



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 29, 2017 – 08:12 AM EDT

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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20029077  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : rb-20029077

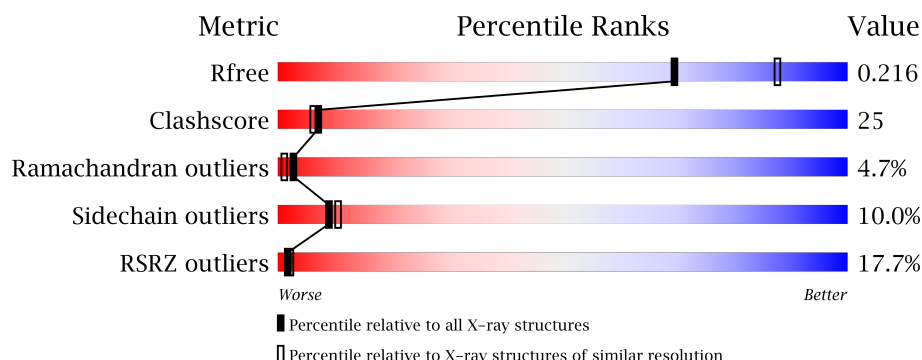
# 1 Overall quality at a glance ⓘ

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))
$R_{free}$	100719	4130 (2.30-2.30)
Clashscore	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)
RSRZ outliers	101464	4156 (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  $\geq 3$ , 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>14%</div> <div>62%</div> <div>23%</div> <div>6%</div> <div>9%</div> </div>
1	B	1022	<div> <div>19%</div> <div>57%</div> <div>24%</div> <div>8%</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: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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		



Chain B:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.46 (at 2.30Å)	Xtriage
Refinement program	REFMAC	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 <sup>2</sup> )	45.5	Xtriage
Anisotropy	0.078	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 52.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	15945	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical 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: 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:1210:PHE:O	1:A:1214:SER:HB2	1.47	1.14
1:A:503:ASP:O	1:A:504:ASN:HB2	1.38	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:A:1315:HIS:CB	1:A:1316:LYS:HB2	1.81	1.10
1:B:459:ARG:N	1:B:460:LEU:HB2	1.67	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:A:1217:SER:CB	1:A:1221:ALA:HB2	1.97	0.94
1:B:452:ASP:O	1:B:454:TRP:N	2.00	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:922:MET:HE1	1:A:1011:ASP:HB3	1.59	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:879:MET:HE3	1:A:885:PRO:HG3	1.60	0.84
1:B:431:LEU:CB	1:B:432:GLU:CB	2.25	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:417:ALA:HB1	1:A:576:VAL:HG13	1.61	0.83
1:A:559:ALA:HB1	1:A:562:GLU:OE1	1.78	0.83
1:B:1134:ARG:O	4:B:2333:HOH:O	1.96	0.83
1:A:454:TRP:O	1:A:458:TYR:HB3	1.77	0.83
1:B:460:LEU:H	1:B:461:ASP:CA	1.92	0.83
1:A:457:LEU:HB3	1:A:458:TYR:HB2	1.60	0.83
1:B:1041:LYS:O	1:B:1123:VAL:HG12	1.80	0.82
1:B:463:PHE:HA	1:B:464:ARG:C	2.00	0.82
1:B:461:ASP:H	1:B:462:ALA:HA	1.43	0.81
1:A:423:LEU:HD11	1:A:458:TYR:CE1	2.16	0.81
1:A:438:LEU:CA	1:A:439:LYS:CB	2.52	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:A:1315:HIS:HB2	1:A:1316:LYS:HB2	0.85	0.80
1:B:460:LEU:N	1:B:461:ASP:CA	2.43	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:419:GLU:H	1:B:422:ARG:HB2	1.48	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:1217:SER:HB3	1:B:1221:ALA:HB2	1.65	0.78
1:B:409:LEU:HD12	1:B:409:LEU:H	1.49	0.78
1:A:503:ASP:O	1:A:504:ASN:CB	2.25	0.78
1:B:460:LEU:H	1:B:461:ASP:HB3	1.49	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:A:828:PHE:CD1	1:A:1178:GLU:HG2	2.19	0.77
1:B:1137:LEU:CB	1:B:1138:GLY:HA3	2.14	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:A:1112:GLY:O	1:A:1115:VAL:HG22	1.84	0.77
1:B:431:LEU:HB2	1:B:432:GLU:HB2	1.61	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:A:829:SER:HA	1:A:832:LYS:HE3	1.68	0.75
1:B:836:ASN:HA	1:B:886:LYS:HD2	1.69	0.75
1:A:488:LYS:HG3	1:B:1373:ASP:N	2.01	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:B:400:ASN:O	1:B:402:TRP:N	2.20	0.75
1:A:576:VAL:HG12	1:A:576:VAL:O	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:400:ASN:CG	1:B:401:ILE:N	2.40	0.74
1:B:879:MET:CE	1:B:885:PRO:CD	2.66	0.74
1:B:879:MET:CE	1:B:885:PRO:HD3	2.18	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:B:456:THR:H	1:B:457:LEU:CB	2.00	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:A:705:GLU:OE2	1:A:1001:LYS:NZ	2.15	0.72
1:B:451:THR:CB	1:B:452:ASP:HB2	2.20	0.72
1:A:826:ARG:NH1	1:A:913:ARG:HH22	1.88	0.72
1:B:391:ALA:HB3	1:B:563:GLU:HG3	1.70	0.72
1:A:457:LEU:H	1:A:459:ARG:HB2	1.55	0.71
1:B:1139:GLY:HA3	1:B:1141:LEU:HB3	1.71	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: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:1315:HIS:O	4:B:2386:HOH:O	2.09	0.70
1:B:626:VAL:O	1:B:626:VAL:HG13	1.91	0.70
1:B:842:ARG:HD2	4:B:2168:HOH:O	1.92	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: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:433:ASP:HA	1:B:434:GLU:CB	2.21	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:1337:THR:HG22	4:B:2395:HOH:O	1.93	0.69
1:B:459:ARG:HB2	1:B:460:LEU:HD23	1.75	0.69
1:B:491:ALA:HB1	1:B:532:PRO:HB3	1.75	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:433:ASP:CA	1:B:434:GLU:CB	2.72	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:A:498:LEU:HD22	1:A:513:VAL:HG22	1.75	0.67
1:B:462:ALA:HB3	1:B:463:PHE:C	2.14	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:A:412:ALA:HB1	1:A:413:PRO:C	2.14	0.67
1:B:424:PHE:HA	1:B:428:LYS:O	1.95	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: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:B:838:PRO:HA	1:B:879:MET:HE1	1.76	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:1159:PRO:HB3	1:B:1164:ASP:HB3	1.76	0.66
1:B:456:THR:N	1:B:457:LEU:HB2	2.11	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:A:1217:SER:OG	1:A:1221:ALA:CB	2.44	0.66
1:B:408:TRP:HE3	1:B:408:TRP:O	1.78	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:A:836:ASN:OD1	1:A:886:LYS:HE3	1.96	0.65
1:B:462:ALA:H	1:B:463:PHE:C	1.99	0.65
1:B:450:VAL:HG12	1:B:451:THR:OG1	1.97	0.65
1:A:399:ARG:HD2	1:A:507:THR:CG2	2.13	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: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:A:942:LYS:HG3	1:A:949:SER:OG	1.97	0.64
1:B:625:ASP:HB3	1:B:643:THR:CG2	2.27	0.64
1:A:796:LEU:HD12	1:A:797:GLN:N	2.12	0.64
1:B:461:ASP:O	1:B:464:ARG:HG3	1.97	0.64
1:A:1220:SER:N	1:A:1221:ALA:CB	2.58	0.64
1:B:429:VAL:O	1:B:430:ASP:CB	2.44	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:405:PHE:CE2	1:B:409:LEU:HD13	2.33	0.63
1:B:450:VAL:N	1:B:451:THR:OG1	2.31	0.63
1:A:1180:GLU:HA	1:A:1180:GLU:OE1	1.99	0.63
1:A:605:LYS:H	1:A:605:LYS:HD2	1.63	0.62
1:B:1041:LYS:HB2	1:B:1123:VAL:HG13	1.80	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:A:626:VAL:N	1:A:627:PHE:HA	2.15	0.61
1:B:393:VAL:HG22	1:B:394:VAL:H	1.64	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:A:1202:ASP:O	1:A:1205:SER:HB2	2.00	0.61
1:B:418:TRP:CD1	1:B:518:LEU:HD13	2.35	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:1300:THR:HA	1:A:1303:LEU:HD23	1.83	0.60
1:A:1207:TYR:CD2	1:A:1311:LYS:HG3	2.36	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:A:820:LEU:HD11	1:A:906:LEU:HD21	1.83	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: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: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:459:ARG:H	1:B:460:LEU:HB2	1.65	0.59
1:A:922:MET:HE2	1:A:1012:MET:C	2.23	0.59
1:B:428:LYS:O	1:B:429:VAL:HG23	2.02	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:A:723:ARG:NH1	1:A:724:ASP:OD1	2.33	0.58
1:B:671:ARG:HH22	1:B:1119:LYS:HZ2	1.51	0.58
1:B:1194:ASP:O	1:B:1196:ALA:N	2.35	0.58
1:B:879:MET:HE2	1:B:885:PRO:CD	2.32	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:1042:LYS:HG2	1:B:1122:ILE:HG12	1.85	0.58
1:B:1147:MET:HA	1:B:1147:MET:CE	2.33	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:1235:GLU:HG2	1:A:1313:TYR:CZ	2.39	0.57
1:A:820:LEU:CD1	1:A:906:LEU:HD21	2.35	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:A:456:THR:O	1:A:459:ARG:NH1	2.38	0.57
1:B:431:LEU:HB3	1:B:432:GLU:HB2	0.60	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:C	1:B:1285:ILE:HD12	2.27	0.56
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:445:SER:O	1:B:446:THR:HG23	2.05	0.55
1:B:400:ASN:C	1:B:401:ILE:HG12	2.27	0.55
1:B:419:GLU:OE2	1:B:419:GLU:HA	2.07	0.55
1:A:1217:SER:OG	1:A:1221:ALA:N	2.40	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
1:B:1363:THR:O	1:B:1367:VAL:HG13	2.06	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:A:393:VAL:N	1:A:394:VAL:C	2.54	0.55
1:B:408:TRP:CE3	1:B:408:TRP:C	2.80	0.55
1:A:395:ALA:CB	1:A:396:ALA:HA	2.31	0.54
1:A:813:ARG:HD2	4:A:2227:HOH:O	2.07	0.54
1:B:456:THR:CA	1:B:457:LEU:HB2	2.37	0.54
1:A:1193:GLU:N	1:A:1194:ASP:O	2.40	0.54
1:A:399:ARG:CB	1:A:400:ASN:CA	2.85	0.54
1:B:1024:GLY:HA3	4:B:2291:HOH:O	2.07	0.54
1:B:1217:SER:CB	1:B:1218:ARG:HA	2.36	0.54
1:B:433:ASP:CA	1:B:434:GLU:HB2	2.35	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:B:1269:THR:HG21	4:B:2377:HOH:O	2.03	0.54
1:B:428:LYS:C	1:B:429:VAL:HG23	2.28	0.54
1:A:466:LYS:HB3	1:A:467:PRO:O	2.08	0.54
1:B:1120:GLN:OE1	1:B:1120:GLN:HA	2.07	0.54
1:B:433:ASP:CB	1:B:434:GLU:CB	2.83	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:438:LEU:CB	1:A:439:LYS:HB3	2.38	0.53
1:A:641:GLN:HB3	1:A:642:ARG:HB2	1.75	0.53
1:A:1210:PHE:O	1:A:1213:ILE:HG22	2.08	0.53
1:A:1213:ILE:O	1:A:1216:LYS:HB3	2.08	0.53
1:A:457:LEU:CB	1:A:458:TYR:CB	2.78	0.53
1:B:860:ARG:HA	1:B:1354:ALA:HB2	1.90	0.53
1:B:406:PRO:CB	1:B:408:TRP:CD1	2.92	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:A:793:GLY:HA2	1:A:914:VAL:H	1.73	0.53
1:B:1089:LYS:HA	1:B:1107:LEU:HD13	1.91	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:A:399:ARG:CD	1:A:507:THR:HG22	2.16	0.53
1:B:1038:ARG:O	1:B:1038:ARG:HG2	2.09	0.53
1:A:555:SER:OG	1:A:555:SER:O	2.21	0.52
1:B:716:ARG:O	1:B:720:LYS:HG2	2.08	0.52
1:A:1146:PRO:HB3	1:A:1148:TYR:CE2	2.44	0.52
1:A:580:TRP:HB3	1:A:614:PHE:HB3	1.90	0.52
1:A:586:LYS:HG2	1:A:587:ASP:N	2.23	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:883:PHE:CE2	1:A:1203:LEU:HD21	2.44	0.52
1:B:546:THR:HA	1:B:547:SER:HB3	1.92	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: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: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: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:427:CYS:O	1:A:428:LYS:HB2	2.10	0.52
1:A:456:THR:HG22	1:A:457:LEU:CA	2.33	0.52
1:A:967:PHE:CD2	1:A:1031:PRO:HG3	2.45	0.52
1:B:829:SER:O	1:B:832:LYS:HG2	2.10	0.52
1:A:451:THR:OG1	1:A:471:LYS:HE3	2.09	0.51
1:A:458:TYR:CZ	1:A:465:GLY:O	2.64	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:B:843:GLN:O	1:B:847:GLU:HG3	2.11	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:828:PHE:CG	1:A:1178:GLU:CG	2.93	0.51
1:A:1219:SER:CA	1:A:1221:ALA:HB3	2.41	0.51
1:B:1088:TYR:CE1	1:B:1143:LEU:HD22	2.46	0.51
1:B:406:PRO:CB	1:B:408:TRP:NE1	2.74	0.51
1:B:468:PHE:HB3	4:B:2007:HOH:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:622:PHE:HA	1:B:642:ARG:O	2.10	0.51
1:A:1194:ASP:N	1:A:1194:ASP:OD2	2.43	0.51
1:B:1189:ALA:O	1:B:1190:LYS:C	2.48	0.51
1:B:403:PRO:HA	1:B:404:LYS:HG2	1.91	0.51
1:B:450:VAL:HG12	1:B:451:THR:HA	1.92	0.51
1:B:552:PRO:N	1:B:553:VAL:HB	2.26	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:462:ALA:N	1:B:463:PHE:C	2.63	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:A:839:VAL:HG13	1:B:1351:PHE:CZ	2.45	0.51
1:B:441:ASP:HB3	1:B:442:PRO:C	2.31	0.51
1:A:1129:TRP:CZ2	1:A:1133:ARG:HD3	2.46	0.51
1:B:1152:SER:O	1:B:1154:LEU:HD13	2.10	0.51
1:B:411:GLU:O	1:B:412:ALA:HB3	2.11	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: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:A:1352:MET:O	1:B:842:ARG:NH2	2.43	0.50
1:B:1140:ALA:O	1:B:1141:LEU:O	2.28	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:1038:ARG:HD2	1:B:1039:TYR:CE2	2.47	0.50
1:B:503:ASP:O	1:B:504:ASN:HB3	2.11	0.50
1:B:1304:LEU:O	1:B:1308:THR:HG23	2.10	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: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:O	1:B:1252:ASP:OD2	2.30	0.50
1:A:1328:GLN:O	1:A:1332:ILE:HG13	2.12	0.50
1:A:400:ASN:OD1	1:A:400:ASN:C	2.50	0.50
1:A:558:PRO:O	1:A:559:ALA:C	2.50	0.49
1:B:509:PRO:O	1:B:510:LEU:CB	2.58	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: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
1:B:460:LEU:HD13	1:B:460:LEU:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:466:LYS:H	1:A:467:PRO:CA	2.18	0.49
1:B:470:GLU:O	1:B:471:LYS:HB3	2.12	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:A:565:ILE:CD1	1:A:1074:HIS:HA	2.43	0.48
1:B:1112:GLY:O	1:B:1115:VAL:CG2	2.57	0.48
1:B:546:THR:HA	1:B:547:SER:CB	2.43	0.48
1:B:861:VAL:HG21	1:B:873:GLU:HG2	1.95	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:A:498:LEU:O	1:A:541:PRO:HD3	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:1195:GLY:O	1:B:1196:ALA:HB3	2.13	0.48
1:B:453:ILE:C	1:B:455:LYS:N	2.67	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:A:456:THR:O	1:A:459:ARG:CD	2.62	0.47
1:B:454:TRP:HA	1:B:457:LEU:HD23	1.95	0.47
1:B:626:VAL:O	1:B:626:VAL:CG1	2.62	0.47
1:A:1211:LYS:O	1:A:1214:SER:HB3	2.14	0.47
1:A:457:LEU:CB	1:A:458:TYR:HB2	2.40	0.47
1:A:900:LYS:HE3	1:A:900:LYS:HB2	1.58	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:464:ARG:HD2	1:A:464:ARG:HA	1.70	0.47
1:A:791:SER:HB3	4:A:2214:HOH:O	2.13	0.47
1:B:424:PHE:HD2	1:B:430:ASP:H	1.62	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: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:A:721:ARG:O	1:A:725:VAL:HG13	2.15	0.47
1:B:1119:LYS:HG3	1:B:1120:GLN:NE2	2.30	0.47
1:B:1214:SER:HA	1:B:1217:SER:HA	1.96	0.47
1:B:460:LEU:HD12	1:B:462:ALA:CB	2.45	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:A:464:ARG:HA	1:A:465:GLY:O	2.15	0.47
1:A:589:GLY:H	1:A:611:ARG:HH21	1.63	0.47
1:B:407:LYS:H	1:B:408:TRP:HD1	1.63	0.47
1:B:942:LYS:HD2	1:B:949:SER:CB	2.44	0.47
1:A:1217:SER:OG	1:A:1221:ALA:CA	2.64	0.46
1:A:1224:PHE:CE2	1:A:1228:LYS:HE3	2.50	0.46
1:B:1254:TYR:HB3	1:B:1255:PRO:HD3	1.97	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:1169:SER:O	1:A:1173:PRO:HG2	2.15	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:A:622:PHE:CD1	1:A:622:PHE:N	2.84	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:B:859:GLY:O	1:B:860:ARG:HB3	2.15	0.46
1:A:456:THR:C	1:A:459:ARG:HB2	2.36	0.46
1:A:458:TYR:H	1:A:459:ARG:C	2.19	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: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:A:966:HIS:ND1	1:A:1089:LYS:HE3	2.31	0.46
1:B:459:ARG:CB	1:B:460:LEU:HB2	2.46	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:426:HIS:HA	1:B:427:CYS:HA	1.57	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:546:THR:O	1:B:546:THR:CG2	2.63	0.45
1:B:589:GLY:O	1:B:590:TYR:HB2	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:462:ALA:H	1:B:464:ARG:N	2.15	0.45
1:B:503:ASP:O	1:B:504:ASN:CB	2.64	0.45
1:B:403:PRO:CB	1:B:404:LYS:HB2	2.45	0.45
1:B:457:LEU:HA	1:B:458:TYR:HA	1.58	0.45
1:B:839:VAL:HG22	4:B:2167:HOH:O	2.16	0.45
1:A:1102:LYS:N	1:A:1103:PRO:HD2	2.32	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:B:610:GLU:HG3	1:B:1077:LEU:HD22	1.99	0.45
1:B:621:THR:HG22	1:B:622:PHE:CD2	2.52	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: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:441:ASP:CB	1:B:442:PRO:HA	2.46	0.45
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:B:447:ALA:CB	1:B:453:ILE:HD11	2.47	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:A:867:LEU:HD22	1:A:874:THR:HG23	1.99	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: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:A:959:LEU:HD22	1:A:1021:ILE:HG22	2.00	0.44
1:B:1063:GLN:CB	4:B:2306:HOH:O	2.65	0.44
1:B:475:ASP:OD1	1:B:476:VAL:N	2.51	0.44
1:A:1134:ARG:HG3	4:A:2232:HOH:O	2.16	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:407:LYS:N	1:B:408:TRP:CD1	2.85	0.44
1:B:861:VAL:HG21	1:B:873:GLU:CG	2.47	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: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:443:SER:CA	1:B:444:TRP:C	2.85	0.44
1:B:1217:SER:CB	1:B:1218:ARG:CA	2.94	0.43
1:B:841:PHE:HB3	1:B:879:MET:HE1	1.99	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:B:429:VAL:HG22	1:B:463:PHE:CE2	2.53	0.43
1:A:467:PRO:HB2	1:A:468:PHE:H	1.53	0.43
1:B:962:ARG:HD3	1:B:1011:ASP:HB3	2.00	0.43
1:B:544:THR:HG21	1:B:1079:PRO:HD3	1.99	0.43
1:B:1289:GLU:O	1:B:1299:ASN:ND2	2.51	0.43
1:B:551:PRO:HA	1:B:552:PRO:HD3	1.67	0.43
1:B:916:ARG:HD3	4:B:2284:HOH:O	2.17	0.43
1:B:772:PHE:O	1:B:778:ARG:CD	2.67	0.43
1:A:665:HIS:HE1	4:A:2366:HOH:O	2.00	0.43
1:A:905:THR:HG23	1:A:909:LYS:HD2	2.01	0.43
1:B:451:THR:N	1:B:452:ASP:CA	2.81	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: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:B:428:LYS:O	1:B:429:VAL:CB	2.66	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:1211:LYS:HB3	1:B:1211:LYS:HE2	1.86	0.43
1:B:451:THR:CA	1:B:452:ASP:HB2	2.49	0.43
1:B:498:LEU:O	1:B:541:PRO:HD3	2.19	0.43
1:B:900:LYS:HB2	1:B:900:LYS:HE3	1.64	0.43
1:A:852:ARG:O	1:A:856:VAL:HG23	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1075:PHE:O	1:B:1078:GLN:HG2	2.19	0.43
1:B:420:VAL:C	1:B:422:ARG:H	2.22	0.43
1:A:1344:ALA:HB1	1:B:1327:ARG:CD	2.48	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:547:SER:CB	1:A:548:PRO:CA	2.96	0.43
1:A:740:GLY:HA3	1:A:772:PHE:CE2	2.54	0.43
1:B:1143:LEU:HD12	1:B:1143:LEU:HA	1.81	0.43
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:423:LEU:HD21	1:B:458:TYR:HE2	1.84	0.42
1:A:1222:LEU:HA	1:A:1222:LEU:HD12	1.86	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:B:1229:ASN:O	1:B:1233:GLU:HG3	2.19	0.42
1:B:459:ARG:HB2	1:B:460:LEU:CB	2.49	0.42
1:B:429:VAL:HG12	1:B:430:ASP:H	1.83	0.42
1:B:580:TRP:HB3	1:B:614:PHE:HB3	1.99	0.42
1:B:530:PHE:CE2	1:B:650:MET:HG2	2.55	0.42
1:B:991:PHE:CD2	1:B:999:LEU:HB3	2.54	0.42
1:A:1190:LYS:HG3	1:A:1191:ASP:N	2.34	0.42
1:A:419:GLU:OE1	1:A:422:ARG:HD3	2.20	0.42
1:A:467:PRO:HG2	1:A:468:PHE:HD2	1.85	0.42
1:B:1187:LYS:HE2	1:B:1187:LYS:HB3	1.89	0.42
1:B:404:LYS:HD3	1:B:404:LYS:HA	1.76	0.42
1:A:454:TRP:HA	1:A:457:LEU:HD23	2.01	0.42
1:A:547:SER:CB	1:A:548:PRO:HA	2.50	0.42
1:B:667:LYS:HB2	1:B:667:LYS:HE2	1.56	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:B:441:ASP:HB2	1:B:444:TRP:CG	2.54	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: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:429:VAL:HG12	1:B:430:ASP:N	2.35	0.42
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:889:LYS:HG2	1:A:1198:PHE:CZ	2.55	0.41
1:A:966:HIS:ND1	1:A:1089:LYS:CE	2.83	0.41
1:A:1189:ALA:O	1:A:1190:LYS:C	2.59	0.41
1:A:1220:SER:H	1:A:1221:ALA:HB3	1.73	0.41
1:B:1075:PHE:HE2	1:B:1118:SER:HA	1.84	0.41
1:B:459:ARG:HB2	1:B:460:LEU:CD2	2.48	0.41
1:B:551:PRO:HB2	1:B:553:VAL:CG1	2.50	0.41
1:B:1153:TRP:NE1	1:B:1157:GLY:O	2.52	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:907:LYS:HG3	1:B:1175:ILE:HD13	2.02	0.41
1:A:922:MET:HE3	1:A:1012:MET:CA	2.51	0.41
1:A:1183:HIS:HA	1:A:1186:MET:HG3	2.03	0.41
1:A:1182:PHE:HA	1:A:1185:ALA:HB1	2.01	0.41
1:A:1334:ALA:HB3	1:B:1347:LEU:HD13	2.01	0.41
1:A:423:LEU:HD11	1:A:458:TYR:CD1	2.54	0.41
1:A:696:ASP:HB3	1:A:706:VAL:HG13	2.02	0.41
1:B:565:ILE:HD13	1:B:1074:HIS:HA	2.03	0.41
1:B:407:LYS:CA	1:B:408:TRP:CB	2.92	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:A:605:LYS:HA	1:A:606:PRO:HD3	1.88	0.41
1:B:393:VAL:O	1:B:394:VAL:CB	2.64	0.41
1:B:400:ASN:OD1	1:B:509:PRO:HB3	2.20	0.41
1:A:794:LEU:HD11	1:A:802:LEU:HD11	2.03	0.41
1:A:799:LEU:HB2	1:A:800:PRO:HD3	2.02	0.41
1:A:869:ASP:HB3	4:A:2264:HOH:O	2.21	0.41
1:B:1203:LEU:HG	1:B:1329:LEU:HD22	2.03	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:A:1141:LEU:HD13	1:A:1141:LEU:HA	1.89	0.41
1:A:1146:PRO:CB	1:A:1148:TYR:CE2	3.04	0.41
1:B:1218:ARG:N	1:B:1219:SER:CB	2.77	0.41
1:B:428:LYS:O	1:B:429:VAL:CG2	2.68	0.41
1:B:400:ASN:HD22	1:B:404:LYS:NZ	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:429:VAL:HG22	1:B:463:PHE:CZ	2.55	0.41
1:A:1089:LYS:HB2	1:A:1107:LEU:HB3	2.03	0.40
1:B:457:LEU:H	1:B:459:ARG:HG2	1.86	0.40
1:B:775:LYS:HG2	4:B:2109:HOH:O	2.20	0.40
1:A:1150:SER:HB2	4:A:2426:HOH:O	2.20	0.40
1:B:1087:ASN:O	1:B:1091:ARG:HG3	2.21	0.40
1:A:488:LYS:HE3	1:B:1371:GLU:O	2.22	0.40
1:B:419:GLU:N	1:B:422:ARG:HB2	2.26	0.40
1:B:456:THR:O	1:B:459:ARG:HG2	2.21	0.40
1:A:454:TRP:O	1:A:458:TYR:CD1	2.75	0.40
1:A:648:SER:HA	1:A:1065:THR:HG21	2.03	0.40
1:B:391:ALA:HB3	1:B:563:GLU:CG	2.45	0.40
1:B:431:LEU:HD13	1:B:432:GLU:OE1	2.21	0.40
1:A:1265:TRP:CZ2	1:A:1325:ALA:HB2	2.56	0.40
1:A:485:PHE:HB3	1:A:532:PRO:HB2	2.02	0.40
1:A:557:GLN:HE21	1:A:557:GLN:HB3	1.68	0.40
1:B:449:ASP:O	1:B:450:VAL:HB	2.22	0.40
1:A:1220:SER:H	1:A:1221:ALA:CB	2.29	0.40
1:A:1207:TYR:CE2	1:A:1311:LYS:HG3	2.55	0.40
1:A:459:ARG:HB3	1:A:460:LEU:H	1.52	0.40
1:A:626:VAL:O	1:A:626:VAL:HG13	2.22	0.40
1:B:547:SER:CB	1:B:548:PRO:CD	2.99	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%)	13	16
1	B	812/891 (91%)	716 (88%)	96 (12%)	6	6
All	All	1627/1782 (91%)	1464 (90%)	163 (10%)	9	10

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	0.89	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	436:LEU	C	437:GLY	N	1.62

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	935/1022 (91%)	0.83	140 (14%) 3 4	39, 50, 65, 78	0
1	B	932/1022 (91%)	1.09	191 (20%) 1 1	38, 51, 64, 77	0
All	All	1867/2044 (91%)	0.96	331 (17%) 2 2	38, 51, 64, 78	0

All (331) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	590	TYR	12.6
1	B	1191	ASP	11.1
1	B	507	THR	10.2
1	B	466	LYS	9.6
1	A	626	VAL	9.3
1	A	1186	MET	9.1
1	B	460	LEU	9.0
1	A	604	PRO	8.8
1	B	1189	ALA	8.7
1	B	464	ARG	8.6
1	B	626	VAL	8.5
1	B	468	PHE	8.5
1	A	1138	GLY	8.0
1	B	443	SER	8.0
1	B	1190	LYS	8.0
1	B	1192	THR	7.9
1	B	459	ARG	7.6
1	A	627	PHE	7.3
1	A	589	GLY	7.2
1	B	1195	GLY	7.2
1	B	508	ALA	7.0
1	B	469	PRO	7.0
1	B	454	TRP	6.8
1	B	1184	ASN	6.5

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Mol	Chain	Res	Type	RSRZ
1	B	1185	ALA	6.2
1	B	607	ILE	6.1
1	A	1141	LEU	6.1
1	B	428	LYS	6.0
1	B	546	THR	6.0
1	A	1191	ASP	5.9
1	A	1218	ARG	5.9
1	A	468	PHE	5.8
1	A	457	LEU	5.8
1	A	849	TYR	5.7
1	B	512	LEU	5.7
1	A	467	PRO	5.6
1	A	1254	TYR	5.6
1	B	1188	ALA	5.5
1	A	1188	ALA	5.5
1	A	1222	LEU	5.5
1	A	1187	LYS	5.4
1	B	488	LYS	5.4
1	B	589	GLY	5.4
1	A	1192	THR	5.3
1	B	1194	ASP	5.3
1	B	1154	LEU	5.3
1	B	396	ALA	5.1
1	B	1156	ARG	5.0
1	A	1185	ALA	5.0
1	B	436	LEU	4.8
1	B	1252	ASP	4.8
1	A	1193	GLU	4.8
1	A	605	LYS	4.6
1	B	1218	ARG	4.6
1	A	1372	GLY	4.6
1	A	399	ARG	4.6
1	A	420	VAL	4.6
1	A	458	TYR	4.5
1	B	425	MET	4.5
1	A	1217	SER	4.5
1	A	558	PRO	4.4
1	A	559	ALA	4.4
1	A	396	ALA	4.4
1	B	1254	TYR	4.3
1	B	739	PHE	4.3
1	A	1166	LEU	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	1215	ASP	4.3
1	B	467	PRO	4.2
1	B	1140	ALA	4.2
1	A	438	LEU	4.2
1	B	1373	ASP	4.2
1	B	440	TYR	4.2
1	A	466	LYS	4.2
1	A	1373	ASP	4.2
1	A	1189	ALA	4.1
1	B	503	ASP	4.1
1	B	429	VAL	4.1
1	B	1186	MET	4.0
1	B	510	LEU	4.0
1	B	1137	LEU	4.0
1	A	469	PRO	4.0
1	A	1304	LEU	4.0
1	B	780	LEU	4.0
1	B	1157	GLY	4.0
1	A	409	LEU	4.0
1	A	588	ALA	4.0
1	B	620	ILE	3.9
1	B	463	PHE	3.9
1	B	553	VAL	3.9
1	B	849	TYR	3.9
1	A	989	ILE	3.9
1	B	947	GLU	3.9
1	B	449	ASP	3.9
1	A	546	THR	3.9
1	A	1190	LYS	3.9
1	B	623	ARG	3.8
1	A	395	ALA	3.8
1	B	456	THR	3.8
1	A	547	SER	3.8
1	A	606	PRO	3.8
1	B	520	PHE	3.8
1	B	1015	VAL	3.8
1	B	439	LYS	3.8
1	B	989	ILE	3.8
1	B	1182	PHE	3.7
1	B	461	ASP	3.7
1	B	1138	GLY	3.7
1	B	470	GLU	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	464	ARG	3.7
1	A	1315	HIS	3.7
1	B	518	LEU	3.6
1	B	1166	LEU	3.6
1	A	641	GLN	3.6
1	B	1187	LYS	3.6
1	A	1163	ILE	3.6
1	B	391	ALA	3.5
1	B	434	GLU	3.5
1	B	442	PRO	3.5
1	B	548	PRO	3.5
1	B	559	ALA	3.5
1	B	398	LEU	3.5
1	B	1151	ASP	3.5
1	A	417	ALA	3.5
1	A	1184	ASN	3.5
1	A	759	ILE	3.4
1	B	651	LEU	3.4
1	B	588	ALA	3.4
1	B	1193	GLU	3.4
1	B	433	ASP	3.4
1	A	400	ASN	3.4
1	B	472	PRO	3.3
1	B	545	SER	3.3
1	B	960	VAL	3.3
1	B	570	MET	3.3
1	A	620	ILE	3.3
1	B	558	PRO	3.3
1	A	1282	SER	3.3
1	A	1107	LEU	3.3
1	B	412	ALA	3.2
1	B	991	PHE	3.2
1	B	1107	LEU	3.2
1	A	463	PHE	3.2
1	B	404	LYS	3.2
1	B	413	PRO	3.2
1	B	755	ASP	3.2
1	A	555	SER	3.2
1	B	505	SER	3.2
1	B	971	ILE	3.1
1	B	502	PRO	3.1
1	A	960	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	511	TYR	3.1
1	A	390	HIS	3.1
1	B	1217	SER	3.1
1	B	1282	SER	3.1
1	B	1216	LYS	3.0
1	A	923	ILE	3.0
1	A	990	ILE	3.0
1	A	991	PHE	3.0
1	B	390	HIS	3.0
1	A	570	MET	3.0
1	B	563	GLU	3.0
1	A	701	SER	3.0
1	A	1015	VAL	3.0
1	B	1016	CYS	3.0
1	B	1257	ARG	3.0
1	B	437	GLY	3.0
1	A	510	LEU	3.0
1	B	1068	MET	3.0
1	B	1222	LEU	3.0
1	A	1210	PHE	3.0
1	B	1065	THR	3.0
1	B	458	TYR	3.0
1	B	409	LEU	3.0
1	B	625	ASP	3.0
1	B	556	LYS	3.0
1	A	780	LEU	2.9
1	B	448	ARG	2.9
1	A	560	ALA	2.9
1	B	432	GLU	2.9
1	B	1074	HIS	2.9
1	B	455	LYS	2.9
1	A	1140	ALA	2.9
1	A	459	ARG	2.9
1	B	1219	SER	2.9
1	A	1139	GLY	2.9
1	B	1215	ASP	2.8
1	B	1253	PRO	2.8
1	B	547	SER	2.8
1	B	1265	TRP	2.8
1	B	494	LEU	2.8
1	A	1110	LEU	2.8
1	B	392	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	501	ASN	2.8
1	A	1162	ILE	2.8
1	B	418	TRP	2.8
1	A	999	LEU	2.7
1	A	394	VAL	2.7
1	B	424	PHE	2.7
1	A	428	LYS	2.7
1	B	482	THR	2.7
1	B	1212	GLU	2.7
1	B	999	LEU	2.7
1	A	1068	MET	2.7
1	A	439	LYS	2.7
1	A	1211	LYS	2.7
1	B	430	ASP	2.7
1	B	988	VAL	2.7
1	B	1141	LEU	2.7
1	A	1321	VAL	2.7
1	B	414	LEU	2.7
1	B	465	GLY	2.6
1	A	461	ASP	2.6
1	A	556	LYS	2.6
1	A	423	LEU	2.6
1	A	1237	GLU	2.6
1	B	1296	ARG	2.6
1	B	506	PRO	2.6
1	B	399	ARG	2.6
1	A	850	SER	2.6
1	A	541	PRO	2.6
1	B	1132	LEU	2.6
1	B	1356	LEU	2.6
1	B	850	SER	2.6
1	B	1177	LYS	2.6
1	A	802	LEU	2.6
1	A	959	LEU	2.6
1	A	1183	HIS	2.6
1	A	755	ASP	2.6
1	B	759	ILE	2.6
1	B	990	ILE	2.6
1	A	1132	LEU	2.5
1	B	427	CYS	2.5
1	B	1063	GLN	2.5
1	A	1316	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	391	ALA	2.5
1	A	506	PRO	2.5
1	A	1137	LEU	2.5
1	B	438	LEU	2.5
1	B	959	LEU	2.5
1	A	465	GLY	2.5
1	A	421	THR	2.5
1	A	548	PRO	2.5
1	B	1139	GLY	2.5
1	B	471	LYS	2.5
1	A	796	LEU	2.5
1	B	1180	GLU	2.5
1	A	511	TYR	2.5
1	A	971	ILE	2.5
1	B	924	ALA	2.4
1	A	801	VAL	2.4
1	A	1252	ASP	2.4
1	A	739	PHE	2.4
1	B	938	GLY	2.4
1	B	1309	ALA	2.4
1	B	1220	SER	2.4
1	A	1239	GLY	2.4
1	B	1223	LEU	2.4
1	A	946	GLU	2.4
1	A	668	LEU	2.3
1	A	416	VAL	2.3
1	B	1155	GLY	2.3
1	A	502	PRO	2.3
1	A	924	ALA	2.3
1	B	492	VAL	2.3
1	A	642	ARG	2.3
1	B	1064	THR	2.3
1	A	1120	GLN	2.3
1	A	424	PHE	2.3
1	B	1133	ARG	2.3
1	A	540	ILE	2.3
1	B	1354	ALA	2.3
1	A	448	ARG	2.3
1	A	1069	ILE	2.3
1	B	951	THR	2.2
1	A	1371	GLU	2.2
1	B	616	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	1163	ILE	2.2
1	A	1116	ASP	2.2
1	A	988	VAL	2.2
1	A	623	ARG	2.2
1	A	1236	LYS	2.2
1	A	1285	ILE	2.2
1	B	740	GLY	2.2
1	A	1032	LEU	2.2
1	A	507	THR	2.2
1	B	395	ALA	2.2
1	A	799	LEU	2.2
1	B	1236	LYS	2.2
1	B	446	THR	2.2
1	B	1149	LYS	2.2
1	B	420	VAL	2.2
1	B	450	VAL	2.2
1	B	457	LEU	2.2
1	A	740	GLY	2.2
1	B	1162	ILE	2.1
1	B	923	ILE	2.1
1	B	403	PRO	2.1
1	B	435	SER	2.1
1	B	1072	SER	2.1
1	A	711	VAL	2.1
1	B	735	VAL	2.1
1	B	473	PRO	2.1
1	B	802	LEU	2.1
1	B	1352	MET	2.1
1	A	746	TRP	2.1
1	A	742	ALA	2.1
1	A	1354	ALA	2.1
1	A	951	THR	2.1
1	B	711	VAL	2.1
1	A	672	ILE	2.1
1	A	434	GLU	2.1
1	B	714	MET	2.1
1	A	937	VAL	2.1
1	B	410	HIS	2.0
1	B	498	LEU	2.0
1	B	1143	LEU	2.0
1	B	1150	SER	2.0
1	B	937	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	820	LEU	2.0
1	B	912	ILE	2.0
1	B	519	MET	2.0
1	A	703	THR	2.0
1	B	1183	HIS	2.0
1	B	444	TRP	2.0
1	A	1229	ASN	2.0
1	B	400	ASN	2.0
1	A	494	LEU	2.0
1	B	453	ILE	2.0
1	B	1110	LEU	2.0
1	B	1231	ILE	2.0
1	B	1035	ASP	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no 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, 95<sup>th</sup> 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(Å <sup>2</sup> )	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.