



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:50 PM UTC

PDB ID : 4N78 / pdb_00004n78
Title : The WAVE Regulatory Complex Links Diverse Receptors to the Actin Cytoskeleton
Authors : Chen, Z.C.
Deposited on : 2013-10-15
Resolution : 2.43 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

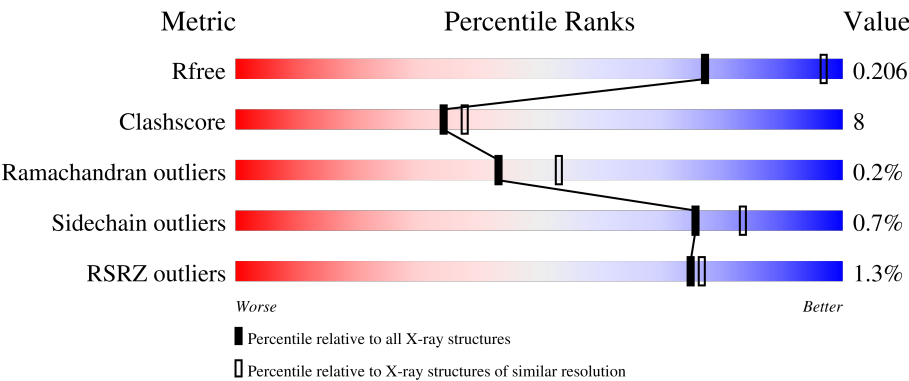
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.43 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	2340 (2.46-2.42)
Clashscore	190562	2400 (2.46-2.42)
Ramachandran outliers	187476	2379 (2.46-2.42)
Sidechain outliers	187428	2379 (2.46-2.42)
RSRZ outliers	180081	2340 (2.46-2.42)

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

Mol	Chain	Length	Quality of chain
1	A	1253	% 75% 19% 6%
2	B	1128	81% 15% .
3	D	559	3% 28% 8% 64%
4	E	75	% 68% 21% 11%
5	F	514	% 24% 6% 70%

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Mol	Chain	Length	Quality of chain
6	P	15	 53%47%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 22843 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 Cytoplasmic FMR1-interacting protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1184	Total	C	N	O	S	7	7	0
			9745	6233	1672	1772	68			

- Molecule 2 is a protein called Nck-associated protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1085	Total	C	N	O	S	0	3	0
			8709	5565	1454	1620	70			

- Molecule 3 is a protein called Wiskott-Aldrich syndrome protein family member 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	202	Total	C	N	O	S	0	0	0
			1657	1043	288	322	4			

- Molecule 4 is a protein called Protein BRICK1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	67	Total	C	N	O	S	0	2	0
			571	356	103	110	2			

- Molecule 5 is a protein called Abl interactor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	156	Total	C	N	O	S	0	0	0
			1253	780	227	241	5			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	0	ALA	-	expression tag	UNP J3KNB2

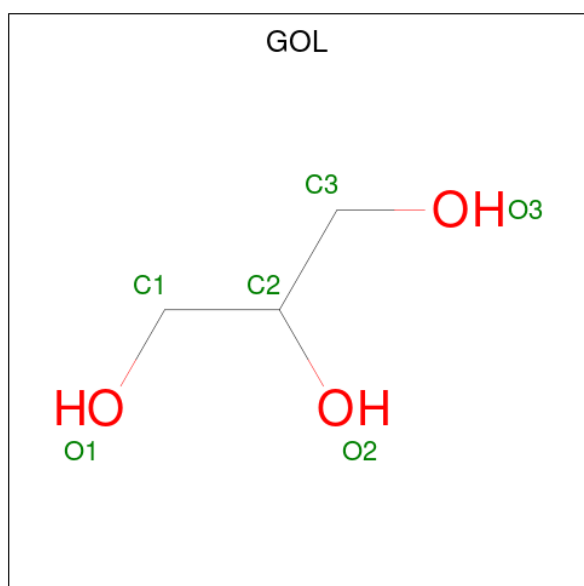
- Molecule 6 is a protein called WIRS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	P	8	Total	C	N	O	S	0	0	0
			62	38	12	11	1			

- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Cl	0	0
			1	1		
7	B	3	Total	Cl	0	0
			3	3		

- Molecule 8 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			6	3	3		
8	A	1	Total	C	O	0	0
			6	3	3		
8	A	1	Total	C	O	0	0
			6	3	3		
8	A	1	Total	C	O	0	0
			6	3	3		
8	A	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		

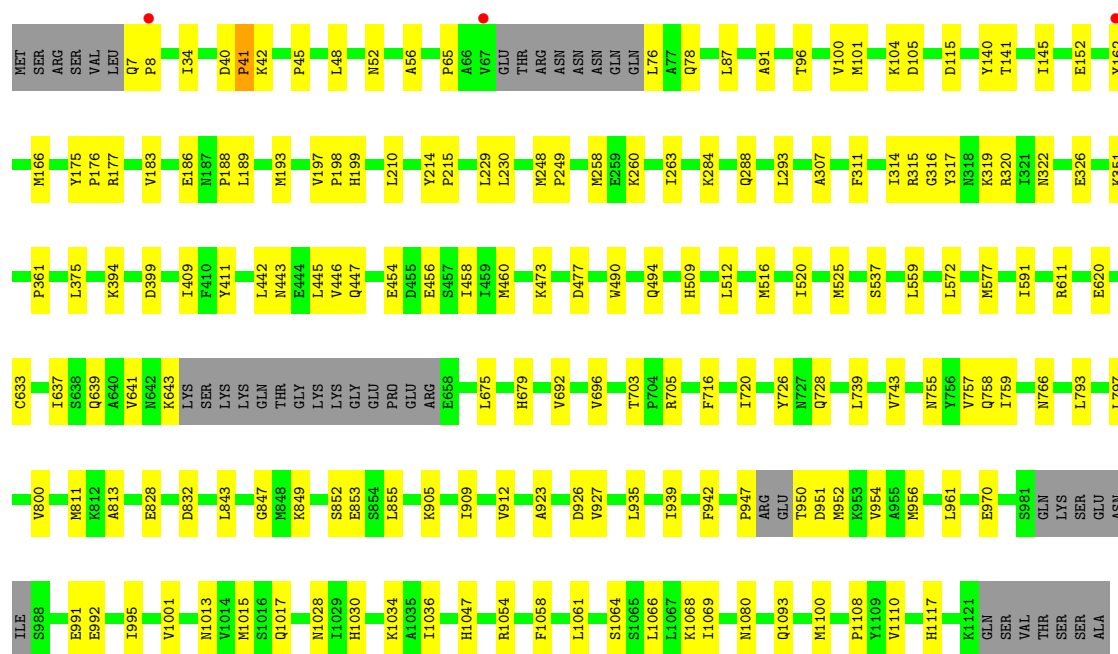
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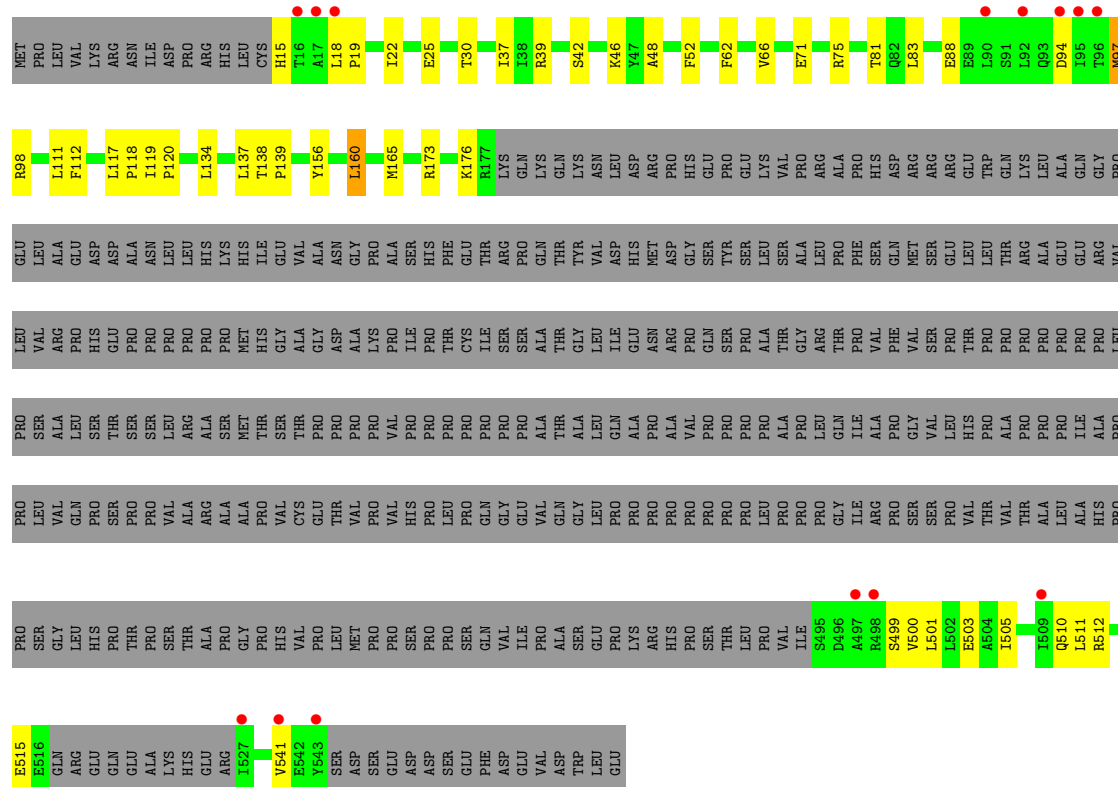
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total C O 6 3 3	0	0
8	B	1	Total C O 6 3 3	0	0
8	B	1	Total C O 6 3 3	0	0
8	B	1	Total C O 6 3 3	0	0
8	B	1	Total C O 6 3 3	0	0
8	B	1	Total C O 6 3 3	0	0
8	B	1	Total C O 6 3 3	0	0
8	B	1	Total C O 6 3 3	0	0
8	F	1	Total C O 6 3 3	0	0
8	F	1	Total C O 6 3 3	0	0

- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	330	Total O 330 330	0	0
9	B	355	Total O 355 355	0	0
9	D	26	Total O 26 26	0	0
9	E	14	Total O 14 14	0	0
9	F	21	Total O 21 21	0	0



• Molecule 3: Wiskott-Aldrich syndrome protein family member 1

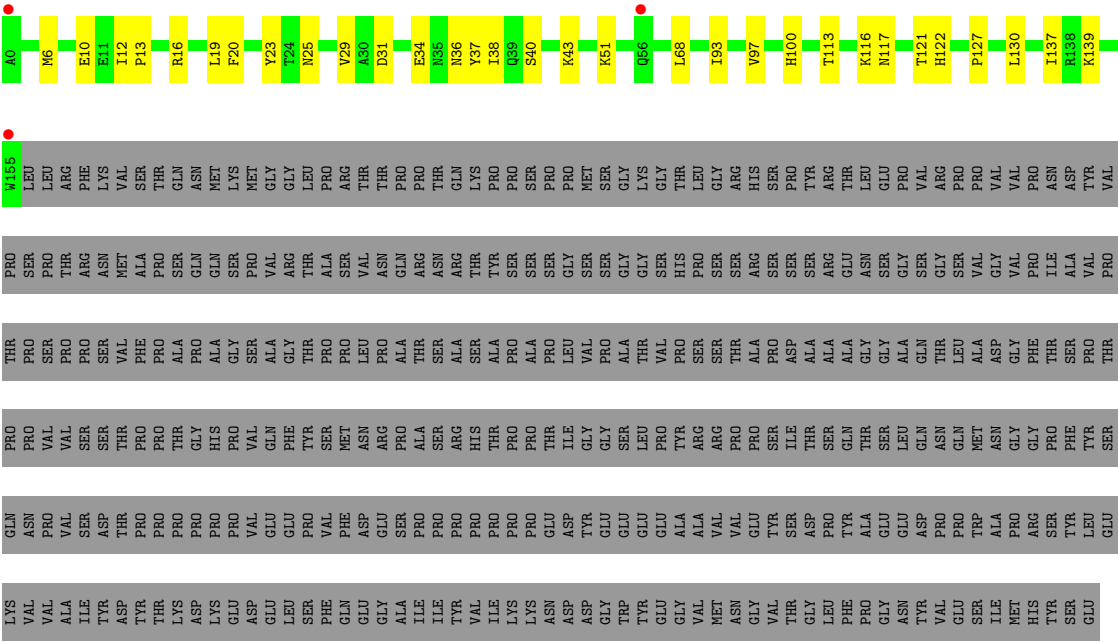


• Molecule 4: Protein BRICK1

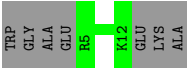




● Molecule 5: Abl interactor 2



● Molecule 6: WIRS



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	97.49Å 114.75Å 323.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.98 – 2.43 19.98 – 2.43	Depositor EDS
% Data completeness (in resolution range)	99.6 (19.98-2.43) 90.2 (19.98-2.43)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 2.34Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.189 , 0.209 0.185 , 0.206	Depositor DCC
R_{free} test set	2000 reflections (1.33%)	wwPDB-VP
Wilson B-factor (Å ²)	40.2	Xtriage
Anisotropy	0.630	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 50.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	22843	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.01% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, GOL

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	0.26	0/9958	0.63	0/13441
2	B	0.26	0/8880	0.66	4/12009 (0.0%)
3	D	0.27	0/1682	0.67	0/2265
4	E	0.27	0/582	0.61	0/782
5	F	0.26	0/1270	0.64	0/1717
6	P	0.20	0/62	0.52	0/79
All	All	0.26	0/22434	0.65	4/30293 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	703	THR	CA-C-N	6.14	125.63	119.24
2	B	703	THR	C-N-CA	6.14	125.63	119.24
2	B	559	LEU	CA-C-N	5.23	124.68	119.24
2	B	559	LEU	C-N-CA	5.23	124.68	119.24

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	9745	0	9753	179	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	8709	0	8766	115	0
3	D	1657	0	1663	41	0
4	E	571	0	568	22	0
5	F	1253	0	1269	25	0
6	P	62	0	63	0	0
7	A	1	0	0	0	0
7	B	3	0	0	1	0
8	A	30	0	40	5	0
8	B	54	0	72	5	0
8	F	12	0	16	2	0
9	A	330	0	0	10	0
9	B	355	0	0	5	0
9	D	26	0	0	0	0
9	E	14	0	0	0	0
9	F	21	0	0	0	0
All	All	22843	0	22210	338	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (338) 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)
2:B:314:ILE:HG22	2:B:315:ARG:H	1.39	0.87
1:A:556:SER:HG	3:D:15:HIS:N	1.72	0.87
1:A:177:MET:HE3	1:A:178:LYS:HG2	1.59	0.83
2:B:446:VAL:HG22	2:B:460:MET:HE2	1.62	0.80
1:A:212:MET:O	1:A:216:ASN:ND2	2.14	0.79
3:D:30:THR:HG21	4:E:18:ASN:HD22	1.48	0.79
2:B:105:ASP:OD2	2:B:177:ARG:NH2	2.18	0.77
5:F:137:ILE:HG22	8:F:602:GOL:H31	1.68	0.74
1:A:660:MET:HE2	1:A:660:MET:HA	1.71	0.72
1:A:660:MET:HE3	2:B:1117:HIS:CD2	2.24	0.72
2:B:473:LYS:NZ	2:B:477:ASP:OD1	2.24	0.71
3:D:18:LEU:HB3	3:D:19:PRO:HD2	1.72	0.71
4:E:69:THR:HG22	4:E:70:LYS:H	1.54	0.71
2:B:166:MET:HA	2:B:166:MET:HE3	1.73	0.70
1:A:513:ALA:HA	1:A:516:LYS:HE3	1.75	0.69
2:B:696:VAL:H	8:B:1211:GOL:HO2	1.40	0.68
4:E:6:ASP:HB3	4:E:7:PRO:HD3	1.74	0.68
2:B:620:GLU:HG2	2:B:675:LEU:HD13	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:7:GLN:N	2:B:8:PRO:HD3	2.10	0.67
4:E:9:GLN:O	4:E:13[B]:HIS:HD2	1.77	0.67
3:D:117:LEU:HD12	3:D:118:PRO:HD2	1.75	0.67
5:F:37:TYR:CZ	5:F:43:LYS:HG3	2.30	0.67
1:A:956:MET:HE1	1:A:1133:ALA:HB2	1.75	0.66
2:B:210:LEU:HD22	2:B:258:MET:HE3	1.76	0.66
5:F:6:MET:O	5:F:10:GLU:HG2	1.95	0.66
3:D:37:ILE:HD11	4:E:22:ILE:HG23	1.78	0.66
1:A:556:SER:OG	3:D:15:HIS:ND1	2.21	0.66
2:B:1015:MET:HE2	2:B:1015:MET:HA	1.78	0.65
2:B:45:PRO:HB2	2:B:48:LEU:HD23	1.79	0.64
2:B:52:ASN:ND2	2:B:78:GLN:OE1	2.30	0.64
2:B:951:ASP:OD2	2:B:952:MET:N	2.31	0.64
3:D:511:LEU:O	3:D:515:GLU:HB3	1.98	0.63
1:A:1135:GLN:HA	1:A:1138:TYR:CE2	2.34	0.63
4:E:40:ASP:O	4:E:44:ARG:HG2	1.98	0.63
3:D:88:GLU:OE1	5:F:100:HIS:NE2	2.25	0.63
2:B:1013:ASN:O	2:B:1080:ASN:ND2	2.30	0.62
2:B:351:LYS:NZ	2:B:411:TYR:OH	2.33	0.62
1:A:212:MET:HE2	1:A:212:MET:HA	1.82	0.62
1:A:494:GLU:HB3	1:A:495:PRO:HD3	1.81	0.62
1:A:556:SER:OG	3:D:15:HIS:N	2.34	0.60
1:A:345:ILE:HD12	1:A:346:CYS:N	2.17	0.60
1:A:307:LEU:HD23	1:A:311:MET:HE3	1.83	0.60
3:D:165:MET:HA	3:D:165:MET:HE2	1.83	0.60
1:A:468:MET:HE2	1:A:468:MET:HA	1.83	0.60
2:B:260:LYS:NZ	9:B:1419:HOH:O	2.35	0.60
1:A:408:VAL:HG12	1:A:409:MET:HE2	1.83	0.60
1:A:116:GLU:HB3	1:A:117:PRO:HD3	1.84	0.60
1:A:1225:TYR:OH	2:B:755:ASN:OD1	2.12	0.59
1:A:932:GLU:OE2	3:D:499:SER:OG	2.12	0.59
2:B:800:VAL:HG11	2:B:912:VAL:HG11	1.85	0.59
2:B:951:ASP:HB3	2:B:954:VAL:HG12	1.84	0.59
4:E:21:TYR:CE1	5:F:51:LYS:HE2	2.37	0.59
2:B:442:LEU:HD13	2:B:516:MET:HE1	1.85	0.58
5:F:139:LYS:HE2	8:F:602:GOL:H11	1.84	0.58
7:B:1201:CL:CL	8:B:1208:GOL:H31	2.40	0.58
1:A:100:GLU:N	1:A:100:GLU:OE1	2.37	0.58
1:A:1004:ILE:HD11	1:A:1100:ILE:CD1	2.33	0.57
1:A:660:MET:HE3	2:B:1117:HIS:HD2	1.67	0.57
1:A:521:TRP:H	4:E:13[B]:HIS:CE1	2.22	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1185:LYS:NZ	9:A:1524:HOH:O	2.37	0.57
3:D:22:ILE:CG1	3:D:25:GLU:HB2	2.36	0.56
5:F:51:LYS:C	5:F:51:LYS:HD3	2.30	0.56
1:A:969:SER:OG	1:A:970:PRO:HD3	2.05	0.56
1:A:304:VAL:HG21	1:A:417:VAL:HG21	1.86	0.56
1:A:162:GLY:O	1:A:165:ILE:HG12	2.05	0.56
1:A:189:LYS:NZ	1:A:207:SER:OG	2.39	0.56
1:A:879:LYS:HD3	1:A:880:GLN:H	1.71	0.56
2:B:726:TYR:CE2	2:B:728:GLN:HG2	2.41	0.56
1:A:59:TYR:HB2	1:A:561:MET:HE1	1.88	0.55
1:A:422:LYS:HB3	1:A:430:ASP:OD1	2.06	0.55
2:B:456:GLU:N	2:B:456:GLU:OE1	2.39	0.55
1:A:382:LYS:HB2	1:A:387:TYR:CZ	2.42	0.55
1:A:1026:ALA:HB3	1:A:1027:PRO:HD3	1.89	0.55
1:A:412:TYR:CZ	1:A:416:LEU:HD11	2.42	0.55
1:A:911:PRO:N	1:A:912:PRO:HD2	2.22	0.54
1:A:1044:ASP:O	1:A:1048:LYS:HE3	2.08	0.54
1:A:1057:LEU:HA	2:B:961:LEU:HD23	1.88	0.54
2:B:314:ILE:HG22	2:B:315:ARG:N	2.17	0.54
2:B:1028:ASN:HA	2:B:1030:HIS:CE1	2.43	0.54
1:A:498:GLN:HE22	1:A:585:GLU:HG3	1.71	0.54
2:B:214:TYR:HB3	2:B:215:PRO:HD3	1.90	0.54
1:A:521:TRP:N	4:E:13[B]:HIS:HE1	2.06	0.54
1:A:521:TRP:N	4:E:13[B]:HIS:CE1	2.76	0.54
1:A:1226:LEU:O	1:A:1227:LYS:C	2.51	0.54
2:B:766:ASN:OD1	9:B:1551:HOH:O	2.18	0.54
1:A:525:HIS:HA	4:E:9:GLN:NE2	2.24	0.53
1:A:263:LEU:O	1:A:267:MET:HG3	2.08	0.53
1:A:762:ILE:HD12	3:D:111:LEU:HD23	1.90	0.53
2:B:443:ASN:O	2:B:447:GLN:HG2	2.08	0.53
2:B:1036:ILE:HD13	2:B:1058:PHE:CZ	2.43	0.53
1:A:1060:VAL:HB	1:A:1061:PRO:HD3	1.91	0.53
2:B:375:LEU:HB3	2:B:537:SER:HB3	1.91	0.52
2:B:992:GLU:HG3	2:B:1047:HIS:NE2	2.24	0.52
3:D:503:GLU:OE1	3:D:503:GLU:N	2.41	0.52
1:A:427:ASP:O	1:A:429:PRO:HD3	2.10	0.52
1:A:301:GLN:HG3	1:A:343:TYR:OH	2.09	0.52
1:A:557:THR:HG23	3:D:15:HIS:N	2.24	0.52
1:A:1043:LEU:HD13	1:A:1044:ASP:H	1.73	0.52
2:B:793:LEU:HD21	2:B:855:LEU:HD23	1.92	0.52
1:A:602:TYR:O	1:A:606:ILE:HG12	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:454:GLU:O	2:B:458:ILE:HG13	2.11	0.51
1:A:754:HIS:O	1:A:754:HIS:ND1	2.43	0.51
1:A:525:HIS:HA	4:E:9:GLN:HE21	1.76	0.51
1:A:1004:ILE:HD11	1:A:1100:ILE:HD12	1.92	0.51
3:D:138:THR:HB	3:D:139:PRO:HD3	1.92	0.51
1:A:382:LYS:HG3	1:A:386:GLU:OE1	2.11	0.51
1:A:966:GLU:OE1	1:A:966:GLU:N	2.35	0.51
2:B:490:TRP:O	2:B:494:GLN:HG3	2.11	0.51
1:A:989:LEU:O	1:A:993:CYS:HB2	2.10	0.51
2:B:394:LYS:HE3	2:B:399:ASP:O	2.11	0.51
1:A:174:LEU:HA	1:A:177:MET:HE2	1.93	0.50
2:B:442:LEU:CD1	2:B:516:MET:HE1	2.41	0.50
3:D:97:MET:HE2	3:D:97:MET:HA	1.92	0.50
1:A:744:ASN:OD1	1:A:745:ARG:N	2.37	0.50
1:A:476:ILE:HD13	1:A:605:LEU:HB3	1.92	0.50
1:A:807:MET:HE3	1:A:811:LEU:HD21	1.93	0.50
2:B:1054:ARG:HA	2:B:1054:ARG:NE	2.26	0.50
2:B:315:ARG:C	2:B:317:TYR:H	2.19	0.50
1:A:566:LEU:HD22	1:A:592:ILE:HG23	1.94	0.50
1:A:1163:MET:HA	1:A:1222:LEU:HD13	1.94	0.50
1:A:345:ILE:O	1:A:349:MET:HG2	2.11	0.50
1:A:1094:GLU:OE2	1:A:1227:LYS:HE3	2.12	0.49
2:B:516:MET:O	2:B:520:ILE:HG12	2.12	0.49
2:B:1093:GLN:OE1	2:B:1100:MET:HE3	2.12	0.49
1:A:791:ASP:OD1	1:A:793:THR:OG1	2.29	0.49
1:A:919:ARG:NH1	1:A:1017:GLU:HG3	2.27	0.49
4:E:69:THR:HG22	4:E:70:LYS:N	2.23	0.49
1:A:308:PHE:CD1	8:A:1304:GOL:H2	2.47	0.49
1:A:521:TRP:H	4:E:13[B]:HIS:HE1	1.59	0.49
1:A:344:ASN:OD1	1:A:346:CYS:HB3	2.13	0.49
2:B:40:ASP:C	2:B:42:LYS:H	2.21	0.49
1:A:1138:TYR:HB2	1:A:1149:VAL:HG11	1.94	0.49
1:A:861:THR:HG22	2:B:675:LEU:HD23	1.94	0.48
2:B:189:LEU:O	2:B:193:MET:HG3	2.12	0.48
2:B:947:PRO:C	2:B:950:THR:HB	2.37	0.48
1:A:710:ILE:HD13	1:A:750:LEU:HD21	1.95	0.48
1:A:941:LEU:O	1:A:946:LEU:HB2	2.13	0.48
2:B:229:LEU:HG	2:B:230:LEU:HG	1.95	0.48
1:A:1066:LEU:HB2	2:B:942:PHE:HZ	1.77	0.48
1:A:1094:GLU:HG2	1:A:1225:TYR:O	2.13	0.48
2:B:115:ASP:OD2	2:B:199:HIS:ND1	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:319:LYS:HG2	2:B:320:ARG:HH12	1.77	0.48
1:A:150:LYS:HE2	1:A:150:LYS:HA	1.95	0.48
1:A:753:ARG:HD3	9:A:1495:HOH:O	2.13	0.48
1:A:399:GLN:O	1:A:403:GLN:HG3	2.14	0.48
1:A:964:ARG:HB3	1:A:966:GLU:OE1	2.14	0.48
2:B:104:LYS:HG3	2:B:140:TYR:CE1	2.48	0.48
2:B:813:ALA:HB2	2:B:832:ASP:HA	1.95	0.48
1:A:511:LEU:O	1:A:515:ARG:HG3	2.13	0.48
2:B:970:GLU:H	2:B:970:GLU:CD	2.21	0.48
1:A:1135:GLN:HA	1:A:1138:TYR:CZ	2.49	0.48
1:A:93:ILE:HG12	3:D:137:LEU:HD22	1.96	0.47
2:B:65:PRO:HD3	2:B:183:VAL:HG11	1.96	0.47
1:A:89:CYS:HB2	1:A:115:LEU:HD21	1.96	0.47
2:B:263:ILE:HD12	2:B:293:LEU:HD11	1.97	0.47
3:D:62:PHE:CZ	4:E:51:ASN:HB2	2.49	0.47
3:D:46:LYS:HD2	5:F:23:TYR:CE2	2.49	0.47
1:A:409:MET:HE1	1:A:621:LEU:HG	1.96	0.47
3:D:42:SER:OG	5:F:23:TYR:O	2.32	0.47
3:D:119:ILE:HB	3:D:120:PRO:HD3	1.96	0.47
2:B:445:LEU:HD22	2:B:512:LEU:HD13	1.97	0.47
2:B:639:GLN:O	2:B:643:LYS:HB2	2.14	0.47
3:D:501:LEU:O	3:D:505:ILE:HG13	2.14	0.47
1:A:345:ILE:HA	1:A:348:GLN:HG3	1.97	0.47
5:F:12:ILE:O	5:F:16:ARG:HB2	2.15	0.47
1:A:644:MET:HB2	1:A:645:PRO:HD3	1.97	0.47
1:A:956:MET:HG3	1:A:957:PRO:HD2	1.97	0.47
1:A:1136:PHE:HA	1:A:1180:CYS:SG	2.55	0.47
4:E:68:VAL:HG12	4:E:68:VAL:O	2.15	0.47
1:A:742:PRO:HB2	8:A:1302:GOL:H32	1.96	0.47
1:A:880:GLN:HB3	9:A:1619:HOH:O	2.14	0.47
2:B:197:VAL:N	2:B:198:PRO:HD2	2.30	0.47
2:B:315:ARG:O	2:B:317:TYR:N	2.45	0.47
3:D:48:ALA:HB3	5:F:19:LEU:HD21	1.97	0.47
1:A:857:TYR:HB2	1:A:864:PHE:CE1	2.50	0.47
3:D:39:ARG:NH2	5:F:31:ASP:OD2	2.47	0.47
3:D:94:ASP:OD1	3:D:98:ARG:HD2	2.15	0.47
1:A:844:PHE:CE1	1:A:932:GLU:HB3	2.50	0.46
2:B:633[B]:CYS:O	2:B:637:ILE:HG12	2.15	0.46
3:D:18:LEU:HB3	3:D:19:PRO:CD	2.44	0.46
4:E:21:TYR:CZ	5:F:51:LYS:HG2	2.50	0.46
1:A:1043:LEU:HD22	1:A:1044:ASP:N	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:526:GLU:H	4:E:9:GLN:NE2	2.13	0.46
1:A:265:LYS:NZ	9:A:1493:HOH:O	2.48	0.46
1:A:869:LEU:N	1:A:870:PRO:HD2	2.31	0.46
5:F:12:ILE:HB	5:F:13:PRO:HD3	1.97	0.46
1:A:143:LEU:HA	1:A:148:ARG:HG2	1.97	0.46
1:A:531:PRO:HB2	1:A:536:GLU:HG3	1.96	0.46
1:A:1135:GLN:OE1	1:A:1215:ASN:ND2	2.48	0.46
2:B:991:GLU:O	2:B:995:ILE:HG12	2.15	0.46
3:D:156:TYR:CE2	3:D:160:LEU:HD22	2.51	0.46
1:A:498:GLN:NE2	1:A:585:GLU:HG3	2.31	0.45
1:A:1119:MET:HE3	1:A:1173:ARG:HD2	1.97	0.45
2:B:1066:LEU:O	2:B:1069:ILE:HG12	2.15	0.45
3:D:46:LYS:HB2	5:F:23:TYR:CD2	2.51	0.45
1:A:356:HIS:CE1	1:A:360:ILE:HD12	2.51	0.45
1:A:932:GLU:O	1:A:936:VAL:HG23	2.17	0.45
2:B:101:MET:SD	2:B:177:ARG:HG2	2.56	0.45
2:B:442:LEU:O	2:B:446:VAL:HG23	2.16	0.45
3:D:52:PHE:CD2	5:F:68:LEU:HD23	2.50	0.45
2:B:1108:PRO:HB2	2:B:1110:VAL:HG22	1.99	0.45
1:A:1045:ALA:O	1:A:1049:ARG:NH2	2.49	0.45
2:B:351:LYS:HG3	2:B:411:TYR:CZ	2.51	0.45
1:A:643:SER:O	1:A:647:ILE:HG13	2.16	0.45
5:F:20:PHE:O	5:F:23:TYR:HB3	2.16	0.45
1:A:200:ASP:HB2	1:A:201:PRO:HD2	1.98	0.45
2:B:525:MET:HA	2:B:525:MET:HE2	1.99	0.45
2:B:692:VAL:HG21	9:B:1490:HOH:O	2.17	0.45
2:B:956:MET:HA	2:B:956:MET:HE2	1.98	0.45
1:A:522:GLU:OE1	1:A:548:PRO:HB3	2.16	0.45
1:A:747:GLU:HG2	9:A:1529:HOH:O	2.15	0.45
1:A:12:SER:O	1:A:16:LEU:HD13	2.17	0.45
1:A:1092:MET:HG2	5:F:113:THR:HG22	1.99	0.45
1:A:99:ASN:O	1:A:104:ARG:NH1	2.50	0.45
1:A:1129:ARG:NH1	1:A:1177:LEU:HB3	2.31	0.45
2:B:490:TRP:CD1	2:B:520:ILE:HG13	2.52	0.45
1:A:1085:ARG:NH1	9:A:1501:HOH:O	2.27	0.44
2:B:577:MET:HE1	2:B:591:ILE:HG22	1.98	0.44
5:F:34:GLU:O	5:F:38:ILE:HG13	2.16	0.44
1:A:730:GLU:HA	1:A:730:GLU:OE2	2.17	0.44
1:A:1045:ALA:O	1:A:1049:ARG:HG3	2.17	0.44
3:D:510:GLN:O	3:D:511:LEU:HD12	2.17	0.44
1:A:1070:GLN:CD	1:A:1070:GLN:H	2.25	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:804:ILE:HD12	1:A:889:HIS:HD2	1.82	0.44
1:A:747:GLU:O	1:A:751:LYS:HG3	2.17	0.44
1:A:751:LYS:NZ	2:B:1093:GLN:OE1	2.51	0.44
1:A:1055:ALA:N	1:A:1056:PRO:CD	2.80	0.44
2:B:96:THR:O	2:B:100:VAL:HG23	2.18	0.44
1:A:8:GLU:CD	1:A:8:GLU:H	2.25	0.44
1:A:411:VAL:O	1:A:415:LYS:HG2	2.17	0.44
1:A:757:LEU:HD23	3:D:112:PHE:CZ	2.53	0.44
1:A:1084:GLU:O	1:A:1085:ARG:HD2	2.17	0.44
1:A:281:ILE:HA	1:A:284:LEU:HD12	1.99	0.44
1:A:129:GLN:O	1:A:133:ILE:HG13	2.18	0.43
1:A:782:LEU:O	1:A:786:ARG:HG2	2.18	0.43
1:A:165:ILE:HD11	1:A:266:VAL:HG13	1.99	0.43
1:A:919:ARG:HH11	1:A:1017:GLU:HG3	1.84	0.43
1:A:1204:MET:O	1:A:1208:ILE:HG13	2.18	0.43
2:B:214:TYR:HB2	2:B:258:MET:HE2	1.99	0.43
1:A:1117:GLY:HA2	9:A:1692:HOH:O	2.16	0.43
2:B:757:VAL:O	2:B:759:ILE:N	2.48	0.43
1:A:20:LEU:HD12	1:A:21:PRO:HD2	1.99	0.43
1:A:497:ARG:NH2	1:A:537:LYS:HE2	2.34	0.43
1:A:852:LEU:HB2	1:A:853:PRO:HD3	1.99	0.43
3:D:83:LEU:HD21	4:E:68:VAL:HG13	1.99	0.43
1:A:388:ARG:O	1:A:391:PHE:HB3	2.18	0.43
1:A:446:GLU:OE1	9:A:1629:HOH:O	2.21	0.43
1:A:533:LEU:O	1:A:533:LEU:HD23	2.18	0.43
2:B:175:TYR:HB3	2:B:176:PRO:HD3	2.01	0.43
2:B:793:LEU:HD23	2:B:797:LEU:HD12	2.01	0.43
1:A:497:ARG:HE	1:A:537:LYS:HG2	1.83	0.43
1:A:1226:LEU:HD12	1:A:1226:LEU:HA	1.87	0.43
2:B:905:LYS:O	2:B:909:ILE:HG13	2.19	0.43
1:A:1187:GLN:OE1	8:A:1303:GOL:O1	2.34	0.43
1:A:725:LYS:HD2	2:B:828:GLU:OE2	2.18	0.43
1:A:1188:LYS:HG2	8:A:1303:GOL:H12	2.01	0.43
2:B:509:HIS:NE2	8:B:1209:GOL:H31	2.33	0.43
3:D:62:PHE:O	3:D:66:VAL:HG23	2.19	0.43
1:A:155:GLU:HG3	1:A:567:GLU:OE2	2.18	0.43
1:A:745:ARG:HA	1:A:747:GLU:OE2	2.19	0.43
3:D:30:THR:HG21	4:E:18:ASN:ND2	2.26	0.43
1:A:725:LYS:HE3	2:B:811[B]:MET:HE2	1.99	0.42
2:B:1034:LYS:HB2	2:B:1034:LYS:HE3	1.82	0.42
5:F:121:THR:OG1	5:F:122:HIS:N	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:ASP:OD1	1:A:289:ARG:NH2	2.35	0.42
1:A:497:ARG:NH1	1:A:498:GLN:HG2	2.34	0.42
1:A:610:GLU:HB2	9:A:1676:HOH:O	2.19	0.42
1:A:1184:LEU:O	1:A:1188:LYS:HG3	2.19	0.42
2:B:409:ILE:HD13	2:B:572:LEU:HD11	2.01	0.42
2:B:843:LEU:HB3	2:B:847:GLY:HA3	2.00	0.42
2:B:716:PHE:O	2:B:720:ILE:HG13	2.20	0.42
2:B:852:SER:HA	2:B:855:LEU:HD12	2.01	0.42
2:B:1015:MET:C	2:B:1017:GLN:H	2.27	0.42
1:A:68:SER:OG	1:A:135:ARG:NH2	2.49	0.42
1:A:1184:LEU:HD11	8:A:1303:GOL:H32	2.01	0.42
1:A:1036:HIS:HD2	1:A:1038:LYS:HE3	1.85	0.42
2:B:611:ARG:HH22	8:B:1208:GOL:H11	1.84	0.42
1:A:265:LYS:NZ	9:A:1506:HOH:O	2.52	0.42
2:B:141:THR:O	2:B:145:ILE:HG13	2.19	0.42
5:F:93:ILE:O	5:F:97:VAL:HG23	2.20	0.42
1:A:101:GLN:HA	1:A:102:PRO:HD3	1.95	0.42
1:A:350:ILE:O	1:A:354:GLU:HG3	2.19	0.42
1:A:767:LEU:HD11	3:D:111:LEU:HD21	2.01	0.42
1:A:839:ILE:O	1:A:843:VAL:HG23	2.20	0.42
2:B:7:GLN:N	2:B:8:PRO:CD	2.82	0.42
3:D:22:ILE:HG12	3:D:25:GLU:HB2	2.02	0.42
1:A:139:GLU:HG2	1:A:157:TYR:OH	2.20	0.41
1:A:1096:ILE:O	1:A:1100:ILE:HG13	2.20	0.41
2:B:923:ALA:O	2:B:927:VAL:HG23	2.20	0.41
1:A:1239:VAL:HG11	2:B:361:PRO:HB2	2.03	0.41
2:B:637:ILE:O	2:B:641:VAL:HG23	2.20	0.41
2:B:849:LYS:O	2:B:853:GLU:HG3	2.21	0.41
2:B:926[A]:ASP:OD1	9:B:1614:HOH:O	2.22	0.41
3:D:71:GLU:O	3:D:75:ARG:HG2	2.20	0.41
4:E:30:LYS:HE3	4:E:30:LYS:HB2	1.82	0.41
2:B:284:LYS:O	2:B:288:GLN:HG3	2.20	0.41
2:B:951:ASP:HB3	2:B:954:VAL:CG1	2.49	0.41
5:F:25:ASN:O	5:F:29:VAL:HG23	2.19	0.41
1:A:254:TYR:CD1	1:A:260:LYS:HB2	2.56	0.41
1:A:401:LEU:HD21	1:A:461:LEU:HB3	2.02	0.41
1:A:1217:GLU:OE2	2:B:679:HIS:NE2	2.50	0.41
2:B:1001:VAL:HG13	2:B:1061:LEU:HD21	2.03	0.41
5:F:36:ASN:O	5:F:40:SER:HB2	2.20	0.41
1:A:1099:ARG:O	1:A:1102:SER:OG	2.35	0.41
1:A:1106:ASP:CG	1:A:1107:PRO:HD2	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:439:THR:OG1	1:A:440:ARG:N	2.54	0.41
1:A:450:ALA:O	1:A:453:GLU:HB2	2.20	0.41
2:B:186:GLU:O	2:B:188:PRO:HD3	2.20	0.41
2:B:1064:SER:O	2:B:1068:LYS:HG3	2.21	0.41
5:F:127:PRO:HG2	5:F:130:LEU:HD23	2.03	0.41
1:A:1008:LEU:O	1:A:1012:GLN:HG3	2.21	0.41
1:A:1055:ALA:HB3	1:A:1056:PRO:HD3	2.01	0.41
2:B:248:MET:N	2:B:249:PRO:HD2	2.35	0.41
1:A:788:GLU:OE2	3:D:512:ARG:NH1	2.44	0.41
1:A:1001:GLY:HA3	1:A:1156:GLY:O	2.21	0.41
2:B:87:LEU:O	2:B:91:ALA:HB2	2.21	0.41
2:B:322:ASN:O	2:B:326:GLU:HG3	2.21	0.41
2:B:961:LEU:HD13	2:B:961:LEU:C	2.46	0.41
1:A:455:ILE:HD13	1:A:670:LEU:HD11	2.03	0.41
1:A:740:LEU:HD22	1:A:740:LEU:N	2.36	0.41
2:B:40:ASP:HA	2:B:41:PRO:HD2	1.86	0.41
3:D:173:ARG:O	3:D:176:LYS:HG2	2.21	0.41
5:F:116:LYS:HG3	5:F:116:LYS:O	2.20	0.41
1:A:513:ALA:O	1:A:516:LYS:HG2	2.22	0.40
2:B:739:LEU:O	2:B:743:VAL:HG23	2.21	0.40
1:A:497:ARG:HB2	1:A:532:ALA:HB1	2.03	0.40
1:A:550:ARG:NH1	4:E:20:GLU:OE1	2.50	0.40
2:B:56:ALA:HB1	2:B:76:LEU:HD23	2.02	0.40
1:A:114:VAL:HG11	3:D:134:LEU:HD23	2.02	0.40
2:B:34:ILE:HG13	8:B:1212:GOL:O1	2.22	0.40
2:B:162:TYR:O	2:B:166:MET:HB2	2.21	0.40
2:B:307:ALA:O	2:B:311:PHE:HD2	2.04	0.40
2:B:757:VAL:HG12	2:B:759:ILE:HG13	2.03	0.40
2:B:935:LEU:O	2:B:939:ILE:HG13	2.21	0.40
2:B:311:PHE:HD1	2:B:317:TYR:HB3	1.85	0.40
1:A:56:ILE:O	1:A:60:ILE:HG13	2.21	0.40
1:A:86:TRP:CD1	1:A:86:TRP:C	3.00	0.40
2:B:705:ARG:HG2	9:B:1522:HOH:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1179/1253 (94%)	1146 (97%)	32 (3%)	1 (0%)	48	60
2	B	1078/1128 (96%)	1053 (98%)	22 (2%)	3 (0%)	36	44
3	D	196/559 (35%)	189 (96%)	7 (4%)	0	100	100
4	E	67/75 (89%)	67 (100%)	0	0	100	100
5	F	154/514 (30%)	151 (98%)	2 (1%)	1 (1%)	21	25
6	P	6/15 (40%)	6 (100%)	0	0	100	100
All	All	2680/3544 (76%)	2612 (98%)	63 (2%)	5 (0%)	43	53

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	758	GLN
1	A	1089	GLY
5	F	117	ASN
2	B	316	GLY
2	B	41	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	1080/1131 (96%)	1070 (99%)	10 (1%)	70	80
2	B	984/1021 (96%)	983 (100%)	1 (0%)	88	93
3	D	188/502 (38%)	183 (97%)	5 (3%)	39	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	E	63/67 (94%)	62 (98%)	1 (2%)	55	68
5	F	137/444 (31%)	137 (100%)	0	100	100
6	P	7/11 (64%)	7 (100%)	0	100	100
All	All	2459/3176 (77%)	2442 (99%)	17 (1%)	76	83

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	164	PHE
1	A	358	ARG
1	A	468	MET
1	A	610	GLU
1	A	747	GLU
1	A	848	ASN
1	A	959	ILE
1	A	977	HIS
1	A	1037	VAL
1	A	1043	LEU
2	B	152	GLU
3	D	81	THR
3	D	97	MET
3	D	160	LEU
3	D	500	VAL
3	D	541	VAL
4	E	36	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	GLN
1	A	166	ASN
1	A	508	GLN
1	A	512	GLN
1	A	596	HIS
1	A	701	GLN
1	A	734	GLN
1	A	880	GLN
1	A	889	HIS
1	A	907	ASN
1	A	915	GLN

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Mol	Chain	Res	Type
1	A	978	HIS
1	A	979	GLN
1	A	1012	GLN
1	A	1036	HIS
2	B	33	ASN
2	B	404	HIS
2	B	858	HIS
2	B	889	GLN
2	B	1038	GLN
2	B	1117	HIS
4	E	9	GLN
4	E	14	GLN
4	E	18	ASN
5	F	79	GLN
5	F	117	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 20 ligands modelled in this entry, 4 are monoatomic - leaving 16 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
8	GOL	A	1305	-	5,5,5	0.37	0	5,5,5	0.33	0
8	GOL	F	601	-	5,5,5	0.37	0	5,5,5	0.28	0
8	GOL	A	1303	-	5,5,5	0.38	0	5,5,5	0.31	0
8	GOL	A	1302	-	5,5,5	0.37	0	5,5,5	0.23	0
8	GOL	B	1208	-	5,5,5	0.36	0	5,5,5	0.33	0
8	GOL	B	1204	-	5,5,5	0.39	0	5,5,5	0.33	0
8	GOL	A	1306	-	5,5,5	0.38	0	5,5,5	0.26	0
8	GOL	B	1209	-	5,5,5	0.37	0	5,5,5	0.38	0
8	GOL	A	1304	-	5,5,5	0.38	0	5,5,5	0.35	0
8	GOL	B	1205	-	5,5,5	0.40	0	5,5,5	0.28	0
8	GOL	B	1210	-	5,5,5	0.37	0	5,5,5	0.31	0
8	GOL	B	1212	-	5,5,5	0.35	0	5,5,5	0.58	0
8	GOL	B	1211	-	5,5,5	0.39	0	5,5,5	0.25	0
8	GOL	F	602	-	5,5,5	0.37	0	5,5,5	0.32	0
8	GOL	B	1207	-	5,5,5	0.36	0	5,5,5	0.30	0
8	GOL	B	1206	-	5,5,5	0.38	0	5,5,5	0.30	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
8	GOL	A	1305	-	-	2/4/4/4	-
8	GOL	F	601	-	-	2/4/4/4	-
8	GOL	A	1303	-	-	2/4/4/4	-
8	GOL	A	1302	-	-	4/4/4/4	-
8	GOL	B	1208	-	-	2/4/4/4	-
8	GOL	B	1204	-	-	2/4/4/4	-
8	GOL	A	1306	-	-	2/4/4/4	-
8	GOL	B	1209	-	-	2/4/4/4	-
8	GOL	A	1304	-	-	2/4/4/4	-
8	GOL	B	1205	-	-	2/4/4/4	-
8	GOL	B	1210	-	-	2/4/4/4	-
8	GOL	B	1212	-	-	4/4/4/4	-
8	GOL	B	1211	-	-	4/4/4/4	-
8	GOL	F	602	-	-	2/4/4/4	-
8	GOL	B	1207	-	-	2/4/4/4	-
8	GOL	B	1206	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	1302	GOL	O1-C1-C2-C3
8	A	1303	GOL	O1-C1-C2-C3
8	A	1305	GOL	O1-C1-C2-C3
8	B	1204	GOL	O1-C1-C2-C3
8	B	1207	GOL	O1-C1-C2-C3
8	B	1208	GOL	O1-C1-C2-O2
8	B	1209	GOL	O1-C1-C2-C3
8	B	1210	GOL	O1-C1-C2-C3
8	B	1211	GOL	O1-C1-C2-C3
8	B	1212	GOL	O1-C1-C2-C3
8	F	602	GOL	O1-C1-C2-C3
8	A	1302	GOL	O1-C1-C2-O2
8	A	1306	GOL	O1-C1-C2-O2
8	A	1302	GOL	C1-C2-C3-O3
8	A	1304	GOL	O1-C1-C2-C3
8	A	1306	GOL	O1-C1-C2-C3
8	B	1205	GOL	O1-C1-C2-C3
8	B	1206	GOL	O1-C1-C2-C3
8	B	1208	GOL	O1-C1-C2-C3
8	B	1211	GOL	C1-C2-C3-O3
8	B	1212	GOL	C1-C2-C3-O3
8	F	601	GOL	O1-C1-C2-C3
8	A	1305	GOL	O1-C1-C2-O2
8	B	1207	GOL	O1-C1-C2-O2
8	B	1209	GOL	O1-C1-C2-O2
8	B	1210	GOL	O1-C1-C2-O2
8	B	1211	GOL	O1-C1-C2-O2
8	B	1212	GOL	O2-C2-C3-O3
8	F	602	GOL	O1-C1-C2-O2
8	A	1304	GOL	O1-C1-C2-O2
8	B	1204	GOL	O1-C1-C2-O2
8	B	1205	GOL	O1-C1-C2-O2
8	B	1206	GOL	O1-C1-C2-O2
8	B	1212	GOL	O1-C1-C2-O2
8	F	601	GOL	O1-C1-C2-O2
8	A	1303	GOL	O1-C1-C2-O2
8	A	1302	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
8	B	1211	GOL	O2-C2-C3-O3

There are no ring outliers.

8 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	1303	GOL	3	0
8	A	1302	GOL	1	0
8	B	1208	GOL	2	0
8	B	1209	GOL	1	0
8	A	1304	GOL	1	0
8	B	1212	GOL	1	0
8	B	1211	GOL	1	0
8	F	602	GOL	2	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	1183/1253 (94%)	-0.33	14 (1%) 76 78	21, 52, 108, 155	6 (0%)
2	B	1085/1128 (96%)	-0.40	3 (0%) 90 91	24, 50, 91, 136	3 (0%)
3	D	202/559 (36%)	0.39	14 (6%) 23 19	44, 79, 145, 162	0
4	E	67/75 (89%)	-0.21	1 (1%) 72 73	32, 55, 104, 142	2 (2%)
5	F	156/514 (30%)	-0.02	3 (1%) 66 67	42, 65, 104, 124	0
6	P	8/15 (53%)	-0.02	0 100 100	52, 71, 101, 118	0
All	All	2701/3544 (76%)	-0.28	35 (1%) 75 77	21, 53, 108, 162	11 (0%)

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	95	ILE	4.5
5	F	155	TRP	4.4
3	D	527	ILE	4.3
3	D	497	ALA	4.3
3	D	17	ALA	3.7
1	A	539	PRO	3.5
1	A	345	ILE	3.5
1	A	881	PRO	3.3
1	A	528	PHE	3.2
3	D	92	LEU	3.0
1	A	875	PHE	3.0
1	A	341	PRO	2.9
3	D	94	ASP	2.9
2	B	162	TYR	2.7
3	D	509	ILE	2.6
3	D	18	LEU	2.6
3	D	543	TYR	2.5
1	A	198	MET	2.5
1	A	527	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
3	D	90	LEU	2.4
1	A	380	ALA	2.3
3	D	541	VAL	2.3
2	B	67	VAL	2.3
1	A	533	LEU	2.3
1	A	430	ASP	2.2
5	F	0	ALA	2.2
2	B	8	PRO	2.2
3	D	96	THR	2.1
3	D	498	ARG	2.0
1	A	1043	LEU	2.0
1	A	55	GLY	2.0
4	E	70	LYS	2.0
1	A	343	TYR	2.0
5	F	56	GLN	2.0
3	D	16	THR	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	GOL	B	1211	6/6	0.69	0.18	104,108,109,109	0
8	GOL	F	601	6/6	0.70	0.12	77,92,95,95	0
8	GOL	B	1208	6/6	0.76	0.16	90,92,93,93	0
8	GOL	A	1305	6/6	0.81	0.19	102,103,104,105	0
8	GOL	A	1302	6/6	0.84	0.16	73,80,85,92	0
8	GOL	B	1207	6/6	0.85	0.19	75,80,86,89	0
8	GOL	A	1303	6/6	0.85	0.15	88,94,96,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	GOL	B	1212	6/6	0.86	0.25	112,114,115,115	0
8	GOL	F	602	6/6	0.87	0.10	73,77,81,84	0
8	GOL	B	1206	6/6	0.88	0.15	84,86,87,88	0
8	GOL	B	1209	6/6	0.88	0.15	94,100,101,102	0
8	GOL	B	1205	6/6	0.88	0.10	77,84,87,88	0
7	CL	B	1201	1/1	0.89	0.08	94,94,94,94	0
8	GOL	B	1210	6/6	0.89	0.15	86,93,100,103	0
7	CL	A	1301	1/1	0.89	0.10	84,84,84,84	0
8	GOL	A	1304	6/6	0.90	0.12	83,84,85,85	0
8	GOL	B	1204	6/6	0.90	0.13	83,86,88,88	0
7	CL	B	1203	1/1	0.91	0.20	100,100,100,100	0
8	GOL	A	1306	6/6	0.92	0.11	59,63,64,67	0
7	CL	B	1202	1/1	0.98	0.04	55,55,55,55	0

6.5 Other polymers [i](#)

There are no such residues in this entry.