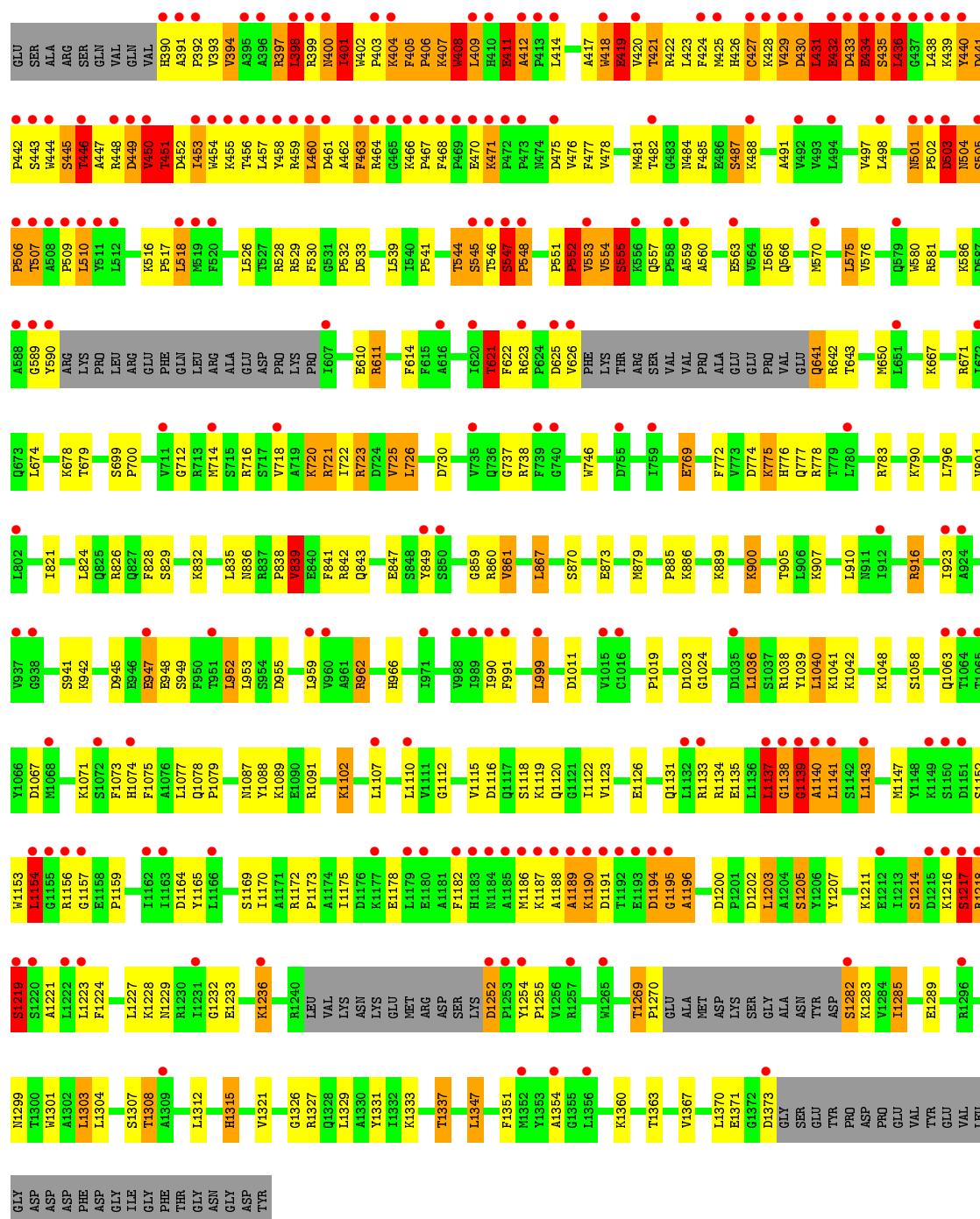
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			5	3	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	499	Total	O	0	0
			499	499		
4	B	421	Total	O	0	0
			421	421		



● Molecule 1: RNA-DEPENDENT RNA POLYMERASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	101.02Å 122.55Å 114.70Å 90.00° 108.90° 90.00°	Depositor
Resolution (Å)	19.98 – 2.30 19.97 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.7 (19.98-2.30) 97.7 (19.97-2.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 2.30Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.217 , 0.264 0.218 , 0.216	Depositor DCC
R_{free} test set	5728 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	45.5	Xtriage
Anisotropy	0.078	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 52.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 114162 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	15945	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 27.58 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 2.1432e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: GOL, MG

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	0.89	10/7713 (0.1%)	0.76	10/10439 (0.1%)
1	B	0.61	12/7689 (0.2%)	0.73	8/10407 (0.1%)
All	All	0.77	22/15402 (0.1%)	0.74	18/20846 (0.1%)

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
1	A	0	16
1	B	0	16
All	All	0	32

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	434	GLU	CD-OE2	50.04	1.80	1.25
1	A	434	GLU	CD-OE1	25.38	1.53	1.25
1	A	432	GLU	CD-OE1	16.68	1.44	1.25
1	A	436	LEU	C-N	16.11	1.62	1.33
1	B	435	SER	CB-OG	-13.76	1.24	1.42
1	B	436	LEU	C-N	11.41	1.53	1.33
1	A	434	GLU	C-O	10.18	1.42	1.23
1	B	432	GLU	CD-OE1	10.04	1.36	1.25
1	B	411	GLU	CD-OE2	9.22	1.35	1.25
1	A	434	GLU	CG-CD	7.65	1.63	1.51
1	A	1257	ARG	CZ-NH1	7.48	1.42	1.33
1	B	434	GLU	C-N	6.85	1.49	1.34
1	B	434	GLU	C-O	6.59	1.35	1.23
1	A	436	LEU	C-O	6.49	1.35	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1219	SER	CB-OG	6.37	1.50	1.42
1	A	435	SER	CA-CB	-6.22	1.43	1.52
1	B	440	TYR	CG-CD1	6.07	1.47	1.39
1	B	405	PHE	CG-CD2	5.69	1.47	1.38
1	A	435	SER	CB-OG	-5.41	1.35	1.42
1	B	436	LEU	C-O	5.39	1.33	1.23
1	B	440	TYR	CE1-CZ	5.32	1.45	1.38
1	B	405	PHE	CE1-CZ	5.00	1.46	1.37

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	434	GLU	OE1-CD-OE2	13.01	138.91	123.30
1	A	436	LEU	O-C-N	7.02	135.13	123.20
1	A	952	LEU	CA-CB-CG	6.91	131.20	115.30
1	A	1316	LYS	N-CA-C	-6.56	93.28	111.00
1	A	1283	LYS	N-CA-C	-6.52	93.40	111.00
1	A	432	GLU	OE1-CD-OE2	6.29	130.85	123.30
1	B	398	LEU	CA-CB-CG	6.26	129.69	115.30
1	B	433	ASP	CB-CG-OD1	6.24	123.92	118.30
1	A	436	LEU	CA-C-N	-6.06	104.09	116.20
1	B	1139	GLY	N-CA-C	-5.88	98.41	113.10
1	B	1154	LEU	CA-CB-CG	5.67	128.33	115.30
1	B	839	VAL	CB-CA-C	-5.65	100.66	111.40
1	B	962	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	A	798	LEU	CA-CB-CG	5.53	128.01	115.30
1	B	433	ASP	CB-CG-OD2	-5.43	113.41	118.30
1	B	952	LEU	CA-CB-CG	5.30	127.49	115.30
1	A	560	ALA	N-CA-C	5.21	125.06	111.00
1	A	459	ARG	N-CA-C	5.07	124.68	111.00

There are no chirality outliers.

All (32) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1138	GLY	Peptide
1	A	1139	GLY	Peptide
1	A	1213	ILE	Peptide
1	A	1217	SER	Peptide
1	A	1220	SER	Peptide
1	A	1252	ASP	Peptide
1	A	1282	SER	Peptide

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Mol	Chain	Res	Type	Group
1	A	1315	HIS	Peptide
1	A	456	THR	Peptide
1	A	504	ASN	Peptide
1	A	506	PRO	Peptide
1	A	545	SER	Peptide
1	A	547	SER	Peptide
1	A	555	SER	Peptide
1	A	559	ALA	Peptide
1	A	624	PRO	Peptide
1	B	1137	LEU	Peptide
1	B	1138	GLY	Peptide
1	B	1139	GLY	Peptide
1	B	1154	LEU	Peptide
1	B	1218	ARG	Peptide
1	B	1252	ASP	Peptide
1	B	1282	SER	Peptide
1	B	436	LEU	Mainchain
1	B	487	SER	Peptide
1	B	506	PRO	Peptide
1	B	545	SER	Peptide
1	B	547	SER	Peptide
1	B	552	PRO	Peptide
1	B	555	SER	Peptide
1	B	559	ALA	Peptide
1	B	641	GLN	Peptide

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	7520	0	7468	365	1
1	B	7498	0	7440	401	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	B	5	0	5	1	0
4	A	499	0	0	20	2
4	B	421	0	0	22	2
All	All	15945	0	14913	757	3

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 25.

All (757) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:431:LEU:CB	1:B:432:GLU:HB2	1.34	1.51
1:B:407:LYS:CB	1:B:408:TRP:HB3	1.41	1.51
1:A:641:GLN:CB	1:A:642:ARG:HB2	1.50	1.41
1:B:407:LYS:HB2	1:B:408:TRP:CB	1.47	1.41
1:B:431:LEU:HB3	1:B:432:GLU:CB	1.48	1.40
1:A:1184:ASN:N	1:A:1185:ALA:HB3	1.49	1.25
1:A:1193:GLU:HA	1:A:1194:ASP:O	1.37	1.25
1:B:462:ALA:HB3	1:B:463:PHE:O	1.29	1.24
1:A:399:ARG:CB	1:A:400:ASN:HB3	1.69	1.21
1:A:434:GLU:CD	1:A:434:GLU:OE2	1.80	1.19
1:A:1315:HIS:HB2	1:A:1316:LYS:CB	1.72	1.18
1:A:438:LEU:HA	1:A:439:LYS:CB	1.71	1.17
1:A:438:LEU:HA	1:A:439:LYS:HB3	1.18	1.15
1:B:418:TRP:CB	1:B:419:GLU:HB2	1.76	1.15
1:A:465:GLY:HA2	1:A:466:LYS:HB2	1.29	1.15
1:A:641:GLN:HB2	1:A:642:ARG:CB	1.77	1.14
1:A:399:ARG:HD2	1:A:507:THR:HG22	1.23	1.14
1:B:505:SER:CB	1:B:506:PRO:HD3	1.75	1.14
1:A:503:ASP:O	1:A:504:ASN:HB2	1.38	1.14
1:A:1210:PHE:O	1:A:1214:SER:HB2	1.47	1.14
1:A:393:VAL:HG23	1:A:394:VAL:HG23	1.14	1.13
1:B:461:ASP:N	1:B:462:ALA:HA	1.63	1.12
1:B:879:MET:HE3	1:B:885:PRO:HG3	1.25	1.12
1:A:439:LYS:HG3	1:A:440:TYR:H	1.06	1.11
1:B:505:SER:HB2	1:B:506:PRO:CD	1.81	1.10
1:A:1186:MET:H	1:A:1187:LYS:HB3	1.01	1.10
1:B:459:ARG:N	1:B:460:LEU:HB2	1.67	1.10
1:A:1315:HIS:CB	1:A:1316:LYS:HB2	1.81	1.10
1:A:723:ARG:HH11	1:A:723:ARG:HG2	0.99	1.07
1:A:439:LYS:HG3	1:A:440:TYR:N	1.65	1.07
1:A:1184:ASN:H	1:A:1185:ALA:CB	1.68	1.07
1:B:505:SER:HB3	1:B:506:PRO:HD3	1.32	1.06
1:B:403:PRO:HA	1:B:404:LYS:HB2	1.28	1.06
1:A:412:ALA:HB1	1:A:413:PRO:HA	1.37	1.06
1:A:438:LEU:CA	1:A:439:LYS:HB3	1.86	1.05
1:B:723:ARG:CG	1:B:723:ARG:HH11	1.70	1.05
1:B:829:SER:HA	1:B:832:LYS:HE3	1.05	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:418:TRP:HB3	1:B:419:GLU:HB2	1.04	1.04
1:A:1194:ASP:HB2	1:A:1195:GLY:HA2	1.36	1.02
1:B:1137:LEU:HB3	1:B:1138:GLY:HA3	1.37	1.02
1:B:545:SER:HA	1:B:546:THR:HG22	1.41	1.01
1:A:457:LEU:HB3	1:A:458:TYR:CB	1.90	1.01
1:B:505:SER:CB	1:B:506:PRO:CD	2.34	1.01
1:B:403:PRO:HA	1:B:404:LYS:CB	1.90	1.01
1:B:433:ASP:HB2	1:B:434:GLU:HB3	1.40	1.01
1:A:412:ALA:HB1	1:A:413:PRO:CA	1.90	1.00
1:B:450:VAL:H	1:B:451:THR:HB	1.27	0.99
1:B:723:ARG:NH1	1:B:723:ARG:HG2	1.65	0.99
1:A:399:ARG:HB3	1:A:400:ASN:CB	1.91	0.99
1:A:412:ALA:CB	1:A:413:PRO:HA	1.92	0.99
1:B:723:ARG:HH11	1:B:723:ARG:HG2	0.82	0.98
1:B:1188:ALA:N	1:B:1189:ALA:HB2	1.78	0.98
1:B:879:MET:HE3	1:B:885:PRO:CG	1.93	0.97
1:B:397:ARG:CG	1:B:397:ARG:HH21	1.77	0.96
1:B:460:LEU:N	1:B:461:ASP:HA	1.77	0.96
1:B:829:SER:CA	1:B:832:LYS:HE3	1.96	0.96
1:A:1220:SER:N	1:A:1221:ALA:HB3	1.80	0.96
1:A:399:ARG:HB3	1:A:400:ASN:HB3	0.96	0.96
1:A:624:PRO:HA	1:A:625:ASP:HB2	1.45	0.95
1:A:723:ARG:NH1	1:A:723:ARG:HG2	1.77	0.95
1:B:397:ARG:HG2	1:B:397:ARG:HH21	1.28	0.95
1:A:399:ARG:HA	1:A:399:ARG:HE	1.29	0.95
1:A:457:LEU:HB3	1:A:458:TYR:HB3	1.48	0.95
1:A:1186:MET:N	1:A:1187:LYS:HB3	1.83	0.94
1:B:451:THR:HB	1:B:452:ASP:HB2	1.49	0.94
1:B:452:ASP:O	1:B:454:TRP:N	2.00	0.94
1:A:1217:SER:CB	1:A:1221:ALA:HB2	1.97	0.94
1:A:1193:GLU:CA	1:A:1194:ASP:O	2.14	0.94
1:B:462:ALA:CB	1:B:463:PHE:O	2.15	0.93
1:B:418:TRP:HB3	1:B:419:GLU:CB	1.97	0.92
1:A:1194:ASP:CB	1:A:1195:GLY:HA2	1.98	0.92
1:B:403:PRO:CA	1:B:404:LYS:HB2	1.99	0.92
1:A:439:LYS:CG	1:A:440:TYR:N	2.33	0.91
1:A:1217:SER:OG	1:A:1221:ALA:HB2	1.70	0.91
1:B:1232:GLY:O	1:B:1236:LYS:HG3	1.72	0.90
1:A:1210:PHE:O	1:A:1214:SER:CB	2.21	0.89
1:A:395:ALA:HB1	1:A:396:ALA:HA	1.52	0.89
1:A:456:THR:HG22	1:A:457:LEU:HA	1.53	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:450:VAL:O	1:B:453:ILE:HB	1.73	0.88
1:A:393:VAL:H	1:A:394:VAL:C	1.77	0.88
1:A:399:ARG:CB	1:A:400:ASN:CB	2.48	0.87
1:A:838:PRO:HA	1:A:879:MET:HE1	1.55	0.87
1:A:1194:ASP:HB2	1:A:1195:GLY:CA	2.04	0.87
1:A:466:LYS:H	1:A:467:PRO:HA	1.39	0.87
1:B:1139:GLY:O	4:B:2339:HOH:O	1.90	0.87
1:A:1140:ALA:O	1:A:1141:LEU:O	1.94	0.86
1:B:451:THR:H	1:B:452:ASP:C	1.80	0.85
1:A:468:PHE:HA	1:A:469:PRO:O	1.76	0.85
1:A:559:ALA:CB	1:A:562:GLU:OE1	2.23	0.85
1:B:576:VAL:O	1:B:576:VAL:HG12	1.75	0.85
1:A:641:GLN:CB	1:A:642:ARG:CB	2.45	0.85
1:B:1112:GLY:O	1:B:1115:VAL:HG22	1.77	0.85
1:B:450:VAL:H	1:B:451:THR:CB	1.90	0.84
1:A:641:GLN:HB2	1:A:642:ARG:HB2	0.85	0.84
1:B:1137:LEU:HB3	1:B:1138:GLY:CA	2.08	0.84
1:A:922:MET:HE1	1:A:1011:ASP:HB3	1.59	0.84
1:B:431:LEU:CB	1:B:432:GLU:CB	2.25	0.84
1:A:879:MET:HE3	1:A:885:PRO:HG3	1.60	0.84
1:A:1217:SER:HB3	1:A:1221:ALA:HB2	1.59	0.84
1:A:723:ARG:HH11	1:A:723:ARG:CG	1.86	0.83
1:A:559:ALA:HB1	1:A:562:GLU:OE1	1.78	0.83
1:A:417:ALA:HB1	1:A:576:VAL:HG13	1.61	0.83
1:B:1134:ARG:O	4:B:2333:HOH:O	1.96	0.83
1:B:460:LEU:H	1:B:461:ASP:CA	1.92	0.83
1:A:454:TRP:O	1:A:458:TYR:HB3	1.77	0.83
1:A:457:LEU:HB3	1:A:458:TYR:HB2	1.60	0.83
1:B:463:PHE:HA	1:B:464:ARG:C	2.00	0.82
1:B:1041:LYS:O	1:B:1123:VAL:HG12	1.80	0.82
1:B:461:ASP:H	1:B:462:ALA:HA	1.43	0.81
1:A:438:LEU:CA	1:A:439:LYS:CB	2.52	0.81
1:A:423:LEU:HD11	1:A:458:TYR:CE1	2.16	0.81
1:B:418:TRP:CA	1:B:419:GLU:HB2	2.11	0.80
1:B:456:THR:N	1:B:457:LEU:O	2.14	0.80
1:B:460:LEU:N	1:B:461:ASP:CA	2.43	0.80
1:A:1315:HIS:HB2	1:A:1316:LYS:HB2	0.85	0.80
1:A:450:VAL:HG11	1:A:472:PRO:HD2	1.64	0.80
1:B:1218:ARG:N	1:B:1219:SER:HB3	1.95	0.80
1:B:1131:GLN:O	1:B:1135:GLU:HG3	1.82	0.80
1:B:829:SER:HA	1:B:832:LYS:CE	2.00	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:942:LYS:HD2	1:B:949:SER:OG	1.82	0.79
1:B:429:VAL:O	1:B:430:ASP:HB2	1.81	0.79
1:A:1186:MET:H	1:A:1187:LYS:CB	1.90	0.78
1:B:433:ASP:HA	1:B:434:GLU:HB2	1.64	0.78
1:B:460:LEU:HB3	1:B:462:ALA:HB2	1.64	0.78
1:B:419:GLU:H	1:B:422:ARG:HB2	1.48	0.78
1:B:1217:SER:HB3	1:B:1221:ALA:HB2	1.65	0.78
1:B:409:LEU:H	1:B:409:LEU:HD12	1.49	0.78
1:B:460:LEU:H	1:B:461:ASP:HB3	1.49	0.78
1:A:503:ASP:O	1:A:504:ASN:CB	2.25	0.78
1:A:1029:GLU:HB3	4:A:2359:HOH:O	1.82	0.78
1:B:407:LYS:CA	1:B:408:TRP:HB3	2.14	0.78
1:B:505:SER:HB2	1:B:506:PRO:HD2	1.62	0.77
1:A:453:ILE:O	1:A:454:TRP:HD1	1.66	0.77
1:B:1137:LEU:CB	1:B:1138:GLY:HA3	2.14	0.77
1:A:828:PHE:CD1	1:A:1178:GLU:HG2	2.19	0.77
1:A:393:VAL:HG23	1:A:394:VAL:CG2	2.07	0.77
1:A:412:ALA:HB2	4:A:2004:HOH:O	1.83	0.77
1:B:667:LYS:HE2	4:B:2033:HOH:O	1.85	0.77
1:B:431:LEU:HB2	1:B:432:GLU:HB2	1.61	0.77
1:A:1112:GLY:O	1:A:1115:VAL:HG22	1.84	0.77
1:B:459:ARG:CA	1:B:460:LEU:HB2	2.15	0.76
1:A:399:ARG:HB2	1:A:400:ASN:O	1.86	0.76
1:A:438:LEU:HA	1:A:439:LYS:HB2	1.66	0.76
1:B:390:HIS:CD2	1:B:566:GLN:HE22	2.02	0.76
1:B:714:MET:HE2	1:B:718:VAL:HG12	1.68	0.75
1:A:457:LEU:HD12	1:A:457:LEU:O	1.85	0.75
1:B:1269:THR:HG23	1:B:1270:PRO:HD2	1.67	0.75
1:B:836:ASN:HA	1:B:886:LYS:HD2	1.69	0.75
1:A:829:SER:HA	1:A:832:LYS:HE3	1.68	0.75
1:A:488:LYS:HG3	1:B:1373:ASP:N	2.01	0.75
1:B:400:ASN:O	1:B:402:TRP:N	2.20	0.75
1:A:796:LEU:HA	1:A:799:LEU:HD12	1.68	0.75
1:B:867:LEU:HD13	1:B:1326:GLY:HA3	1.66	0.75
1:A:576:VAL:O	1:A:576:VAL:HG12	1.86	0.75
1:A:423:LEU:HD21	1:A:458:TYR:HD1	1.52	0.74
1:B:879:MET:HE3	1:B:885:PRO:CD	2.17	0.74
1:B:433:ASP:HB2	1:B:434:GLU:CB	2.17	0.74
1:B:460:LEU:H	1:B:461:ASP:CB	2.00	0.74
1:B:723:ARG:HD3	1:B:730:ASP:C	2.08	0.74
1:B:801:VAL:HG23	4:B:2130:HOH:O	1.88	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:879:MET:CE	1:B:885:PRO:CD	2.66	0.74
1:B:400:ASN:CG	1:B:401:ILE:N	2.40	0.74
1:B:879:MET:CE	1:B:885:PRO:HD3	2.18	0.73
1:B:456:THR:H	1:B:457:LEU:CB	2.00	0.73
1:A:1315:HIS:ND1	4:A:2470:HOH:O	2.21	0.73
1:A:408:TRP:HZ3	1:A:431:LEU:O	1.71	0.73
1:A:393:VAL:CG2	1:A:394:VAL:HG23	2.08	0.73
1:B:1270:PRO:HG2	1:B:1289:GLU:HG3	1.69	0.73
1:A:1214:SER:HA	1:A:1217:SER:OG	1.89	0.72
1:A:879:MET:HE3	1:A:885:PRO:CG	2.20	0.72
1:B:1188:ALA:HB3	1:B:1189:ALA:HA	1.70	0.72
1:B:433:ASP:CB	1:B:434:GLU:HB3	2.18	0.72
1:A:465:GLY:CA	1:A:466:LYS:HB2	2.16	0.72
1:A:470:GLU:O	1:A:471:LYS:HB3	1.89	0.72
1:B:431:LEU:HB3	1:B:432:GLU:CA	2.19	0.72
1:B:451:THR:CB	1:B:452:ASP:HB2	2.20	0.72
1:A:705:GLU:OE2	1:A:1001:LYS:NZ	2.15	0.72
1:B:391:ALA:HB3	1:B:563:GLU:HG3	1.70	0.72
1:A:826:ARG:NH1	1:A:913:ARG:HH22	1.88	0.72
1:A:457:LEU:H	1:A:459:ARG:HB2	1.55	0.71
1:B:449:ASP:HB3	1:B:451:THR:HB	1.72	0.71
1:B:450:VAL:N	1:B:451:THR:CB	2.53	0.71
1:B:1139:GLY:HA3	1:B:1141:LEU:HB3	1.71	0.71
1:A:1253:PRO:HD2	1:A:1256:VAL:HB	1.72	0.71
1:A:457:LEU:N	1:A:459:ARG:HB2	2.06	0.71
1:B:398:LEU:HD13	1:B:510:LEU:HD23	1.71	0.70
1:A:879:MET:HE3	1:A:885:PRO:CD	2.22	0.70
1:B:435:SER:HB2	1:B:436:LEU:HB2	1.72	0.70
1:B:774:ASP:HB3	1:B:777:GLN:HG2	1.73	0.70
1:A:1184:ASN:N	1:A:1185:ALA:CB	2.41	0.70
1:B:576:VAL:O	1:B:576:VAL:CG1	2.40	0.70
1:B:1269:THR:CG2	4:B:2377:HOH:O	2.39	0.70
1:B:842:ARG:HD2	4:B:2168:HOH:O	1.92	0.70
1:B:626:VAL:O	1:B:626:VAL:HG13	1.91	0.70
1:B:1315:HIS:O	4:B:2386:HOH:O	2.09	0.70
1:A:465:GLY:HA2	1:A:466:LYS:CB	2.15	0.70
1:A:879:MET:CE	1:A:885:PRO:HD3	2.22	0.70
1:A:641:GLN:CA	1:A:642:ARG:HB2	2.21	0.69
1:A:395:ALA:HB1	1:A:396:ALA:CA	2.23	0.69
1:B:397:ARG:HG2	1:B:397:ARG:NH2	1.99	0.69
1:A:459:ARG:O	1:A:461:ASP:N	2.23	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:466:LYS:N	1:A:467:PRO:HA	2.06	0.69
1:B:433:ASP:HA	1:B:434:GLU:CB	2.21	0.69
1:A:1184:ASN:CA	1:A:1185:ALA:HB3	2.22	0.69
1:A:1344:ALA:HB1	1:B:1327:ARG:HD3	1.75	0.69
1:B:456:THR:H	1:B:457:LEU:HB2	1.57	0.69
1:A:1219:SER:C	1:A:1221:ALA:HB3	2.13	0.69
1:B:459:ARG:HB2	1:B:460:LEU:HD23	1.75	0.69
1:B:1337:THR:HG22	4:B:2395:HOH:O	1.93	0.69
1:B:491:ALA:HB1	1:B:532:PRO:HB3	1.75	0.68
1:B:433:ASP:CA	1:B:434:GLU:CB	2.72	0.68
1:A:408:TRP:CZ3	1:A:431:LEU:O	2.45	0.68
1:B:1304:LEU:O	1:B:1308:THR:CG2	2.41	0.68
1:B:461:ASP:N	1:B:462:ALA:CA	2.51	0.68
1:B:406:PRO:HB3	1:B:408:TRP:NE1	2.09	0.68
1:B:462:ALA:HB3	1:B:463:PHE:C	2.14	0.67
1:A:498:LEU:HD22	1:A:513:VAL:HG22	1.75	0.67
1:A:391:ALA:HB3	1:A:392:PRO:HA	1.75	0.67
1:B:546:THR:O	1:B:546:THR:HG23	1.94	0.67
1:B:424:PHE:HA	1:B:428:LYS:O	1.95	0.67
1:A:412:ALA:HB1	1:A:413:PRO:C	2.14	0.67
1:B:843:GLN:HG3	1:B:1363:THR:HG21	1.77	0.67
1:A:399:ARG:HB2	1:A:400:ASN:CB	2.23	0.67
1:B:1188:ALA:H	1:B:1189:ALA:HB2	1.59	0.67
1:B:1304:LEU:O	1:B:1308:THR:HG22	1.95	0.67
1:B:838:PRO:HA	1:B:879:MET:HE1	1.76	0.67
1:A:412:ALA:CB	1:A:413:PRO:CA	2.55	0.67
1:B:555:SER:HA	1:B:557:GLN:H	1.60	0.67
1:A:456:THR:O	1:A:459:ARG:HD2	1.95	0.67
1:A:397:ARG:O	1:A:398:LEU:HB2	1.93	0.66
1:B:547:SER:OG	1:B:548:PRO:HD3	1.95	0.66
1:A:453:ILE:O	1:A:454:TRP:CD1	2.48	0.66
1:A:828:PHE:CG	1:A:1178:GLU:HG2	2.29	0.66
1:B:403:PRO:HA	1:B:404:LYS:CG	2.25	0.66
1:B:456:THR:N	1:B:457:LEU:HB2	2.11	0.66
1:B:1159:PRO:HB3	1:B:1164:ASP:HB3	1.76	0.66
1:B:1217:SER:HB2	1:B:1218:ARG:C	2.16	0.66
1:B:505:SER:HB2	1:B:506:PRO:HD3	1.55	0.66
1:B:408:TRP:HE3	1:B:408:TRP:O	1.78	0.66
1:A:1217:SER:OG	1:A:1221:ALA:CB	2.44	0.66
1:B:509:PRO:O	1:B:510:LEU:HB3	1.96	0.66
1:A:1044:LYS:HD2	4:A:2207:HOH:O	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:ARG:NH2	4:A:2002:HOH:O	2.29	0.65
1:B:402:TRP:HB3	1:B:575:LEU:HD23	1.78	0.65
1:B:667:LYS:CE	4:B:2033:HOH:O	2.40	0.65
1:A:560:ALA:HB1	1:A:563:GLU:HB3	1.78	0.65
1:B:400:ASN:CG	1:B:401:ILE:H	1.98	0.65
1:A:418:TRP:CD1	1:A:518:LEU:HD13	2.32	0.65
1:B:462:ALA:H	1:B:463:PHE:C	1.99	0.65
1:A:836:ASN:OD1	1:A:886:LYS:HE3	1.96	0.65
1:B:450:VAL:HG12	1:B:451:THR:OG1	1.97	0.65
1:B:443:SER:H	1:B:445:SER:N	1.95	0.65
1:B:429:VAL:HG21	1:B:463:PHE:CZ	2.32	0.65
1:A:399:ARG:HD2	1:A:507:THR:CG2	2.13	0.65
1:B:406:PRO:HB3	1:B:408:TRP:CD1	2.32	0.65
1:B:879:MET:HE2	1:B:885:PRO:HD3	1.78	0.65
1:B:625:ASP:HB3	1:B:643:THR:CG2	2.27	0.64
1:A:942:LYS:HG3	1:A:949:SER:OG	1.97	0.64
1:B:461:ASP:O	1:B:464:ARG:HG3	1.97	0.64
1:A:796:LEU:HD12	1:A:797:GLN:N	2.12	0.64
1:B:429:VAL:O	1:B:430:ASP:CB	2.44	0.64
1:A:1220:SER:N	1:A:1221:ALA:CB	2.58	0.64
1:B:429:VAL:CG2	1:B:463:PHE:CZ	2.81	0.64
1:A:550:VAL:HG22	4:A:2058:HOH:O	1.96	0.63
1:B:444:TRP:H	1:B:453:ILE:HG13	1.63	0.63
1:B:394:VAL:HG21	1:B:560:ALA:HB1	1.80	0.63
1:B:450:VAL:N	1:B:451:THR:OG1	2.31	0.63
1:B:405:PHE:CE2	1:B:409:LEU:HD13	2.33	0.63
1:A:1180:GLU:HA	1:A:1180:GLU:OE1	1.99	0.63
1:B:1041:LYS:HB2	1:B:1123:VAL:HG13	1.80	0.62
1:A:605:LYS:H	1:A:605:LYS:HD2	1.63	0.62
1:A:423:LEU:HD11	1:A:458:TYR:HE1	1.63	0.62
1:A:565:ILE:HD13	1:A:1074:HIS:HA	1.81	0.62
1:B:836:ASN:OD1	1:B:886:LYS:HE3	1.98	0.62
1:A:1216:LYS:HE3	1:A:1216:LYS:HA	1.81	0.62
1:B:1203:LEU:O	1:B:1307:SER:HB2	2.00	0.62
1:B:393:VAL:HG22	1:B:394:VAL:H	1.64	0.61
1:A:626:VAL:N	1:A:627:PHE:HA	2.15	0.61
1:B:431:LEU:CA	1:B:432:GLU:HB2	2.27	0.61
1:B:431:LEU:CA	1:B:432:GLU:CB	2.79	0.61
1:B:516:LYS:HD3	1:B:517:PRO:HD2	1.83	0.61
1:B:418:TRP:CD1	1:B:518:LEU:HD13	2.35	0.61
1:A:1202:ASP:O	1:A:1205:SER:HB2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:390:HIS:CE1	1:A:566:GLN:HE22	2.18	0.61
1:A:879:MET:HE3	1:A:885:PRO:HD3	1.82	0.61
1:A:624:PRO:CA	1:A:625:ASP:HB2	2.27	0.61
1:A:408:TRP:CH2	1:A:438:LEU:HD13	2.36	0.60
1:A:457:LEU:O	1:A:460:LEU:HB2	2.01	0.60
1:B:460:LEU:HD12	1:B:462:ALA:HB1	1.82	0.60
1:A:412:ALA:HB3	1:A:413:PRO:HA	1.82	0.60
1:B:941:SER:HB2	4:B:2225:HOH:O	2.01	0.60
1:A:1207:TYR:CD2	1:A:1311:LYS:HG3	2.36	0.60
1:A:1300:THR:HA	1:A:1303:LEU:HD23	1.83	0.60
1:A:797:GLN:HG3	1:A:797:GLN:O	1.97	0.60
1:A:423:LEU:HD21	1:A:458:TYR:CD1	2.35	0.60
1:A:509:PRO:O	1:A:510:LEU:HB3	2.01	0.60
1:B:503:ASP:O	1:B:504:ASN:ND2	2.29	0.60
1:B:916:ARG:HH21	1:B:1019:PRO:CD	2.15	0.60
1:A:1186:MET:HB2	1:A:1187:LYS:HB2	1.82	0.60
1:B:393:VAL:O	1:B:394:VAL:HB	2.02	0.60
1:A:1184:ASN:CA	1:A:1185:ALA:CB	2.79	0.60
1:B:1207:TYR:HD1	1:B:1308:THR:HB	1.66	0.60
1:B:641:GLN:HB3	1:B:642:ARG:HG2	1.84	0.60
1:A:820:LEU:HD11	1:A:906:LEU:HD21	1.83	0.60
1:A:460:LEU:O	1:A:461:ASP:CB	2.49	0.60
1:A:922:MET:HE1	1:A:1011:ASP:CB	2.31	0.60
1:B:459:ARG:H	1:B:460:LEU:HB2	1.65	0.59
1:A:399:ARG:HA	1:A:399:ARG:NE	2.11	0.59
1:A:884:ASP:HB3	1:A:887:LYS:HB2	1.84	0.59
1:B:428:LYS:O	1:B:429:VAL:HG23	2.02	0.59
1:A:922:MET:HE2	1:A:1012:MET:C	2.23	0.59
1:A:453:ILE:HG22	1:A:453:ILE:O	2.02	0.59
1:A:393:VAL:N	1:A:394:VAL:O	2.25	0.59
1:A:491:ALA:HB1	1:A:532:PRO:HB3	1.84	0.59
1:A:1141:LEU:HD12	4:A:2421:HOH:O	2.02	0.59
1:A:835:LEU:HD13	1:A:841:PHE:CE1	2.38	0.58
1:B:879:MET:HE2	1:B:885:PRO:CD	2.32	0.58
1:A:723:ARG:NH1	1:A:724:ASP:OD1	2.33	0.58
1:B:1194:ASP:O	1:B:1196:ALA:N	2.35	0.58
1:B:671:ARG:HH22	1:B:1119:LYS:HZ2	1.51	0.58
1:B:1218:ARG:H	1:B:1219:SER:HB3	1.66	0.58
1:A:1285:ILE:O	1:A:1289:GLU:HB2	2.03	0.58
1:B:1147:MET:HA	1:B:1147:MET:CE	2.33	0.58
1:B:1042:LYS:HG2	1:B:1122:ILE:HG12	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:922:MET:CE	1:A:1012:MET:C	2.71	0.58
1:B:1227:LEU:HD13	1:B:1301:TRP:CZ2	2.38	0.58
1:B:1217:SER:HB2	1:B:1218:ARG:CA	2.34	0.58
1:B:417:ALA:O	1:B:421:THR:OG1	2.20	0.58
1:B:453:ILE:C	1:B:455:LYS:H	2.05	0.58
1:A:624:PRO:HA	1:A:625:ASP:CB	2.28	0.58
1:B:1333:LYS:O	1:B:1337:THR:HB	2.04	0.58
1:B:528:ARG:NH2	1:B:679:THR:O	2.37	0.57
1:B:723:ARG:CG	1:B:723:ARG:NH1	2.41	0.57
1:B:772:PHE:O	1:B:778:ARG:HD2	2.04	0.57
1:A:674:LEU:CD1	4:A:2095:HOH:O	2.53	0.57
1:A:509:PRO:O	1:A:510:LEU:CB	2.53	0.57
1:A:1259:ASN:O	1:A:1263:GLU:HG3	2.05	0.57
1:B:916:ARG:HH21	1:B:1019:PRO:HD3	1.69	0.57
1:A:820:LEU:CD1	1:A:906:LEU:HD21	2.35	0.57
1:A:1235:GLU:HG2	1:A:1313:TYR:CZ	2.39	0.57
1:B:400:ASN:O	1:B:401:ILE:HG12	2.05	0.57
1:A:439:LYS:HA	4:A:2013:HOH:O	2.04	0.57
1:A:861:VAL:HG13	1:A:873:GLU:HG2	1.86	0.57
1:B:431:LEU:HB3	1:B:432:GLU:HB2	0.60	0.57
1:A:456:THR:O	1:A:459:ARG:NH1	2.38	0.57
1:B:721:ARG:O	1:B:725:VAL:HG13	2.04	0.57
1:B:418:TRP:CA	1:B:419:GLU:CB	2.83	0.56
1:A:622:PHE:HA	1:A:642:ARG:O	2.05	0.56
1:A:879:MET:CE	1:A:885:PRO:CD	2.81	0.56
1:B:397:ARG:CG	1:B:397:ARG:NH2	2.49	0.56
1:B:589:GLY:H	1:B:611:ARG:HH21	1.53	0.56
1:B:419:GLU:H	1:B:422:ARG:CB	2.17	0.56
1:B:441:ASP:HB3	1:B:442:PRO:CA	2.36	0.56
1:B:450:VAL:CG1	1:B:451:THR:HA	2.35	0.56
1:A:454:TRP:O	1:A:458:TYR:CB	2.52	0.56
1:B:1285:ILE:HD12	1:B:1285:ILE:C	2.27	0.56
1:B:445:SER:O	1:B:446:THR:HG23	2.05	0.55
1:A:408:TRP:C	1:A:408:TRP:CD1	2.78	0.55
1:B:411:GLU:HG2	1:B:412:ALA:N	2.21	0.55
1:B:419:GLU:OE2	1:B:419:GLU:HA	2.07	0.55
1:B:400:ASN:C	1:B:401:ILE:HG12	2.27	0.55
1:A:1217:SER:OG	1:A:1221:ALA:N	2.40	0.55
1:B:1363:THR:O	1:B:1367:VAL:HG13	2.06	0.55
1:B:1116:ASP:HB3	1:B:1120:GLN:HG2	1.87	0.55
1:B:1172:ARG:HB3	1:B:1173:PRO:HD3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1315:HIS:HB2	1:A:1316:LYS:CA	2.36	0.55
1:B:769:GLU:HG3	4:B:2030:HOH:O	2.07	0.55
1:B:397:ARG:HG3	1:B:397:ARG:HH21	1.69	0.55
1:B:533:ASP:OD1	1:B:642:ARG:NH2	2.39	0.55
1:B:1270:PRO:HG3	1:B:1301:TRP:CD2	2.41	0.55
1:B:1327:ARG:HD2	1:B:1331:TYR:OH	2.07	0.55
1:A:547:SER:HB2	1:A:548:PRO:CA	2.35	0.55
1:B:408:TRP:CE3	1:B:408:TRP:C	2.80	0.55
1:A:393:VAL:N	1:A:394:VAL:C	2.54	0.55
1:A:395:ALA:CB	1:A:396:ALA:HA	2.31	0.54
1:B:456:THR:CA	1:B:457:LEU:HB2	2.37	0.54
1:A:813:ARG:HD2	4:A:2227:HOH:O	2.07	0.54
1:A:1193:GLU:N	1:A:1194:ASP:O	2.40	0.54
1:B:433:ASP:CA	1:B:434:GLU:HB2	2.35	0.54
1:A:399:ARG:CB	1:A:400:ASN:CA	2.85	0.54
1:B:1217:SER:CB	1:B:1218:ARG:HA	2.36	0.54
1:B:1024:GLY:HA3	4:B:2291:HOH:O	2.07	0.54
1:B:428:LYS:C	1:B:429:VAL:HG23	2.28	0.54
1:B:1269:THR:HG21	4:B:2377:HOH:O	2.03	0.54
1:A:899:GLN:OE1	1:A:899:GLN:HA	2.07	0.54
1:B:1036:LEU:HB3	1:B:1040:LEU:HD22	1.89	0.54
1:A:466:LYS:HB3	1:A:467:PRO:O	2.08	0.54
1:B:433:ASP:CB	1:B:434:GLU:CB	2.83	0.54
1:B:1120:GLN:OE1	1:B:1120:GLN:HA	2.07	0.54
1:A:1186:MET:N	1:A:1187:LYS:CB	2.60	0.54
1:A:470:GLU:HB2	4:A:2020:HOH:O	2.06	0.54
1:B:1269:THR:HG23	1:B:1270:PRO:CD	2.35	0.54
1:B:451:THR:N	1:B:452:ASP:C	2.55	0.54
1:B:1165:TYR:O	1:B:1169:SER:HB2	2.08	0.53
1:A:942:LYS:CG	1:A:949:SER:OG	2.56	0.53
1:B:484:ASN:O	1:B:485:PHE:HB2	2.08	0.53
1:A:397:ARG:O	1:A:398:LEU:CB	2.56	0.53
1:A:723:ARG:NH1	1:A:723:ARG:CG	2.53	0.53
1:A:838:PRO:HA	1:A:879:MET:CE	2.31	0.53
1:A:641:GLN:HB3	1:A:642:ARG:HB2	1.75	0.53
1:A:438:LEU:CB	1:A:439:LYS:HB3	2.38	0.53
1:A:1210:PHE:O	1:A:1213:ILE:HG22	2.08	0.53
1:B:406:PRO:CB	1:B:408:TRP:CD1	2.92	0.53
1:A:457:LEU:CB	1:A:458:TYR:CB	2.78	0.53
1:A:1213:ILE:O	1:A:1216:LYS:HB3	2.08	0.53
1:B:860:ARG:HA	1:B:1354:ALA:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:391:ALA:HB1	1:A:393:VAL:HG22	1.90	0.53
1:B:1089:LYS:HA	1:B:1107:LEU:HD13	1.91	0.53
1:A:793:GLY:HA2	1:A:914:VAL:H	1.73	0.53
1:A:399:ARG:CD	1:A:507:THR:HG22	2.16	0.53
1:A:1315:HIS:H	1:A:1315:HIS:CD2	2.26	0.53
1:A:1343:GLY:HA3	1:B:860:ARG:HD2	1.91	0.53
1:B:1038:ARG:HG2	1:B:1038:ARG:O	2.09	0.53
1:B:716:ARG:O	1:B:720:LYS:HG2	2.08	0.52
1:A:555:SER:OG	1:A:555:SER:O	2.21	0.52
1:A:580:TRP:HB3	1:A:614:PHE:HB3	1.90	0.52
1:A:1146:PRO:HB3	1:A:1148:TYR:CE2	2.44	0.52
1:B:394:VAL:HG21	1:B:560:ALA:CB	2.39	0.52
1:B:466:LYS:O	1:B:468:PHE:N	2.43	0.52
1:A:586:LYS:HG2	1:A:587:ASP:N	2.23	0.52
1:B:546:THR:HA	1:B:547:SER:HB3	1.92	0.52
1:A:883:PHE:CE2	1:A:1203:LEU:HD21	2.44	0.52
1:A:417:ALA:CB	1:A:576:VAL:HG13	2.37	0.52
1:B:916:ARG:HD2	1:B:945:ASP:OD2	2.09	0.52
1:B:408:TRP:CE3	1:B:408:TRP:O	2.63	0.52
1:B:545:SER:HA	1:B:546:THR:CG2	2.29	0.52
1:A:576:VAL:CG1	1:A:576:VAL:O	2.58	0.52
1:A:605:LYS:HD2	1:A:605:LYS:N	2.25	0.52
1:A:774:ASP:OD1	1:A:776:HIS:N	2.43	0.52
1:B:452:ASP:HA	1:B:455:LYS:HB2	1.92	0.52
1:A:456:THR:HG22	1:A:457:LEU:CA	2.33	0.52
1:B:829:SER:O	1:B:832:LYS:HG2	2.10	0.52
1:A:967:PHE:CD2	1:A:1031:PRO:HG3	2.45	0.52
1:A:427:CYS:O	1:A:428:LYS:HB2	2.10	0.52
1:A:458:TYR:CZ	1:A:465:GLY:O	2.64	0.51
1:A:451:THR:OG1	1:A:471:LYS:HE3	2.09	0.51
1:B:843:GLN:O	1:B:847:GLU:HG3	2.11	0.51
1:A:1203:LEU:O	1:A:1307:SER:HB2	2.10	0.51
1:B:1303:LEU:HD13	4:B:2381:HOH:O	2.10	0.51
1:A:1189:ALA:HB1	1:A:1195:GLY:HA3	1.92	0.51
1:A:439:LYS:O	1:A:440:TYR:HB2	2.11	0.51
1:A:890:TYR:CE2	1:A:894:ILE:HD11	2.45	0.51
1:A:1219:SER:CA	1:A:1221:ALA:HB3	2.41	0.51
1:A:828:PHE:CG	1:A:1178:GLU:CG	2.93	0.51
1:B:406:PRO:CB	1:B:408:TRP:NE1	2.74	0.51
1:B:1088:TYR:CE1	1:B:1143:LEU:HD22	2.46	0.51
1:B:622:PHE:HA	1:B:642:ARG:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:468:PHE:HB3	4:B:2007:HOH:O	2.10	0.51
1:A:1194:ASP:N	1:A:1194:ASP:OD2	2.43	0.51
1:B:450:VAL:HG12	1:B:451:THR:HA	1.92	0.51
1:B:403:PRO:HA	1:B:404:LYS:HG2	1.91	0.51
1:B:1189:ALA:O	1:B:1190:LYS:C	2.48	0.51
1:B:552:PRO:N	1:B:553:VAL:HB	2.26	0.51
1:B:462:ALA:N	1:B:463:PHE:C	2.63	0.51
1:A:1312:LEU:O	1:A:1315:HIS:CD2	2.64	0.51
1:B:1194:ASP:C	1:B:1196:ALA:H	2.13	0.51
1:B:923:ILE:HB	1:B:990:ILE:HD13	1.92	0.51
1:A:534:ARG:HD2	1:A:642:ARG:HD2	1.92	0.51
1:B:441:ASP:HB3	1:B:442:PRO:C	2.31	0.51
1:A:839:VAL:HG13	1:B:1351:PHE:CZ	2.45	0.51
1:B:456:THR:H	1:B:457:LEU:CA	2.23	0.51
1:B:449:ASP:O	1:B:477:PHE:CD2	2.63	0.51
1:B:411:GLU:O	1:B:412:ALA:HB3	2.11	0.51
1:B:1152:SER:O	1:B:1154:LEU:HD13	2.10	0.51
1:A:1129:TRP:CZ2	1:A:1133:ARG:HD3	2.46	0.51
1:A:391:ALA:HB3	1:A:392:PRO:CA	2.40	0.50
1:A:1335:GLN:HE21	3:B:3375:GOL:H2	1.76	0.50
1:B:1140:ALA:O	1:B:1141:LEU:O	2.28	0.50
1:A:1352:MET:O	1:B:842:ARG:NH2	2.43	0.50
1:B:714:MET:CE	1:B:718:VAL:HG12	2.39	0.50
1:A:450:VAL:HG12	1:A:471:LYS:HE2	1.94	0.50
1:B:503:ASP:O	1:B:504:ASN:HB3	2.11	0.50
1:B:1038:ARG:HD2	1:B:1039:TYR:CE2	2.47	0.50
1:B:407:LYS:CB	1:B:408:TRP:CB	2.37	0.50
1:B:443:SER:HA	1:B:444:TRP:C	2.32	0.50
1:B:1304:LEU:O	1:B:1308:THR:HG23	2.10	0.50
1:A:705:GLU:HG2	1:A:998:PRO:HD2	1.93	0.50
1:B:497:VAL:HG23	1:B:539:LEU:HB2	1.93	0.50
1:B:1252:ASP:OD2	1:B:1252:ASP:O	2.30	0.50
1:A:400:ASN:OD1	1:A:400:ASN:C	2.50	0.50
1:A:1328:GLN:O	1:A:1332:ILE:HG13	2.12	0.50
1:B:509:PRO:O	1:B:510:LEU:CB	2.58	0.49
1:A:558:PRO:O	1:A:559:ALA:C	2.50	0.49
1:A:1186:MET:CA	1:A:1187:LYS:CB	2.90	0.49
1:B:1023:ASP:HB2	4:B:2285:HOH:O	2.11	0.49
1:B:460:LEU:HD13	1:B:460:LEU:O	2.12	0.49
1:A:457:LEU:CB	1:A:458:TYR:HB3	2.33	0.49
1:B:1194:ASP:CG	1:B:1195:GLY:H	2.15	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:470:GLU:O	1:B:471:LYS:HB3	2.12	0.49
1:A:466:LYS:H	1:A:467:PRO:CA	2.18	0.49
1:A:904:ASP:HA	1:A:907:LYS:HE2	1.94	0.49
1:A:917:SER:HA	1:A:1015:VAL:O	2.12	0.49
1:A:667:LYS:HE2	1:A:1119:LYS:O	2.13	0.49
1:A:859:GLY:O	1:A:860:ARG:HB3	2.11	0.49
1:B:678:LYS:H	1:B:783:ARG:NH1	2.11	0.49
1:B:570:MET:HG3	1:B:570:MET:O	2.11	0.49
1:A:991:PHE:CD2	1:A:999:LEU:HB3	2.48	0.49
1:B:1200:ASP:OD1	1:B:1202:ASP:HB2	2.13	0.49
1:A:524:CYS:SG	1:A:527:THR:HG23	2.53	0.48
1:B:546:THR:HA	1:B:547:SER:CB	2.43	0.48
1:B:1112:GLY:O	1:B:1115:VAL:CG2	2.57	0.48
1:A:565:ILE:CD1	1:A:1074:HIS:HA	2.43	0.48
1:B:861:VAL:HG21	1:B:873:GLU:HG2	1.95	0.48
1:A:498:LEU:O	1:A:541:PRO:HD3	2.13	0.48
1:A:1300:THR:HA	1:A:1303:LEU:CD2	2.43	0.48
1:A:1317:SER:O	1:A:1321:VAL:HG12	2.13	0.48
1:B:1102:LYS:HG3	4:B:2324:HOH:O	2.13	0.48
1:A:458:TYR:CE2	1:A:465:GLY:O	2.67	0.48
1:B:453:ILE:C	1:B:455:LYS:N	2.67	0.48
1:B:1195:GLY:O	1:B:1196:ALA:HB3	2.13	0.48
1:B:551:PRO:C	1:B:553:VAL:HB	2.34	0.48
1:B:456:THR:HB	1:B:457:LEU:HB2	1.96	0.47
1:B:459:ARG:N	1:B:460:LEU:CB	2.58	0.47
1:B:454:TRP:HA	1:B:457:LEU:HD23	1.95	0.47
1:A:456:THR:O	1:A:459:ARG:CD	2.62	0.47
1:B:626:VAL:O	1:B:626:VAL:CG1	2.62	0.47
1:B:408:TRP:O	1:B:439:LYS:HG3	2.14	0.47
1:B:450:VAL:HG11	1:B:471:LYS:HG2	1.96	0.47
1:A:457:LEU:CB	1:A:458:TYR:HB2	2.40	0.47
1:A:1211:LYS:O	1:A:1214:SER:HB3	2.14	0.47
1:A:900:LYS:HB2	1:A:900:LYS:HE3	1.58	0.47
1:B:424:PHE:HD2	1:B:430:ASP:H	1.62	0.47
1:A:464:ARG:HD2	1:A:464:ARG:HA	1.70	0.47
1:B:448:ARG:HG2	1:B:478:VAL:HG22	1.97	0.47
1:B:529:ARG:HD3	1:B:776:HIS:CD2	2.49	0.47
1:A:791:SER:HB3	4:A:2214:HOH:O	2.13	0.47
1:A:458:TYR:N	1:A:459:ARG:C	2.68	0.47
1:A:1186:MET:CB	1:A:1187:LYS:HB2	2.45	0.47
1:A:723:ARG:NH2	1:B:947:GLU:HG2	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1119:LYS:HG3	1:B:1120:GLN:NE2	2.30	0.47
1:A:721:ARG:O	1:A:725:VAL:HG13	2.15	0.47
1:B:460:LEU:HD12	1:B:462:ALA:CB	2.45	0.47
1:B:1214:SER:HA	1:B:1217:SER:HA	1.96	0.47
1:A:1200:ASP:OD1	1:A:1202:ASP:HB2	2.15	0.47
1:A:774:ASP:C	1:A:774:ASP:OD1	2.53	0.47
1:B:407:LYS:H	1:B:408:TRP:HD1	1.63	0.47
1:A:464:ARG:HA	1:A:465:GLY:O	2.15	0.47
1:B:942:LYS:HD2	1:B:949:SER:CB	2.44	0.47
1:A:589:GLY:H	1:A:611:ARG:HH21	1.63	0.47
1:A:1217:SER:OG	1:A:1221:ALA:CA	2.64	0.46
1:B:1254:TYR:HB3	1:B:1255:PRO:HD3	1.97	0.46
1:A:1224:PHE:CE2	1:A:1228:LYS:HE3	2.50	0.46
1:A:444:TRP:CE2	1:A:453:ILE:HG23	2.50	0.46
1:A:466:LYS:N	1:A:467:PRO:CA	2.77	0.46
1:B:821:ILE:HG13	1:B:1170:ILE:HG23	1.97	0.46
1:A:622:PHE:CD1	1:A:622:PHE:N	2.84	0.46
1:A:1182:PHE:N	1:A:1182:PHE:CD2	2.83	0.46
1:A:395:ALA:HA	1:A:397:ARG:O	2.15	0.46
1:A:406:PRO:HG3	1:A:431:LEU:HB3	1.97	0.46
1:B:859:GLY:O	1:B:860:ARG:HB3	2.15	0.46
1:A:1169:SER:O	1:A:1173:PRO:HG2	2.15	0.46
1:A:712:GLY:O	1:A:746:TRP:HA	2.16	0.46
1:B:501:ASN:HD22	1:B:502:PRO:HD2	1.79	0.46
1:A:456:THR:C	1:A:459:ARG:HB2	2.36	0.46
1:B:433:ASP:OD2	1:B:438:LEU:HD11	2.16	0.46
1:B:447:ALA:HB3	1:B:453:ILE:HD11	1.98	0.46
1:A:458:TYR:H	1:A:459:ARG:C	2.19	0.46
1:B:503:ASP:HB3	1:B:504:ASN:H	1.45	0.46
1:B:459:ARG:HB2	1:B:460:LEU:HB2	1.98	0.46
1:A:723:ARG:HD3	1:A:730:ASP:C	2.36	0.46
1:B:1270:PRO:HG3	1:B:1301:TRP:CE3	2.50	0.46
1:A:456:THR:O	1:A:459:ARG:CZ	2.64	0.46
1:A:484:ASN:O	1:A:485:PHE:HB2	2.16	0.46
1:B:459:ARG:CB	1:B:460:LEU:HB2	2.46	0.46
1:A:966:HIS:ND1	1:A:1089:LYS:HE3	2.31	0.46
1:A:434:GLU:OE2	1:A:434:GLU:N	2.48	0.45
1:A:559:ALA:HB2	1:A:562:GLU:OE1	2.13	0.45
1:A:738:ARG:HD3	1:A:743:LYS:HG2	1.98	0.45
1:A:1185:ALA:H	1:A:1188:ALA:HB2	1.81	0.45
1:B:546:THR:O	1:B:546:THR:CG2	2.63	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:589:GLY:O	1:B:590:TYR:HB2	2.15	0.45
1:B:426:HIS:HA	1:B:427:CYS:HA	1.57	0.45
1:B:462:ALA:H	1:B:464:ARG:N	2.15	0.45
1:A:879:MET:HE2	1:A:885:PRO:HD3	1.95	0.45
1:B:1041:LYS:HB2	1:B:1123:VAL:CG1	2.45	0.45
1:B:503:ASP:O	1:B:504:ASN:CB	2.64	0.45
1:B:457:LEU:HA	1:B:458:TYR:HA	1.58	0.45
1:B:403:PRO:CB	1:B:404:LYS:HB2	2.45	0.45
1:B:839:VAL:HG22	4:B:2167:HOH:O	2.16	0.45
1:A:456:THR:O	1:A:459:ARG:HB2	2.16	0.45
1:B:557:GLN:HG3	1:B:557:GLN:O	2.17	0.45
1:A:1102:LYS:N	1:A:1103:PRO:HD2	2.32	0.45
1:B:621:THR:HG22	1:B:622:PHE:CD2	2.52	0.45
1:B:610:GLU:HG3	1:B:1077:LEU:HD22	1.99	0.45
1:A:399:ARG:HB2	1:A:400:ASN:CA	2.46	0.45
1:B:828:PHE:CD2	1:B:1178:GLU:HG2	2.51	0.45
1:A:1140:ALA:O	1:A:1141:LEU:C	2.54	0.45
1:B:966:HIS:ND1	1:B:1089:LYS:HE2	2.32	0.45
1:B:826:ARG:NH1	1:B:826:ARG:HB3	2.32	0.45
1:B:441:ASP:CB	1:B:442:PRO:HA	2.46	0.45
1:A:674:LEU:HD11	4:A:2095:HOH:O	2.17	0.45
1:A:952:LEU:HG	1:A:978:PHE:CD1	2.52	0.45
1:B:447:ALA:CB	1:B:453:ILE:HD11	2.47	0.44
1:A:391:ALA:CB	1:A:393:VAL:HG22	2.47	0.44
1:A:394:VAL:HA	1:A:395:ALA:HA	1.76	0.44
1:A:396:ALA:HB1	1:A:399:ARG:CZ	2.48	0.44
1:B:400:ASN:OD1	1:B:401:ILE:N	2.39	0.44
1:A:1182:PHE:HA	1:A:1185:ALA:CB	2.47	0.44
1:A:414:LEU:HD13	1:A:485:PHE:CZ	2.53	0.44
1:B:551:PRO:HB2	1:B:553:VAL:HG11	1.99	0.44
1:B:861:VAL:CG2	1:B:873:GLU:HG2	2.48	0.44
1:A:867:LEU:HD22	1:A:874:THR:HG23	1.99	0.44
1:B:407:LYS:HB2	1:B:408:TRP:HB3	0.56	0.44
1:B:451:THR:H	1:B:452:ASP:CA	2.31	0.44
1:A:1193:GLU:H	1:A:1194:ASP:C	2.20	0.44
1:A:883:PHE:CZ	1:A:1203:LEU:HD21	2.53	0.44
1:B:1063:GLN:CB	4:B:2306:HOH:O	2.65	0.44
1:A:959:LEU:HD22	1:A:1021:ILE:HG22	2.00	0.44
1:B:475:ASP:OD1	1:B:476:VAL:N	2.51	0.44
1:B:407:LYS:N	1:B:408:TRP:CD1	2.85	0.44
1:A:406:PRO:O	1:A:410:HIS:CD2	2.71	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:861:VAL:HG21	1:B:873:GLU:CG	2.47	0.44
1:A:1134:ARG:HG3	4:A:2232:HOH:O	2.16	0.44
1:A:1190:LYS:HG3	1:A:1191:ASP:H	1.81	0.44
1:A:839:VAL:HG22	4:A:2246:HOH:O	2.18	0.44
1:B:481:MET:HE3	4:B:2003:HOH:O	2.18	0.44
1:A:1184:ASN:H	1:A:1185:ALA:HB3	0.71	0.44
1:A:468:PHE:CA	1:A:469:PRO:O	2.56	0.44
1:B:1252:ASP:O	1:B:1252:ASP:CG	2.55	0.44
1:B:554:VAL:O	1:B:555:SER:C	2.55	0.44
1:B:737:GLY:C	1:B:738:ARG:HD2	2.38	0.44
1:B:443:SER:CA	1:B:444:TRP:C	2.85	0.44
1:A:624:PRO:CA	1:A:625:ASP:CB	2.93	0.44
1:A:931:GLU:OE2	1:A:994:LYS:NZ	2.51	0.44
1:B:841:PHE:HB3	1:B:879:MET:HE1	1.99	0.43
1:B:1217:SER:CB	1:B:1218:ARG:CA	2.94	0.43
1:B:429:VAL:HG22	1:B:463:PHE:CE2	2.53	0.43
1:A:1094:TYR:CE2	1:A:1146:PRO:HA	2.53	0.43
1:A:947:GLU:HG2	1:A:947:GLU:H	1.65	0.43
1:A:467:PRO:HB2	1:A:468:PHE:H	1.53	0.43
1:B:1289:GLU:O	1:B:1299:ASN:ND2	2.51	0.43
1:B:916:ARG:HD3	4:B:2284:HOH:O	2.17	0.43
1:B:551:PRO:HA	1:B:552:PRO:HD3	1.67	0.43
1:B:544:THR:HG21	1:B:1079:PRO:HD3	1.99	0.43
1:B:962:ARG:HD3	1:B:1011:ASP:HB3	2.00	0.43
1:B:772:PHE:O	1:B:778:ARG:CD	2.67	0.43
1:B:451:THR:N	1:B:452:ASP:CA	2.81	0.43
1:A:905:THR:HG23	1:A:909:LYS:HD2	2.01	0.43
1:A:665:HIS:HE1	4:A:2366:HOH:O	2.00	0.43
1:B:432:GLU:O	1:B:433:ASP:HB3	2.18	0.43
1:B:456:THR:O	1:B:456:THR:CG2	2.67	0.43
1:A:1299:ASN:O	1:A:1303:LEU:HD22	2.19	0.43
1:B:1073:PHE:O	1:B:1077:LEU:HG	2.18	0.43
1:B:428:LYS:O	1:B:429:VAL:CB	2.66	0.43
1:B:451:THR:CA	1:B:452:ASP:HB2	2.49	0.43
1:A:444:TRP:HZ2	1:A:456:THR:HG21	1.84	0.43
1:A:464:ARG:HA	1:A:465:GLY:C	2.38	0.43
1:A:835:LEU:HD13	1:A:841:PHE:CZ	2.54	0.43
1:B:498:LEU:O	1:B:541:PRO:HD3	2.19	0.43
1:B:1211:LYS:HB3	1:B:1211:LYS:HE2	1.86	0.43
1:B:900:LYS:HB2	1:B:900:LYS:HE3	1.64	0.43
1:B:420:VAL:C	1:B:422:ARG:H	2.22	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:852:ARG:O	1:A:856:VAL:HG23	2.19	0.43
1:B:1075:PHE:O	1:B:1078:GLN:HG2	2.19	0.43
1:A:444:TRP:CD1	1:A:453:ILE:HG23	2.53	0.43
1:A:457:LEU:C	1:A:457:LEU:HD12	2.35	0.43
1:A:1344:ALA:HB1	1:B:1327:ARG:CD	2.48	0.43
1:A:547:SER:CB	1:A:548:PRO:CA	2.96	0.43
1:B:1143:LEU:HD12	1:B:1143:LEU:HA	1.81	0.43
1:A:740:GLY:HA3	1:A:772:PHE:CE2	2.54	0.43
1:B:423:LEU:HD21	1:B:458:TYR:HE2	1.84	0.42
1:A:408:TRP:CH2	1:A:431:LEU:HD23	2.54	0.42
1:B:1139:GLY:HA2	1:B:1140:ALA:HB3	2.01	0.42
1:B:459:ARG:HB2	1:B:460:LEU:CB	2.49	0.42
1:A:399:ARG:HB2	1:A:400:ASN:C	2.38	0.42
1:A:460:LEU:O	1:A:461:ASP:HB3	2.19	0.42
1:A:654:LEU:HD12	4:A:2200:HOH:O	2.19	0.42
1:A:1222:LEU:HA	1:A:1222:LEU:HD12	1.86	0.42
1:B:1229:ASN:O	1:B:1233:GLU:HG3	2.19	0.42
1:B:429:VAL:HG12	1:B:430:ASP:H	1.83	0.42
1:B:991:PHE:CD2	1:B:999:LEU:HB3	2.54	0.42
1:B:530:PHE:CE2	1:B:650:MET:HG2	2.55	0.42
1:B:580:TRP:HB3	1:B:614:PHE:HB3	1.99	0.42
1:A:1190:LYS:HG3	1:A:1191:ASP:N	2.34	0.42
1:A:467:PRO:HG2	1:A:468:PHE:HD2	1.85	0.42
1:B:404:LYS:HD3	1:B:404:LYS:HA	1.76	0.42
1:B:1187:LYS:HE2	1:B:1187:LYS:HB3	1.89	0.42
1:A:419:GLU:OE1	1:A:422:ARG:HD3	2.20	0.42
1:A:454:TRP:HA	1:A:457:LEU:HD23	2.01	0.42
1:B:667:LYS:HB2	1:B:667:LYS:HE2	1.56	0.42
1:A:547:SER:CB	1:A:548:PRO:HA	2.50	0.42
1:B:441:ASP:HB2	1:B:444:TRP:CG	2.54	0.42
1:A:454:TRP:O	1:A:458:TYR:CG	2.72	0.42
1:A:772:PHE:O	1:A:778:ARG:CD	2.67	0.42
1:B:1224:PHE:CE2	1:B:1228:LYS:HE3	2.55	0.42
1:A:426:HIS:HB3	1:A:469:PRO:HD3	2.02	0.42
1:A:444:TRP:CD2	1:A:453:ILE:HG23	2.54	0.42
1:B:1182:PHE:O	1:B:1186:MET:HG2	2.19	0.42
1:B:429:VAL:HG12	1:B:430:ASP:N	2.35	0.42
1:A:472:PRO:HA	1:A:473:PRO:HD3	1.90	0.42
1:A:796:LEU:HA	1:A:799:LEU:CD1	2.46	0.42
1:B:441:ASP:CB	1:B:442:PRO:CA	2.96	0.42
1:B:455:LYS:C	1:B:457:LEU:O	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:456:THR:HG22	1:A:457:LEU:HD13	2.01	0.42
1:A:705:GLU:HG2	1:A:998:PRO:CD	2.50	0.42
1:B:555:SER:CA	1:B:557:GLN:H	2.32	0.42
1:B:712:GLY:O	1:B:746:TRP:HA	2.20	0.42
1:A:966:HIS:ND1	1:A:1089:LYS:CE	2.83	0.41
1:A:889:LYS:HG2	1:A:1198:PHE:CZ	2.55	0.41
1:A:1189:ALA:O	1:A:1190:LYS:C	2.59	0.41
1:B:459:ARG:HB2	1:B:460:LEU:CD2	2.48	0.41
1:A:1220:SER:H	1:A:1221:ALA:HB3	1.73	0.41
1:B:551:PRO:HB2	1:B:553:VAL:CG1	2.50	0.41
1:B:1075:PHE:HE2	1:B:1118:SER:HA	1.84	0.41
1:B:449:ASP:HB3	1:B:450:VAL:H	1.65	0.41
1:B:456:THR:H	1:B:457:LEU:C	2.24	0.41
1:B:1153:TRP:NE1	1:B:1157:GLY:O	2.52	0.41
1:B:907:LYS:HG3	1:B:1175:ILE:HD13	2.02	0.41
1:A:1182:PHE:HA	1:A:1185:ALA:HB1	2.01	0.41
1:A:423:LEU:HD11	1:A:458:TYR:CD1	2.54	0.41
1:A:1183:HIS:HA	1:A:1186:MET:HG3	2.03	0.41
1:A:922:MET:HE3	1:A:1012:MET:CA	2.51	0.41
1:A:1334:ALA:HB3	1:B:1347:LEU:HD13	2.01	0.41
1:A:696:ASP:HB3	1:A:706:VAL:HG13	2.02	0.41
1:B:407:LYS:CA	1:B:408:TRP:CB	2.92	0.41
1:B:565:ILE:HD13	1:B:1074:HIS:HA	2.03	0.41
1:B:722:ILE:O	1:B:726:LEU:HB2	2.20	0.41
1:A:514:LYS:HE3	1:A:514:LYS:HB3	1.88	0.41
1:A:581:ARG:NH1	4:A:2068:HOH:O	2.54	0.41
1:B:400:ASN:OD1	1:B:509:PRO:HB3	2.20	0.41
1:B:393:VAL:O	1:B:394:VAL:CB	2.64	0.41
1:A:605:LYS:HA	1:A:606:PRO:HD3	1.88	0.41
1:B:441:ASP:HB3	1:B:442:PRO:O	2.20	0.41
1:B:458:TYR:HB3	1:B:463:PHE:O	2.21	0.41
1:B:462:ALA:HB1	1:B:463:PHE:CD2	2.56	0.41
1:B:428:LYS:O	1:B:429:VAL:CG2	2.68	0.41
1:A:1141:LEU:HD13	1:A:1141:LEU:HA	1.89	0.41
1:B:1218:ARG:N	1:B:1219:SER:CB	2.77	0.41
1:A:799:LEU:HB2	1:A:800:PRO:HD3	2.02	0.41
1:B:1203:LEU:HG	1:B:1329:LEU:HD22	2.03	0.41
1:A:1146:PRO:CB	1:A:1148:TYR:CE2	3.04	0.41
1:A:869:ASP:HB3	4:A:2264:HOH:O	2.21	0.41
1:A:794:LEU:HD11	1:A:802:LEU:HD11	2.03	0.41
1:B:429:VAL:HG22	1:B:463:PHE:CZ	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:400:ASN:HD22	1:B:404:LYS:NZ	2.19	0.41
1:B:457:LEU:H	1:B:459:ARG:HG2	1.86	0.40
1:A:1089:LYS:HB2	1:A:1107:LEU:HB3	2.03	0.40
1:B:775:LYS:HG2	4:B:2109:HOH:O	2.20	0.40
1:B:456:THR:O	1:B:459:ARG:HG2	2.21	0.40
1:B:419:GLU:N	1:B:422:ARG:HB2	2.26	0.40
1:A:488:LYS:HE3	1:B:1371:GLU:O	2.22	0.40
1:B:1087:ASN:O	1:B:1091:ARG:HG3	2.21	0.40
1:A:1150:SER:HB2	4:A:2426:HOH:O	2.20	0.40
1:B:431:LEU:HD13	1:B:432:GLU:OE1	2.21	0.40
1:A:454:TRP:O	1:A:458:TYR:CD1	2.75	0.40
1:B:391:ALA:HB3	1:B:563:GLU:CG	2.45	0.40
1:A:648:SER:HA	1:A:1065:THR:HG21	2.03	0.40
1:B:449:ASP:O	1:B:450:VAL:HB	2.22	0.40
1:A:485:PHE:HB3	1:A:532:PRO:HB2	2.02	0.40
1:A:1265:TRP:CZ2	1:A:1325:ALA:HB2	2.56	0.40
1:A:557:GLN:HB3	1:A:557:GLN:HE21	1.68	0.40
1:A:459:ARG:HB3	1:A:460:LEU:H	1.52	0.40
1:A:1220:SER:H	1:A:1221:ALA:CB	2.29	0.40
1:B:547:SER:CB	1:B:548:PRO:CD	2.99	0.40
1:A:626:VAL:O	1:A:626:VAL:HG13	2.22	0.40
1:A:1207:TYR:CE2	1:A:1311:LYS:HG3	2.55	0.40
1:B:699:SER:HA	1:B:700:PRO:HD3	1.98	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:2389:HOH:O	4:B:2333:HOH:O[1_455]	1.90	0.30
1:A:1156:ARG:NH1	1:B:1126:GLU:OE2[1_455]	2.07	0.13
4:A:2109:HOH:O	4:B:2384:HOH:O[2_746]	2.16	0.04

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	925/1022 (90%)	836 (90%)	51 (6%)	38 (4%)	3	1
1	B	922/1022 (90%)	811 (88%)	63 (7%)	48 (5%)	2	1
All	All	1847/2044 (90%)	1647 (89%)	114 (6%)	86 (5%)	3	1

All (86) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	399	ARG
1	A	412	ALA
1	A	439	LYS
1	A	440	TYR
1	A	459	ARG
1	A	460	LEU
1	A	466	LYS
1	A	467	PRO
1	A	504	ASN
1	A	510	LEU
1	A	547	SER
1	A	553	VAL
1	A	621	THR
1	A	625	ASP
1	A	642	ARG
1	A	1140	ALA
1	A	1141	LEU
1	A	1193	GLU
1	A	1194	ASP
1	B	401	ILE
1	B	406	PRO
1	B	411	GLU
1	B	419	GLU
1	B	429	VAL
1	B	430	ASP
1	B	432	GLU
1	B	434	GLU
1	B	446	THR
1	B	453	ILE
1	B	460	LEU
1	B	463	PHE
1	B	467	PRO
1	B	504	ASN

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Mol	Chain	Res	Type
1	B	505	SER
1	B	547	SER
1	B	548	PRO
1	B	1141	LEU
1	B	1190	LYS
1	B	1217	SER
1	B	1219	SER
1	A	394	VAL
1	A	398	LEU
1	A	461	ASP
1	A	503	ASP
1	A	1138	GLY
1	A	1185	ALA
1	A	1187	LYS
1	A	1214	SER
1	A	1316	LYS
1	B	407	LYS
1	B	408	TRP
1	B	431	LEU
1	B	450	VAL
1	B	451	THR
1	B	503	ASP
1	B	510	LEU
1	B	555	SER
1	B	621	THR
1	B	1196	ALA
1	B	1214	SER
1	A	559	ALA
1	A	1218	ARG
1	A	1315	HIS
1	B	404	LYS
1	B	441	ASP
1	B	1189	ALA
1	B	1194	ASP
1	A	458	TYR
1	A	469	PRO
1	A	471	LYS
1	A	488	LYS
1	B	471	LYS
1	B	553	VAL
1	B	1195	GLY
1	B	1205	SER

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Mol	Chain	Res	Type
1	B	412	ALA
1	B	418	TRP
1	B	445	SER
1	B	507	THR
1	B	1140	ALA
1	A	468	PHE
1	B	392	PRO
1	B	394	VAL
1	A	453	ILE
1	A	1253	PRO
1	B	552	PRO

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	815/891 (92%)	748 (92%)	67 (8%)	14	17
1	B	812/891 (91%)	716 (88%)	96 (12%)	6	7
All	All	1627/1782 (91%)	1464 (90%)	163 (10%)	9	11

All (163) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	393	VAL
1	A	394	VAL
1	A	399	ARG
1	A	408	TRP
1	A	409	LEU
1	A	414	LEU
1	A	456	THR
1	A	457	LEU
1	A	458	TYR
1	A	482	THR
1	A	504	ASN
1	A	507	THR

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Mol	Chain	Res	Type
1	A	515	LEU
1	A	518	LEU
1	A	526	LEU
1	A	546	THR
1	A	547	SER
1	A	553	VAL
1	A	555	SER
1	A	605	LYS
1	A	622	PHE
1	A	623	ARG
1	A	701	SER
1	A	716	ARG
1	A	725	VAL
1	A	726	LEU
1	A	730	ASP
1	A	755	ASP
1	A	774	ASP
1	A	796	LEU
1	A	797	GLN
1	A	798	LEU
1	A	835	LEU
1	A	839	VAL
1	A	891	LEU
1	A	896	TRP
1	A	947	GLU
1	A	949	SER
1	A	952	LEU
1	A	953	LEU
1	A	955	ASP
1	A	959	LEU
1	A	999	LEU
1	A	1032	LEU
1	A	1056	THR
1	A	1134	ARG
1	A	1137	LEU
1	A	1141	LEU
1	A	1172	ARG
1	A	1182	PHE
1	A	1187	LYS
1	A	1193	GLU
1	A	1194	ASP
1	A	1203	LEU

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Mol	Chain	Res	Type
1	A	1211	LYS
1	A	1214	SER
1	A	1216	LYS
1	A	1217	SER
1	A	1218	ARG
1	A	1223	LEU
1	A	1235	GLU
1	A	1240	ARG
1	A	1269	THR
1	A	1282	SER
1	A	1303	LEU
1	A	1317	SER
1	A	1321	VAL
1	B	397	ARG
1	B	398	LEU
1	B	399	ARG
1	B	400	ASN
1	B	401	ILE
1	B	408	TRP
1	B	409	LEU
1	B	414	LEU
1	B	419	GLU
1	B	421	THR
1	B	425	MET
1	B	427	CYS
1	B	431	LEU
1	B	440	TYR
1	B	446	THR
1	B	449	ASP
1	B	450	VAL
1	B	451	THR
1	B	482	THR
1	B	487	SER
1	B	488	LYS
1	B	501	ASN
1	B	503	ASP
1	B	507	THR
1	B	518	LEU
1	B	526	LEU
1	B	544	THR
1	B	554	VAL
1	B	575	LEU

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Mol	Chain	Res	Type
1	B	581	ARG
1	B	586	LYS
1	B	611	ARG
1	B	621	THR
1	B	623	ARG
1	B	674	LEU
1	B	720	LYS
1	B	721	ARG
1	B	723	ARG
1	B	725	VAL
1	B	726	LEU
1	B	769	GLU
1	B	775	LYS
1	B	790	LYS
1	B	796	LEU
1	B	824	LEU
1	B	835	LEU
1	B	839	VAL
1	B	849	TYR
1	B	861	VAL
1	B	867	LEU
1	B	870	SER
1	B	889	LYS
1	B	900	LYS
1	B	905	THR
1	B	910	LEU
1	B	916	ARG
1	B	947	GLU
1	B	948	GLU
1	B	952	LEU
1	B	953	LEU
1	B	955	ASP
1	B	959	LEU
1	B	999	LEU
1	B	1036	LEU
1	B	1040	LEU
1	B	1048	LYS
1	B	1058	SER
1	B	1067	ASP
1	B	1071	LYS
1	B	1102	LYS
1	B	1110	LEU

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Mol	Chain	Res	Type
1	B	1133	ARG
1	B	1137	LEU
1	B	1143	LEU
1	B	1154	LEU
1	B	1156	ARG
1	B	1191	ASP
1	B	1203	LEU
1	B	1205	SER
1	B	1216	LYS
1	B	1217	SER
1	B	1223	LEU
1	B	1236	LYS
1	B	1269	THR
1	B	1282	SER
1	B	1283	LYS
1	B	1285	ILE
1	B	1303	LEU
1	B	1308	THR
1	B	1312	LEU
1	B	1315	HIS
1	B	1321	VAL
1	B	1337	THR
1	B	1347	LEU
1	B	1360	LYS
1	B	1370	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	390	HIS
1	A	557	GLN
1	A	566	GLN
1	A	579	GLN
1	A	827	GLN
1	A	843	GLN
1	B	390	HIS
1	B	501	ASN
1	B	566	GLN
1	B	665	HIS
1	B	776	HIS
1	B	777	GLN
1	B	822	ASN

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Mol	Chain	Res	Type
1	B	1113	ASN
1	B	1299	ASN
1	B	1315	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	GOL	B	3375	-	4,4,5	0.49	0	2,4,5	0.86	0

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	GOL	B	3375	-	-	0/2/2/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	3375	GOL	1	0

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	935/1022 (91%)	0.91	158 (16%) 2 3	39, 50, 65, 78	0
1	B	932/1022 (91%)	1.17	197 (21%) 1 2	38, 51, 64, 77	0
All	All	1867/2044 (91%)	1.04	355 (19%) 2 2	38, 51, 64, 78	0

All (355) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	590	TYR	12.9
1	B	1191	ASP	11.4
1	B	507	THR	10.6
1	B	466	LYS	9.8
1	A	626	VAL	9.6
1	A	1186	MET	9.3
1	B	460	LEU	9.3
1	A	604	PRO	9.1
1	B	1189	ALA	9.0
1	B	626	VAL	8.9
1	B	464	ARG	8.8
1	B	468	PHE	8.8
1	A	1138	GLY	8.3
1	B	443	SER	8.2
1	B	1192	THR	8.2
1	B	1190	LYS	8.2
1	B	459	ARG	7.8
1	A	627	PHE	7.6
1	A	589	GLY	7.5
1	B	1195	GLY	7.5
1	B	508	ALA	7.3
1	B	469	PRO	7.3
1	B	454	TRP	7.0
1	B	1184	ASN	6.7

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Mol	Chain	Res	Type	RSRZ
1	B	1185	ALA	6.4
1	B	607	ILE	6.4
1	A	1141	LEU	6.3
1	B	546	THR	6.2
1	B	428	LYS	6.2
1	A	1191	ASP	6.1
1	A	468	PHE	6.0
1	A	457	LEU	6.0
1	A	1218	ARG	6.0
1	A	467	PRO	5.9
1	B	512	LEU	5.9
1	A	849	TYR	5.8
1	B	1188	ALA	5.8
1	A	1254	TYR	5.7
1	A	1188	ALA	5.7
1	A	1222	LEU	5.6
1	B	589	GLY	5.6
1	A	1187	LYS	5.6
1	A	1192	THR	5.5
1	B	488	LYS	5.5
1	B	1194	ASP	5.5
1	B	1154	LEU	5.5
1	B	396	ALA	5.3
1	A	1185	ALA	5.2
1	B	1156	ARG	5.2
1	B	436	LEU	5.0
1	B	1252	ASP	4.9
1	A	1193	GLU	4.9
1	A	1372	GLY	4.8
1	A	420	VAL	4.8
1	B	1218	ARG	4.8
1	A	605	LYS	4.8
1	A	399	ARG	4.7
1	A	458	TYR	4.7
1	B	425	MET	4.7
1	A	1217	SER	4.6
1	A	558	PRO	4.6
1	A	559	ALA	4.6
1	A	396	ALA	4.5
1	B	739	PHE	4.5
1	A	1166	LEU	4.5
1	B	1254	TYR	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	1215	ASP	4.4
1	B	467	PRO	4.4
1	B	1140	ALA	4.4
1	A	438	LEU	4.3
1	B	1373	ASP	4.3
1	A	1373	ASP	4.3
1	A	1189	ALA	4.3
1	B	440	TYR	4.3
1	B	429	VAL	4.3
1	A	466	LYS	4.2
1	B	503	ASP	4.2
1	A	469	PRO	4.2
1	B	510	LEU	4.2
1	B	1137	LEU	4.2
1	B	1186	MET	4.2
1	A	1304	LEU	4.1
1	B	780	LEU	4.1
1	B	1157	GLY	4.1
1	A	588	ALA	4.1
1	B	553	VAL	4.1
1	B	620	ILE	4.1
1	A	409	LEU	4.1
1	B	463	PHE	4.1
1	A	989	ILE	4.1
1	A	546	THR	4.1
1	B	849	TYR	4.1
1	B	449	ASP	4.0
1	B	947	GLU	4.0
1	B	1015	VAL	4.0
1	A	395	ALA	4.0
1	B	456	THR	4.0
1	A	606	PRO	4.0
1	A	1190	LYS	4.0
1	B	520	PHE	4.0
1	A	547	SER	4.0
1	B	989	ILE	3.9
1	B	623	ARG	3.9
1	B	439	LYS	3.9
1	B	1182	PHE	3.9
1	B	1138	GLY	3.9
1	B	461	ASP	3.9
1	B	470	GLU	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	1315	HIS	3.8
1	A	464	ARG	3.8
1	B	518	LEU	3.8
1	B	1166	LEU	3.8
1	A	641	GLN	3.7
1	A	1163	ILE	3.7
1	B	391	ALA	3.7
1	B	1187	LYS	3.7
1	B	442	PRO	3.7
1	B	548	PRO	3.7
1	B	434	GLU	3.7
1	B	559	ALA	3.7
1	A	417	ALA	3.6
1	B	398	LEU	3.6
1	B	1151	ASP	3.6
1	A	759	ILE	3.6
1	A	1184	ASN	3.6
1	B	588	ALA	3.6
1	B	651	LEU	3.6
1	B	433	ASP	3.5
1	B	1193	GLU	3.5
1	A	400	ASN	3.5
1	B	960	VAL	3.5
1	B	472	PRO	3.5
1	B	545	SER	3.5
1	A	620	ILE	3.4
1	B	558	PRO	3.4
1	A	1282	SER	3.4
1	A	1107	LEU	3.4
1	B	570	MET	3.4
1	B	412	ALA	3.4
1	B	991	PHE	3.4
1	B	1107	LEU	3.3
1	A	463	PHE	3.3
1	B	413	PRO	3.3
1	B	971	ILE	3.3
1	B	755	ASP	3.3
1	A	555	SER	3.3
1	B	505	SER	3.3
1	B	404	LYS	3.3
1	A	960	VAL	3.3
1	B	502	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	390	HIS	3.2
1	B	1217	SER	3.2
1	B	1282	SER	3.2
1	B	511	TYR	3.2
1	B	1016	CYS	3.2
1	A	923	ILE	3.2
1	A	990	ILE	3.2
1	A	1015	VAL	3.2
1	A	991	PHE	3.2
1	B	390	HIS	3.2
1	B	437	GLY	3.1
1	A	510	LEU	3.1
1	A	570	MET	3.1
1	A	701	SER	3.1
1	B	1222	LEU	3.1
1	A	1210	PHE	3.1
1	B	1216	LYS	3.1
1	B	1068	MET	3.1
1	B	563	GLU	3.1
1	B	1065	THR	3.1
1	B	409	LEU	3.1
1	B	1257	ARG	3.1
1	A	780	LEU	3.1
1	B	625	ASP	3.1
1	B	458	TYR	3.1
1	A	560	ALA	3.1
1	B	1074	HIS	3.1
1	A	1140	ALA	3.0
1	B	556	LYS	3.0
1	B	448	ARG	3.0
1	B	432	GLU	3.0
1	A	1139	GLY	3.0
1	B	1219	SER	3.0
1	B	455	LYS	3.0
1	A	459	ARG	3.0
1	B	1215	ASP	3.0
1	B	1253	PRO	2.9
1	B	1265	TRP	2.9
1	B	547	SER	2.9
1	B	494	LEU	2.9
1	A	1162	ILE	2.9
1	A	1110	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	392	PRO	2.9
1	B	501	ASN	2.9
1	A	394	VAL	2.9
1	B	418	TRP	2.9
1	A	999	LEU	2.9
1	B	482	THR	2.9
1	B	424	PHE	2.9
1	B	988	VAL	2.8
1	B	999	LEU	2.8
1	A	1321	VAL	2.8
1	B	1212	GLU	2.8
1	A	428	LYS	2.8
1	A	1068	MET	2.8
1	B	1141	LEU	2.8
1	B	430	ASP	2.8
1	B	414	LEU	2.8
1	B	465	GLY	2.8
1	A	439	LYS	2.8
1	A	1211	LYS	2.8
1	A	461	ASP	2.7
1	A	423	LEU	2.7
1	B	506	PRO	2.7
1	A	1237	GLU	2.7
1	B	427	CYS	2.7
1	B	1132	LEU	2.7
1	B	1356	LEU	2.7
1	A	541	PRO	2.7
1	A	556	LYS	2.7
1	A	850	SER	2.7
1	B	1296	ARG	2.7
1	A	802	LEU	2.7
1	A	959	LEU	2.7
1	B	759	ILE	2.7
1	B	990	ILE	2.7
1	B	850	SER	2.7
1	A	1183	HIS	2.7
1	B	399	ARG	2.7
1	A	755	ASP	2.7
1	A	1132	LEU	2.7
1	A	391	ALA	2.7
1	A	506	PRO	2.7
1	A	1137	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	438	LEU	2.6
1	B	959	LEU	2.6
1	A	465	GLY	2.6
1	A	421	THR	2.6
1	B	1177	LYS	2.6
1	A	548	PRO	2.6
1	B	1063	GLN	2.6
1	B	1139	GLY	2.6
1	A	796	LEU	2.6
1	A	1316	LYS	2.6
1	A	971	ILE	2.6
1	A	511	TYR	2.6
1	B	1180	GLU	2.6
1	A	801	VAL	2.6
1	B	924	ALA	2.6
1	B	471	LYS	2.6
1	A	1252	ASP	2.5
1	A	739	PHE	2.5
1	B	938	GLY	2.5
1	B	1309	ALA	2.5
1	A	1239	GLY	2.5
1	B	1220	SER	2.5
1	B	1223	LEU	2.5
1	A	416	VAL	2.5
1	A	668	LEU	2.5
1	B	492	VAL	2.5
1	A	924	ALA	2.4
1	B	1155	GLY	2.4
1	A	502	PRO	2.4
1	A	946	GLU	2.4
1	B	1064	THR	2.4
1	A	540	ILE	2.4
1	A	424	PHE	2.4
1	B	1354	ALA	2.4
1	A	642	ARG	2.4
1	A	1120	GLN	2.4
1	A	1069	ILE	2.4
1	B	951	THR	2.4
1	A	988	VAL	2.4
1	B	1163	ILE	2.4
1	B	616	ALA	2.4
1	B	1133	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	1285	ILE	2.3
1	A	448	ARG	2.3
1	A	1116	ASP	2.3
1	B	740	GLY	2.3
1	A	1032	LEU	2.3
1	A	1371	GLU	2.3
1	A	507	THR	2.3
1	B	395	ALA	2.3
1	A	799	LEU	2.3
1	B	420	VAL	2.3
1	B	450	VAL	2.3
1	B	446	THR	2.3
1	A	623	ARG	2.3
1	A	1236	LYS	2.3
1	B	457	LEU	2.3
1	A	740	GLY	2.3
1	B	1162	ILE	2.3
1	B	1236	LYS	2.3
1	B	923	ILE	2.2
1	A	711	VAL	2.2
1	B	735	VAL	2.2
1	B	1149	LYS	2.2
1	B	403	PRO	2.2
1	B	435	SER	2.2
1	B	1072	SER	2.2
1	B	802	LEU	2.2
1	B	473	PRO	2.2
1	A	742	ALA	2.2
1	A	746	TRP	2.2
1	A	1354	ALA	2.2
1	B	711	VAL	2.2
1	B	1352	MET	2.2
1	A	951	THR	2.2
1	A	672	ILE	2.2
1	A	937	VAL	2.2
1	B	937	VAL	2.2
1	B	498	LEU	2.2
1	B	714	MET	2.2
1	B	1143	LEU	2.2
1	B	410	HIS	2.2
1	B	912	ILE	2.1
1	A	434	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	820	LEU	2.1
1	B	1150	SER	2.1
1	A	703	THR	2.1
1	B	453	ILE	2.1
1	B	1231	ILE	2.1
1	B	444	TRP	2.1
1	B	1183	HIS	2.1
1	A	494	LEU	2.1
1	B	519	MET	2.1
1	B	1110	LEU	2.1
1	A	1021	ILE	2.1
1	A	1229	ASN	2.1
1	B	400	ASN	2.1
1	B	509	PRO	2.1
1	B	1035	ASP	2.1
1	A	456	THR	2.1
1	B	672	ILE	2.1
1	A	869	ASP	2.1
1	B	475	ASP	2.1
1	A	952	LEU	2.1
1	A	1207	TYR	2.1
1	A	1142	SER	2.1
1	A	1194	ASP	2.1
1	B	718	VAL	2.1
1	A	1320	PHE	2.1
1	A	1143	LEU	2.1
1	A	1305	ARG	2.1
1	A	1016	CYS	2.0
1	A	1240	ARG	2.0
1	A	1369	ARG	2.0
1	B	579	GLN	2.0
1	A	714	MET	2.0
1	B	1179	LEU	2.0
1	A	1257	ARG	2.0
1	A	625	ASP	2.0
1	A	718	VAL	2.0
1	A	518	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
3	GOL	B	3375	5/6	0.89	0.21	3.11	66,67,67,67	0
2	MG	B	3374	1/1	0.98	0.10	-	31,31,31,31	0
2	MG	A	3374	1/1	0.95	0.05	-	50,50,50,50	0

6.5 Other polymers [i](#)

There are no such residues in this entry.