



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:56 PM GMT

PDB ID : 4N78
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

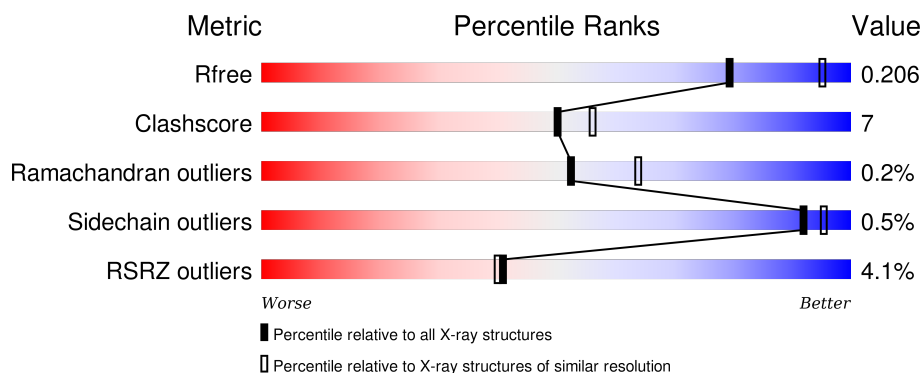
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.43 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}	91344	1003 (2.46-2.42)
Clashscore	102246	1071 (2.46-2.42)
Ramachandran outliers	100387	1065 (2.46-2.42)
Sidechain outliers	100360	1065 (2.46-2.42)
RSRZ outliers	91569	1005 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1253	<div> <div>3%</div> <div>76%</div> <div>18%</div> <div>6%</div> </div>
2	B	1128	<div> <div>2%</div> <div>82%</div> <div>14%</div> <div>.</div> </div>
3	D	559	<div> <div>8%</div> <div>29%</div> <div>8%</div> <div>64%</div> </div>
4	E	75	<div> <div>5%</div> <div>69%</div> <div>20%</div> <div>11%</div> </div>
5	F	514	<div> <div>%</div> <div>24%</div> <div>6%</div> <div>70%</div> </div>

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Mol	Chain	Length	Quality of chain
6	P	15	

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
7	CL	B	1203	-	-	-	X
8	GOL	A	1302	-	-	-	X
8	GOL	A	1303	-	-	-	X
8	GOL	A	1304	-	-	-	X
8	GOL	B	1204	-	-	-	X
8	GOL	B	1207	-	-	-	X
8	GOL	B	1209	-	-	-	X
8	GOL	B	1211	-	-	-	X
8	GOL	B	1212	-	-	-	X

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

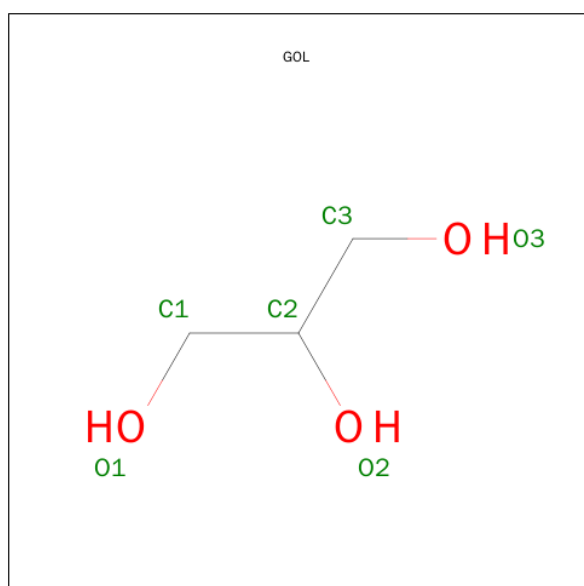
- Molecule 6 is a protein called WIRS.

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 (three-letter code: CL) (formula: Cl).

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

- Molecule 8 is GLYCEROL (three-letter code: 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	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		
8	F	1	Total	C	O	0	0
			6	3	3		
8	F	1	Total	C	O	0	0
			6	3	3		

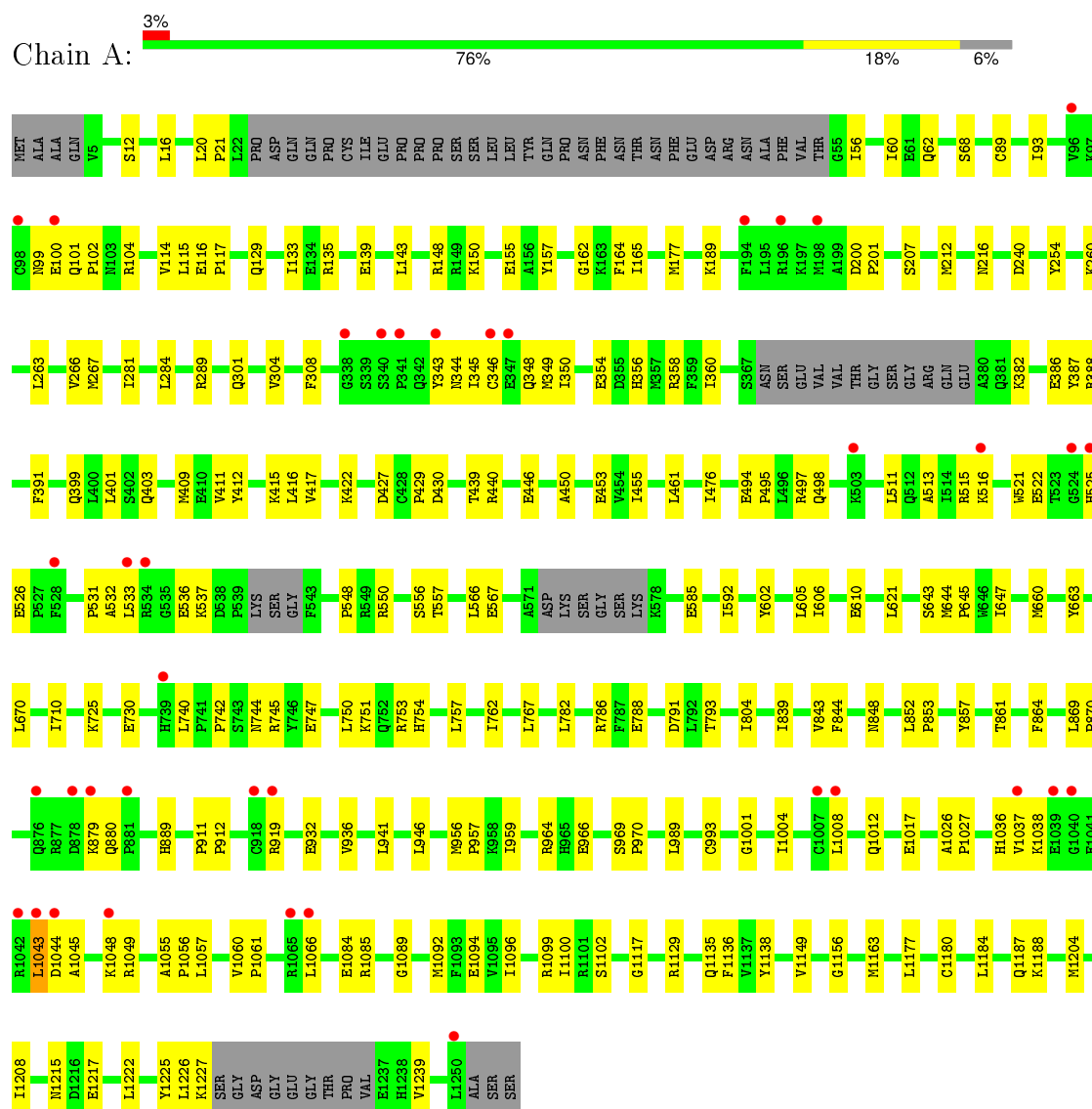
- Molecule 9 is water.

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

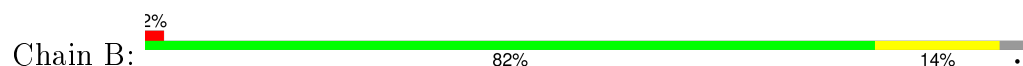
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Cytoplasmic FMR1-interacting protein 1



• Molecule 2: Nck-associated protein 1





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	97.49 Å 114.75 Å 323.61 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.98 – 2.43 43.23 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.6 (19.98-2.43) 86.9 (43.23-2.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.09 (at 2.34 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.189 , 0.209 0.183 , 0.206	Depositor DCC
R_{free} test set	3522 reflections (1.34%)	DCC
Wilson B-factor (Å ²)	41.0	Xtriage
Anisotropy	0.610	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 49.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 148108 reflections	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, 0.375 respectively for untwinned datasets, and 0.333, 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: GOL, CL

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	0.21	0/9958	0.34	0/13441
2	B	0.21	0/8880	0.35	0/12009
3	D	0.20	0/1682	0.35	0/2265
4	E	0.20	0/582	0.32	0/782
5	F	0.20	0/1270	0.35	0/1717
6	P	0.24	0/62	0.31	0/79
All	All	0.21	0/22434	0.34	0/30293

There are no bond length outliers.

There are no bond angle outliers.

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	162	0
2	B	8709	0	8766	104	0
3	D	1657	0	1663	39	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	7	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	311	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 7.

All (311) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:556:SER:HG	3:D:15:HIS:N	1.67	0.92
2:B:314:ILE:HG22	2:B:315:ARG:H	1.39	0.87
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
2:B:473:LYS:NZ	2:B:477:ASP:OD1	2.24	0.71
4:E:69:THR:HG22	4:E:70:LYS:H	1.54	0.71
3:D:18:LEU:HB3	3:D:19:PRO:HD2	1.72	0.71
1:A:513:ALA:HA	1:A:516:LYS:HE3	1.75	0.69
4:E:6:ASP:HB3	4:E:7:PRO:HD3	1.74	0.68
2:B:696:VAL:H	8:B:1211:GOL:HO2	1.39	0.68
2:B:620:GLU:HG2	2:B:675:LEU:HD13	1.75	0.68
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
5:F:37:TYR:CZ	5:F:43:LYS:HG3	2.30	0.67
3:D:117:LEU:HD12	3:D:118:PRO:HD2	1.75	0.67
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:494:GLU:HB3	1:A:495:PRO:HD3	1.81	0.62
1:A:345:ILE:HD12	1:A:346:CYS:N	2.17	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
2:B:800:VAL:HG11	2:B:912:VAL:HG11	1.85	0.59
1:A:932:GLU:OE2	3:D:499:SER:OG	2.12	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
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
2:B:214:TYR:HB2	2:B:258:MET:HE1	1.86	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:556:SER:OG	3:D:15:HIS:N	2.34	0.57
1:A:521:TRP:H	4:E:13[B]:HIS:CE1	2.22	0.57
3:D:22:ILE:CG1	3:D:25:GLU:HB2	2.36	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:189:LYS:NZ	1:A:207:SER:OG	2.39	0.56
1:A:162:GLY:O	1:A:165:ILE:HG12	2.05	0.56
2:B:726:TYR:CE2	2:B:728:GLN:HG2	2.41	0.56
1:A:879:LYS:HD3	1:A:880:GLN:H	1.71	0.56
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
2:B:314:ILE:HG22	2:B:315:ARG:N	2.17	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:1028:ASN:HA	2:B:1030:HIS:CE1	2.43	0.54
2:B:214:TYR:HB3	2:B:215:PRO:HD3	1.90	0.54
1:A:498:GLN:HE22	1:A:585:GLU:HG3	1.71	0.54
1:A:521:TRP:N	4:E:13[B]:HIS:CE1	2.76	0.54
1:A:521:TRP:N	4:E:13[B]:HIS:HE1	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:443:ASN:O	2:B:447:GLN:HG2	2.08	0.53
1:A:762:ILE:HD12	3:D:111:LEU:HD23	1.90	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:557:THR:HG23	3:D:15:HIS:N	2.24	0.52
1:A:301:GLN:HG3	1:A:343:TYR:OH	2.09	0.52
1:A:1043:LEU:HD13	1:A:1044:ASP:H	1.73	0.52
5:F:51:LYS:HD3	5:F:51:LYS:C	2.30	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
2:B:454:GLU:O	2:B:458:ILE:HG13	2.11	0.51
1:A:754:HIS:ND1	1:A:754:HIS:O	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
2:B:490:TRP:O	2:B:494:GLN:HG3	2.11	0.51
1:A:966:GLU:N	1:A:966:GLU:OE1	2.35	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: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
2:B:1054:ARG:HA	2:B:1054:ARG:NE	2.26	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
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:1226:LEU:O	1:A:1227:LYS:C	2.51	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:1094:GLU:HG2	1:A:1225:TYR:O	2.13	0.48
1:A:1066:LEU:HB2	2:B:942:PHE:HZ	1.77	0.48
2:B:115:ASP:OD2	2:B:199:HIS:ND1	2.44	0.48
2:B:319:LYS:HG2	2:B:320:ARG:HH12	1.77	0.48
1:A:753:ARG:HD3	9:A:1495:HOH:O	2.13	0.48
1:A:150:LYS:HA	1:A:150:LYS:HE2	1.95	0.48
1:A:964:ARG:HB3	1:A:966:GLU:OE1	2.14	0.48
2:B:813:ALA:HB2	2:B:832:ASP:HA	1.95	0.48
1:A:399:GLN:O	1:A:403:GLN:HG3	2.14	0.48
2:B:104:LYS:HG3	2:B:140:TYR:CE1	2.48	0.48
1:A:511:LEU:O	1:A:515:ARG:HG3	2.13	0.48
1:A:1135:GLN:HA	1:A:1138:TYR:CZ	2.49	0.48
2:B:65:PRO:HD3	2:B:183:VAL:HG11	1.96	0.47
1:A:93:ILE:HG12	3:D:137:LEU:HD22	1.96	0.47
2:B:263:ILE:HD12	2:B:293:LEU:HD11	1.97	0.47
1:A:89:CYS:HB2	1:A:115:LEU:HD21	1.96	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
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
3:D:501:LEU:O	3:D:505:ILE:HG13	2.14	0.47
2:B:639:GLN:O	2:B:643:LYS:HB2	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
4:E:68:VAL:HG12	4:E:68:VAL:O	2.15	0.47
1:A:1136:PHE:HA	1:A:1180:CYS:SG	2.55	0.47
1:A:956:MET:HG3	1:A:957:PRO:HD2	1.97	0.47
1:A:644:MET:HB2	1:A:645:PRO:HD3	1.97	0.47
2:B:315:ARG:O	2:B:317:TYR:N	2.45	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
3:D:48:ALA:HB3	5:F:19:LEU:HD21	1.97	0.47
1:A:742:PRO:HB2	8:A:1302:GOL:H32	1.96	0.47
1:A:857:TYR:HB2	1:A:864:PHE:CE1	2.50	0.47
3:D:94:ASP:OD1	3:D:98:ARG:HD2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:39:ARG:NH2	5:F:31:ASP:OD2	2.47	0.47
3:D:18:LEU:HB3	3:D:19:PRO:CD	2.44	0.46
1:A:844:PHE:CE1	1:A:932:GLU:HB3	2.50	0.46
4:E:21:TYR:CZ	5:F:51:LYS:HG2	2.50	0.46
2:B:633[B]:CYS:O	2:B:637:ILE:HG12	2.15	0.46
1:A:1043:LEU:HD22	1:A:1044:ASP:N	2.31	0.46
1:A:660:MET:HE1	1:A:663:TYR:CG	2.51	0.46
1:A:526:GLU:H	4:E:9:GLN:NE2	2.13	0.46
5:F:12:ILE:HB	5:F:13:PRO:HD3	1.97	0.46
1:A:869:LEU:N	1:A:870:PRO:HD2	2.31	0.46
1:A:1135:GLN:OE1	1:A:1215:ASN:ND2	2.48	0.46
1:A:531:PRO:HB2	1:A:536:GLU:HG3	1.96	0.46
2:B:991:GLU:O	2:B:995:ILE:HG12	2.15	0.46
1:A:143:LEU:HA	1:A:148:ARG:HG2	1.97	0.46
2:B:446:VAL:HG22	2:B:460:MET:CE	2.45	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
3:D:46:LYS:HB2	5:F:23:TYR:CD2	2.51	0.45
2:B:1066:LEU:O	2:B:1069:ILE:HG12	2.15	0.45
2:B:101:MET:SD	2:B:177:ARG:HG2	2.56	0.45
1:A:932:GLU:O	1:A:936:VAL:HG23	2.17	0.45
2:B:442:LEU:O	2:B:446:VAL:HG23	2.16	0.45
1:A:356:HIS:CE1	1:A:360:ILE:HD12	2.51	0.45
3:D:52:PHE:CD2	5:F:68:LEU:HD23	2.50	0.45
2:B:315:ARG:C	2:B:317:TYR:H	2.19	0.45
2:B:1108:PRO:HB2	2:B:1110:VAL:HG22	1.99	0.45
2:B:351:LYS:HG3	2:B:411:TYR:CZ	2.51	0.45
1:A:1045:ALA:O	1:A:1049:ARG:NH2	2.49	0.45
5:F:20:PHE:O	5:F:23:TYR:HB3	2.16	0.45
1:A:643:SER:O	1:A:647:ILE:HG13	2.16	0.45
1:A:200:ASP:HB2	1:A:201:PRO:HD2	1.98	0.45
2:B:692:VAL:HG21	9:B:1490:HOH:O	2.17	0.45
1:A:747:GLU:HG2	9:A:1529:HOH:O	2.15	0.45
1:A:522:GLU:OE1	1:A:548:PRO:HB3	2.16	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
2:B:490:TRP:CD1	2:B:520:ILE:HG13	2.52	0.45
1:A:1129:ARG:NH1	1:A:1177:LEU:HB3	2.31	0.45
1:A:99:ASN:O	1:A:104:ARG:NH1	2.50	0.45
1:A:1085:ARG:NH1	9:A:1501:HOH:O	2.27	0.44
5:F:34:GLU:O	5:F:38:ILE:HG13	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:510:GLN:O	3:D:511:LEU:HD12	2.17	0.44
1:A:1045:ALA:O	1:A:1049:ARG:HG3	2.17	0.44
1:A:730:GLU:HA	1:A:730:GLU:OE2	2.17	0.44
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
2:B:40:ASP:C	2:B:42:LYS:H	2.21	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
2:B:880:MET:HB3	2:B:890:MET:HE1	1.99	0.44
2:B:947:PRO:C	2:B:950:THR:HB	2.37	0.44
1:A:411:VAL:O	1:A:415:LYS:HG2	2.17	0.44
1:A:1084:GLU:O	1:A:1085:ARG:HD2	2.17	0.44
1:A:757:LEU:HD23	3:D:112:PHE:CZ	2.53	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
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:497:ARG:NH2	1:A:537:LYS:HE2	2.34	0.43
3:D:83:LEU:HD21	4:E:68:VAL:HG13	1.99	0.43
1:A:20:LEU:HD12	1:A:21:PRO:HD2	1.99	0.43
1:A:852:LEU:HB2	1:A:853:PRO:HD3	1.99	0.43
2:B:793:LEU:HD23	2:B:797:LEU:HD12	2.01	0.43
1:A:446:GLU:OE1	9:A:1629:HOH:O	2.21	0.43
2:B:175:TYR:HB3	2:B:176:PRO:HD3	2.01	0.43
1:A:388:ARG:O	1:A:391:PHE:HB3	2.18	0.43
1:A:533:LEU:O	1:A:533:LEU:HD23	2.18	0.43
1:A:1226:LEU:HD12	1:A:1226:LEU:HA	1.87	0.43
1:A:497:ARG:HE	1:A:537:LYS:HG2	1.83	0.43
2:B:905:LYS:O	2:B:909:ILE:HG13	2.19	0.43
1:A:409:MET:HE1	1:A:621:LEU:HD21	2.00	0.43
1:A:1187:GLN:OE1	8:A:1303:GOL:O1	2.34	0.43
3:D:62:PHE:O	3:D:66:VAL:HG23	2.19	0.43
1:A:1188:LYS:HG2	8:A:1303:GOL:H12	2.01	0.43
1:A:725:LYS:HD2	2:B:828:GLU:OE2	2.18	0.43
2:B:509:HIS:NE2	8:B:1209:GOL:H31	2.33	0.43
3:D:30:THR:HG21	4:E:18:ASN:ND2	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:745:ARG:HA	1:A:747:GLU:OE2	2.19	0.43
1:A:660:MET:HE1	1:A:663:TYR:CD2	2.53	0.43
1:A:155:GLU:HG3	1:A:567:GLU:OE2	2.18	0.43
5:F:121:THR:OG1	5:F:122:HIS:N	2.51	0.42
2:B:1034:LYS:HE3	2:B:1034:LYS:HB2	1.82	0.42
1:A:497:ARG:NH1	1:A:498:GLN:HG2	2.34	0.42
2:B:166:MET:CE	2:B:166:MET:HA	2.49	0.42
1:A:240:ASP:OD1	1:A:289:ARG:NH2	2.35	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:852:SER:HA	2:B:855:LEU:HD12	2.01	0.42
2:B:716:PHE:O	2:B:720:ILE:HG13	2.20	0.42
1:A:1184:LEU:HD11	8:A:1303:GOL:H32	2.01	0.42
1:A:68:SER:OG	1:A:135:ARG:NH2	2.49	0.42
1:A:791:ASP:OD1	1:A:793:THR:OG1	2.29	0.42
2:B:611:ARG:HH22	8:B:1208:GOL:H11	1.84	0.42
1:A:1036:HIS:HD2	1:A:1038:LYS:HE3	1.85	0.42
5:F:93:ILE:O	5:F:97:VAL:HG23	2.20	0.42
2:B:141:THR:O	2:B:145:ILE:HG13	2.19	0.42
1:A:101:GLN:HA	1:A:102:PRO:HD3	1.95	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:767:LEU:HD11	3:D:111:LEU:HD21	2.01	0.42
1:A:350:ILE:O	1:A:354:GLU:HG3	2.19	0.42
1:A:839:ILE:O	1:A:843:VAL:HG23	2.20	0.42
1:A:1096:ILE:O	1:A:1100:ILE:HG13	2.20	0.41
1:A:139:GLU:HG2	1:A:157:TYR:OH	2.20	0.41
2:B:923:ALA:O	2:B:927:VAL:HG23	2.20	0.41
2:B:637:ILE:O	2:B:641:VAL:HG23	2.20	0.41
3:D:71:GLU:O	3:D:75:ARG:HG2	2.20	0.41
2:B:926[A]:ASP:OD1	9:B:1614:HOH:O	2.22	0.41
4:E:30:LYS:HB2	4:E:30:LYS:HE3	1.82	0.41
2:B:849:LYS:O	2:B:853:GLU:HG3	2.21	0.41
1:A:1239:VAL:HG11	2:B:361:PRO:HB2	2.03	0.41
2:B:951:ASP:HB3	2:B:954:VAL:CG1	2.49	0.41
2:B:284:LYS:O	2:B:288:GLN:HG3	2.20	0.41
5:F:25:ASN:O	5:F:29:VAL:HG23	2.19	0.41
2:B:1001:VAL:HG13	2:B:1061:LEU:HD21	2.03	0.41
1:A:254:TYR:CD1	1:A:260:LYS:HB2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1217:GLU:OE2	2:B:679:HIS:NE2	2.50	0.41
1:A:401:LEU:HD21	1:A:461:LEU:HB3	2.02	0.41
5:F:36:ASN:O	5:F:40:SER:HB2	2.20	0.41
1:A:660:MET:HE2	1:A:660:MET:HA	2.02	0.41
2:B:1064:SER:O	2:B:1068:LYS:HG3	2.21	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
5:F:127:PRO:HG2	5:F:130:LEU:HD23	2.03	0.41
1:A:439:THR:OG1	1:A:440:ARG:N	2.54	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
2:B:260:LYS:NZ	9:B:1419:HOH:O	2.35	0.41
1:A:1008:LEU:O	1:A:1012:GLN:HG3	2.21	0.41
3:D:42:SER:OG	5:F:23:TYR:O	2.32	0.41
2:B:322:ASN:O	2:B:326:GLU:HG3	2.21	0.41
1:A:1099:ARG:O	1:A:1102:SER:OG	2.35	0.41
1:A:1001:GLY:HA3	1:A:1156:GLY:O	2.21	0.41
1:A:788:GLU:OE2	3:D:512:ARG:NH1	2.44	0.41
2:B:87:LEU:O	2:B:91:ALA:HB2	2.21	0.41
2:B:40:ASP:HA	2:B:41:PRO:HD2	1.86	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
5:F:116:LYS:O	5:F:116:LYS:HG3	2.20	0.41
3:D:173:ARG:O	3:D:176:LYS:HG2	2.21	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
2:B:56:ALA:HB1	2:B:76:LEU:HD23	2.02	0.40
1:A:550:ARG:NH1	4:E:20:GLU:OE1	2.50	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:162:TYR:O	2:B:166:MET:HB2	2.21	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:577:MET:HE1	2:B:592:GLY:HA2	2.02	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:660:MET:HA	1:A:660:MET:CE	2.51	0.40
2:B:970:GLU:H	2:B:970:GLU:CD	2.21	0.40
2:B:705:ARG:HG2	9:B:1522:HOH:O	2.21	0.40
1:A:56:ILE:O	1:A:60:ILE:HG13	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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%)	56	70
2	B	1078/1128 (96%)	1053 (98%)	22 (2%)	3 (0%)	46	56
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%)	30	36
6	P	6/15 (40%)	6 (100%)	0	0	100	100
All	All	2680/3544 (76%)	2612 (98%)	63 (2%)	5 (0%)	52	64

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 [i](#)

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%)	1072 (99%)	8 (1%)	88	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	984/1021 (96%)	979 (100%)	5 (0%)	92	95
3	D	188/502 (38%)	188 (100%)	0	100	100
4	E	63/67 (94%)	63 (100%)	0	100	100
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%)	2446 (100%)	13 (0%)	92	95

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	GLN
1	A	164	PHE
1	A	177	MET
1	A	358	ARG
1	A	848	ASN
1	A	959	ILE
1	A	1037	VAL
1	A	1043	LEU
2	B	152	GLU
2	B	433	TYR
2	B	491	PHE
2	B	832	ASP
2	B	1002	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	GLN
1	A	701	GLN
1	A	889	HIS
1	A	1012	GLN
2	B	33	ASN
2	B	889	GLN
2	B	1038	GLN
2	B	1117	HIS
4	E	9	GLN
4	E	14	GLN
4	E	18	ASN

5.3.3 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 carbohydrates 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	1302	-	5,5,5	0.34	0	5,5,5	0.16	0
8	GOL	A	1303	-	5,5,5	0.35	0	5,5,5	0.24	0
8	GOL	A	1304	-	5,5,5	0.36	0	5,5,5	0.27	0
8	GOL	A	1305	-	5,5,5	0.34	0	5,5,5	0.24	0
8	GOL	A	1306	-	5,5,5	0.35	0	5,5,5	0.21	0
8	GOL	B	1204	-	5,5,5	0.36	0	5,5,5	0.26	0
8	GOL	B	1205	-	5,5,5	0.37	0	5,5,5	0.22	0
8	GOL	B	1206	-	5,5,5	0.35	0	5,5,5	0.22	0
8	GOL	B	1207	-	5,5,5	0.34	0	5,5,5	0.22	0
8	GOL	B	1208	-	5,5,5	0.33	0	5,5,5	0.25	0
8	GOL	B	1209	-	5,5,5	0.34	0	5,5,5	0.30	0
8	GOL	B	1210	-	5,5,5	0.34	0	5,5,5	0.23	0
8	GOL	B	1211	-	5,5,5	0.36	0	5,5,5	0.16	0
8	GOL	B	1212	-	5,5,5	0.34	0	5,5,5	0.45	0
8	GOL	F	601	-	5,5,5	0.34	0	5,5,5	0.21	0
8	GOL	F	602	-	5,5,5	0.35	0	5,5,5	0.24	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	1302	-	-	0/4/4/4	0/0/0/0
8	GOL	A	1303	-	-	0/4/4/4	0/0/0/0
8	GOL	A	1304	-	-	0/4/4/4	0/0/0/0
8	GOL	A	1305	-	-	0/4/4/4	0/0/0/0
8	GOL	A	1306	-	-	0/4/4/4	0/0/0/0
8	GOL	B	1204	-	-	0/4/4/4	0/0/0/0
8	GOL	B	1205	-	-	0/4/4/4	0/0/0/0
8	GOL	B	1206	-	-	0/4/4/4	0/0/0/0
8	GOL	B	1207	-	-	0/4/4/4	0/0/0/0
8	GOL	B	1208	-	-	0/4/4/4	0/0/0/0
8	GOL	B	1209	-	-	0/4/4/4	0/0/0/0
8	GOL	B	1210	-	-	0/4/4/4	0/0/0/0
8	GOL	B	1211	-	-	0/4/4/4	0/0/0/0
8	GOL	B	1212	-	-	0/4/4/4	0/0/0/0
8	GOL	F	601	-	-	0/4/4/4	0/0/0/0
8	GOL	F	602	-	-	0/4/4/4	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.

8 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	1302	GOL	1	0
8	A	1303	GOL	3	0
8	A	1304	GOL	1	0
8	B	1208	GOL	2	0
8	B	1209	GOL	1	0
8	B	1211	GOL	1	0
8	B	1212	GOL	1	0
8	F	602	GOL	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	1184/1253 (94%)	-0.06	38 (3%) 51 49	33, 52, 108, 155	0
2	B	1085/1128 (96%)	-0.18	23 (2%) 67 67	34, 50, 91, 136	0
3	D	202/559 (36%)	0.95	42 (20%) 1 1	44, 79, 145, 162	0
4	E	67/75 (89%)	-0.21	4 (5%) 25 23	37, 56, 104, 142	0
5	F	156/514 (30%)	-0.00	4 (2%) 59 59	42, 65, 104, 124	0
6	P	8/15 (53%)	0.52	1 (12%) 5 4	52, 71, 101, 118	0
All	All	2702/3544 (76%)	-0.03	112 (4%) 41 40	33, 53, 109, 162	0

All (112) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	528	PHE	8.3
3	D	514	VAL	6.4
1	A	881	PRO	6.3
1	A	198	MET	5.8
3	D	541	VAL	5.8
3	D	509	ILE	5.8
3	D	16	THR	5.6
2	B	8	PRO	5.4
5	F	155	TRP	5.2
3	D	176	LYS	5.0
3	D	174	LYS	5.0
3	D	17	ALA	5.0
1	A	1042	ARG	4.9
4	E	71	GLY	4.8
2	B	641	VAL	4.7
1	A	1040	GLY	4.6
3	D	177	ARG	4.4
3	D	527	ILE	4.3
2	B	952	MET	4.3

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Mol	Chain	Res	Type	RSRZ
3	D	98	ARG	4.3
3	D	512	ARG	4.3
3	D	175	GLU	4.0
3	D	96	THR	4.0
3	D	172	LYS	3.9
3	D	87	GLU	3.8
3	D	137	LEU	3.8
3	D	497	ALA	3.7
2	B	78	GLN	3.7
1	A	503	LYS	3.7
3	D	507	LYS	3.6
2	B	67	VAL	3.6
5	F	45	ARG	3.5
1	A	96	VAL	3.5
3	D	18	LEU	3.5
2	B	162	TYR	3.5
1	A	343	TYR	3.5
3	D	516	GLU	3.4
3	D	35	ALA	3.4
1	A	1250	LEU	3.4
3	D	515	GLU	3.4
3	D	95	ILE	3.3
3	D	171	ASP	3.3
2	B	642	ASN	3.3
4	E	72	GLU	3.2
3	D	513	LYS	3.2
1	A	878	ASP	3.1
3	D	97	MET	3.1
3	D	119	ILE	3.1
2	B	951	ASP	3.1
3	D	94	ASP	3.1
3	D	91	SER	3.1
1	A	525	HIS	3.1
1	A	1039	GLU	3.1
2	B	950	THR	3.0
3	D	93	GLN	2.9
1	A	194	PHE	2.9
6	P	5	ARG	2.8
1	A	534	ARG	2.8
1	A	341	PRO	2.8
1	A	918	CYS	2.8
1	A	340	SER	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	49	ILE	2.7
1	A	1043	LEU	2.7
4	E	6	ASP	2.7
3	D	34	LEU	2.7
4	E	70	LYS	2.7
2	B	639	GLN	2.7
3	D	510	GLN	2.7
1	A	739	HIS	2.6
2	B	315	ARG	2.6
5	F	132	ARG	2.6
1	A	196	ARG	2.6
2	B	947	PRO	2.5
1	A	879	LYS	2.5
1	A	1037	VAL	2.5
1	A	98	CYS	2.5
1	A	346	CYS	2.5
1	A	347	GLU	2.5
2	B	80	GLN	2.5
1	A	100	GLU	2.5
2	B	55	SER	2.5
3	D	140	TYR	2.4
3	D	511	LEU	2.4
1	A	1008	LEU	2.4
2	B	62	ARG	2.4
2	B	1048	LYS	2.4
1	A	1044	ASP	2.4
5	F	49	GLU	2.3
1	A	1007	CYS	2.3
3	D	144	GLY	2.3
1	A	876	GLN	2.3
1	A	919	ARG	2.3
3	D	142	ASP	2.2
3	D	15	HIS	2.2
1	A	516	LYS	2.2
1	A	533	LEU	2.2
3	D	500	VAL	2.2
3	D	543	TYR	2.2
1	A	1066	LEU	2.2
1	A	1065	ARG	2.2
2	B	954	VAL	2.1
3	D	50	ASP	2.1
3	D	136	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	1048	LYS	2.1
2	B	7	GLN	2.1
1	A	524	GLY	2.0
2	B	51	LYS	2.0
1	A	338	GLY	2.0
2	B	9	SER	2.0
2	B	930	TYR	2.0
2	B	1075	LYS	2.0
3	D	86	LYS	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
7	CL	B	1203	1/1	0.89	0.78	24.45	100,100,100,100	0
8	GOL	B	1211	6/6	0.51	0.32	9.61	104,108,109,109	0
8	GOL	B	1212	6/6	0.78	0.36	9.41	112,114,115,115	0
8	GOL	A	1302	6/6	0.78	0.29	8.64	73,80,85,92	0
8	GOL	B	1207	6/6	0.79	0.29	6.61	75,80,86,89	0
8	GOL	A	1303	6/6	0.91	0.31	6.08	88,94,96,96	0
8	GOL	A	1304	6/6	0.88	0.46	5.77	83,84,85,85	0
8	GOL	B	1209	6/6	0.88	0.29	5.56	94,100,101,102	0
8	GOL	B	1204	6/6	0.91	0.34	3.91	83,86,88,88	0
8	GOL	B	1210	6/6	0.92	0.21	1.88	86,93,100,103	0
8	GOL	F	602	6/6	0.92	0.19	0.93	73,77,81,84	0
8	GOL	B	1205	6/6	0.89	0.20	0.69	77,84,87,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
8	GOL	A	1306	6/6	0.92	0.13	0.49	59,63,64,67	0
8	GOL	B	1206	6/6	0.88	0.15	0.36	84,86,87,88	0
7	CL	B	1202	1/1	0.99	0.06	-3.29	55,55,55,55	0
8	GOL	F	601	6/6	0.88	0.23	-	77,92,95,95	0
8	GOL	A	1305	6/6	0.86	0.33	-	102,103,104,105	0
7	CL	B	1201	1/1	0.90	0.16	-	94,94,94,94	0
7	CL	A	1301	1/1	0.88	0.13	-	84,84,84,84	0
8	GOL	B	1208	6/6	0.83	0.11	-	90,92,93,93	0

6.5 Other polymers

There are no such residues in this entry.