



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:28 PM UTC

PDB ID : 3P8C / pdb_00003p8c
Title : Structure and Control of the Actin Regulatory WAVE Complex
Authors : Chen, Z.; Borek, D.; Padrick, S.B.; Gomez, T.S.; Metlagel, Z.; Ismail, A.M.;
Umetani, J.; Billadeau, D.D.; Otwinowski, Z.; Rosen, M.K.
Deposited on : 2010-10-13
Resolution : 2.29 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

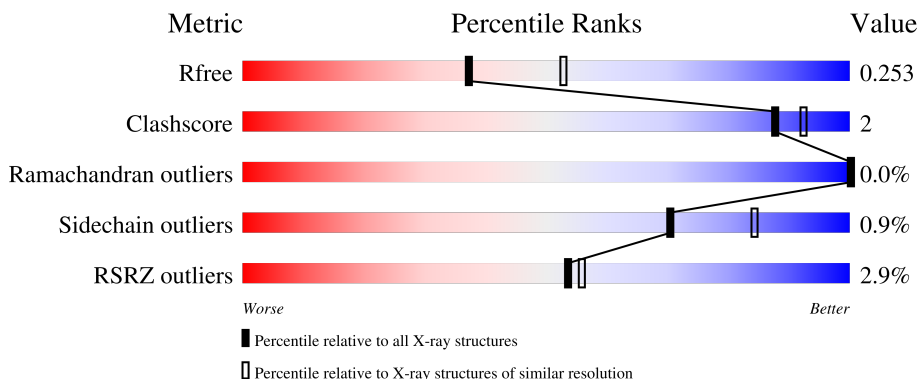
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.29 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (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 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	3% 88% 6% 6%
2	B	1128	2% 90% 6% .
3	D	279	8% 68% 5% 27%
4	E	75	5% 75% 11% 15%
5	F	159	% 95% . .

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	A	1258	-	-	-	X
7	CL	B	1129	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 23017 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	1175	Total	C	N	O	S	0	14	0
			9753	6235	1681	1768	69			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1086	Total	C	N	O	S	0	10	0
			8782	5605	1473	1634	70			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	204	Total	C	N	O	S	0	1	0
			1690	1060	296	330	4			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	187	GLY	-	linker	UNP Q92558
D	188	GLY	-	linker	UNP Q92558
D	189	SER	-	linker	UNP Q92558
D	190	GLY	-	linker	UNP Q92558
D	191	GLY	-	linker	UNP Q92558
D	192	SER	-	linker	UNP Q92558
D	193	GLY	-	linker	UNP Q92558
D	194	GLY	-	linker	UNP Q92558
D	195	SER	-	linker	UNP Q92558
D	196	GLY	-	linker	UNP Q92558
D	197	GLY	-	linker	UNP Q92558
D	198	SER	-	linker	UNP Q92558
D	199	GLY	-	linker	UNP Q92558
D	200	GLY	-	linker	UNP Q92558

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Chain	Residue	Modelled	Actual	Comment	Reference
D	201	SER	-	linker	UNP Q92558
D	202	GLY	-	linker	UNP Q92558
D	203	GLY	-	linker	UNP Q92558
D	204	SER	-	linker	UNP Q92558

- Molecule 4 is a protein called Probable protein BRICK1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	64	Total	C	N	O	S	0	1	0
			541	337	99	103	2			

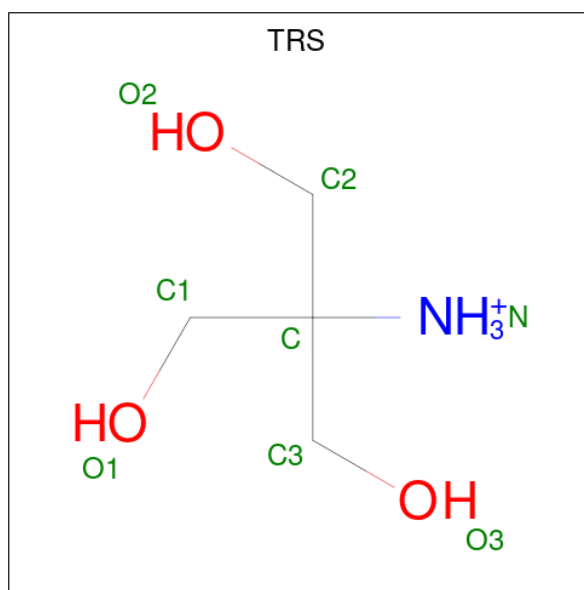
- Molecule 5 is a protein called Abl interactor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	156	Total	C	N	O	S	0	1	0
			1255	779	227	244	5			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	0	ALA	-	expression tag	UNP B4DSN1

- Molecule 6 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: $C_4H_{12}NO_3$).

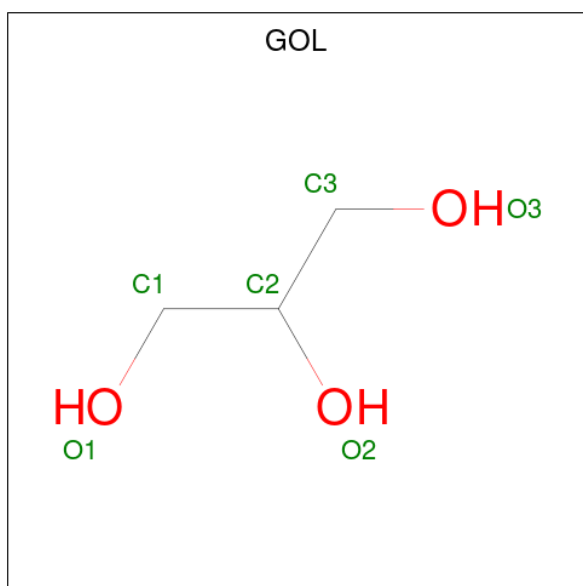


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			8	4	1	3		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	4	Total	Cl	0	0
			4	4		
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	B	1	Total	C	O	0	0
			6	3	3		

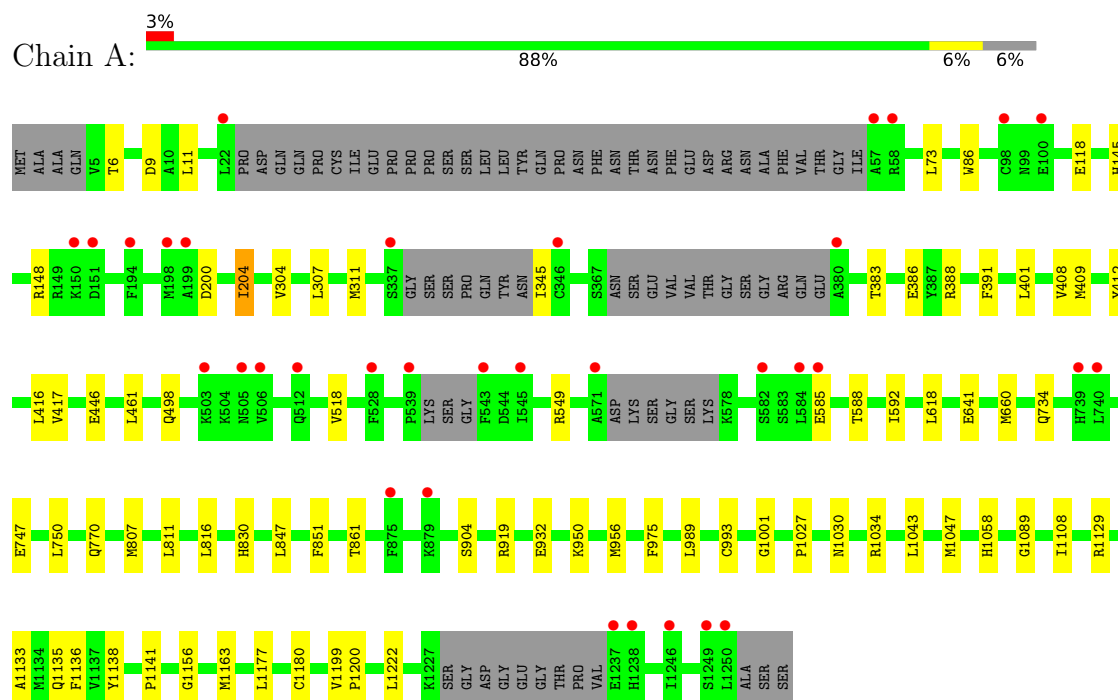
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	404	Total 404	O 404	0	0
9	B	426	Total 426	O 426	0	0
9	D	57	Total 57	O 57	0	0
9	E	12	Total 12	O 12	0	0
9	F	58	Total 58	O 58	0	0

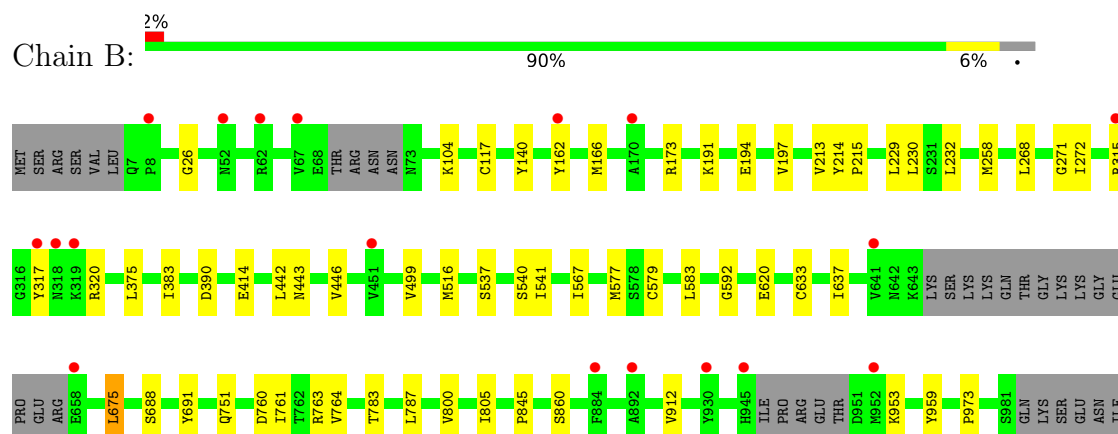
3 Residue-property plots [i](#)

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

• Molecule 1: Cytoplasmic FMR1-interacting protein 1

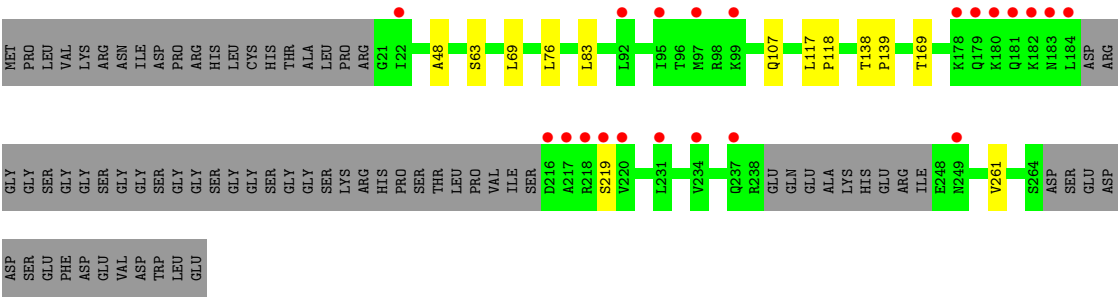


• Molecule 2: Nck-associated protein 1

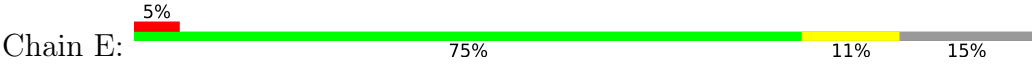




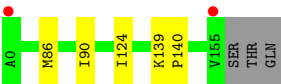
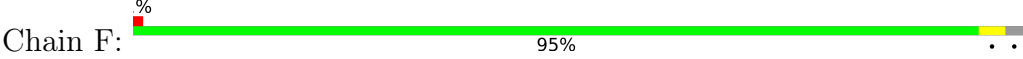
● Molecule 3: Wiskott-Aldrich syndrome protein family member 1



● Molecule 4: Probable protein BRICK1



● Molecule 5: Abl interactor 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	97.01Å 113.98Å 327.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.98 – 2.29 47.98 – 2.29	Depositor EDS
% Data completeness (in resolution range)	86.9 (47.98-2.29) 87.0 (47.98-2.29)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.57 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.188 , 0.237 0.208 , 0.253	Depositor DCC
R_{free} test set	7144 reflections (4.36%)	wwPDB-VP
Wilson B-factor (Å ²)	31.7	Xtriage
Anisotropy	0.150	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 19.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	23017	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.86% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.43	0/9960	0.79	1/13440 (0.0%)
2	B	0.43	1/8956 (0.0%)	0.79	0/12108
3	D	0.44	0/1713	0.76	0/2301
4	E	0.41	0/548	0.79	0/735
5	F	0.42	0/1270	0.82	0/1716
All	All	0.43	1/22447 (0.0%)	0.79	1/30300 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	197	VAL	CA-CB	5.00	1.56	1.54

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	518	VAL	N-CA-C	5.01	117.97	112.96

There are no chirality outliers.

There are no planarity outliers.

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	9753	0	9748	46	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	8782	0	8827	35	0
3	D	1690	0	1698	9	0
4	E	541	0	541	6	0
5	F	1255	0	1273	4	0
6	A	8	0	12	2	0
7	A	4	0	0	0	0
7	B	3	0	0	0	0
8	A	18	0	24	1	0
8	B	6	0	8	1	0
9	A	404	0	0	1	0
9	B	426	0	0	0	0
9	D	57	0	0	0	0
9	E	12	0	0	0	0
9	F	58	0	0	0	0
All	All	23017	0	22131	88	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 2.

All (88) 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:660:MET:HE3	2:B:1117:HIS:CD2	1.87	1.07
1:A:660:MET:HE3	2:B:1117:HIS:HD2	1.27	0.98
1:A:660:MET:HE2	1:A:660:MET:HA	1.69	0.74
1:A:409:MET:HE3	1:A:618:LEU:HD22	1.68	0.74
1:A:660:MET:CE	2:B:1117:HIS:CD2	2.71	0.71
1:A:956:MET:HE1	1:A:1133:ALA:HB2	1.76	0.68
1:A:498:GLN:HE22	1:A:585:GLU:HG3	1.58	0.67
1:A:409:MET:HE3	1:A:618:LEU:CD2	2.26	0.64
1:A:408:VAL:HG12	1:A:409:MET:HE2	1.78	0.64
1:A:641[B]:GLU:CD	1:A:641[B]:GLU:H	2.07	0.62
1:A:1034:ARG:HD2	1:A:1043:LEU:HD11	1.83	0.60
2:B:751:GLN:HA	2:B:761:ILE:HG21	1.85	0.59
2:B:213:VAL:CG1	2:B:258:MET:HE1	2.32	0.59
1:A:145:HIS:HB3	1:A:148:ARG:HB3	1.86	0.58
2:B:213:VAL:HB	2:B:258:MET:HE1	1.88	0.56
1:A:588:THR:O	1:A:592:ILE:HD12	2.07	0.55
1:A:919[B]:ARG:HA	1:A:919[B]:ARG:HE	1.71	0.55
2:B:567[B]:ILE:O	2:B:567[B]:ILE:HD13	2.07	0.54
2:B:375:LEU:HB3	2:B:537:SER:HB3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:40:ASP:O	4:E:44:ARG:HG2	2.07	0.54
8:A:1261:GOL:H31	4:E:59:ARG:HD3	1.90	0.53
1:A:446[A]:GLU:H	1:A:446[A]:GLU:CD	2.18	0.52
1:A:1108[A]:ILE:C	1:A:1108[A]:ILE:HD12	2.35	0.52
2:B:104:LYS:HG3	2:B:140:TYR:CE1	2.45	0.51
2:B:577:MET:HE1	2:B:592:GLY:HA2	1.91	0.51
2:B:633[B]:CYS:O	2:B:637:ILE:HG12	2.11	0.51
2:B:383:ILE:HG22	2:B:541:ILE:HG21	1.93	0.51
4:E:61:ILE:HD11	5:F:90:ILE:HG12	1.93	0.51
1:A:989:LEU:O	1:A:993:CYS:HB2	2.12	0.50
3:D:117:LEU:HD12	3:D:118:PRO:HD2	1.93	0.49
1:A:750:LEU:HD22	1:A:816:LEU:HD21	1.94	0.49
2:B:959:TYR:HB3	2:B:973:PRO:HG3	1.94	0.48
2:B:271:GLY:HA2	2:B:317:TYR:OH	2.14	0.48
2:B:760:ASP:OD2	2:B:763:ARG:HD2	2.13	0.48
2:B:1034[B]:LYS:HE3	2:B:1034[B]:LYS:HB2	1.71	0.48
2:B:577:MET:CE	2:B:592:GLY:HA2	2.44	0.47
1:A:1129:ARG:HH21	1:A:1177:LEU:HB3	1.79	0.47
3:D:83:LEU:HD21	4:E:68:VAL:HG13	1.95	0.47
1:A:1047:MET:HA	1:A:1047:MET:HE2	1.97	0.47
8:B:1132:GOL:H2	5:F:124:ILE:HD13	1.97	0.47
1:A:770:GLN:HB3	3:D:107:GLN:HG2	1.98	0.46
1:A:861:THR:HG22	2:B:675:LEU:HD23	1.97	0.46
1:A:807:MET:HE3	1:A:811:LEU:HD21	1.97	0.46
1:A:932:GLU:OE2	3:D:219:SER:HB2	2.15	0.46
1:A:304:VAL:HG21	1:A:417:VAL:HG21	1.99	0.45
1:A:1027:PRO:HG2	2:B:845:PRO:HB2	1.97	0.45
2:B:620:GLU:HG2	2:B:675:LEU:HD22	1.99	0.45
1:A:86:TRP:CH2	1:A:118:GLU:HB3	2.53	0.44
1:A:383:THR:HG23	1:A:386:GLU:H	1.82	0.44
1:A:847:LEU:HA	1:A:851:PHE:HB3	1.99	0.44
1:A:975:PHE:CD1	6:A:1254:TRS:H32	2.52	0.44
2:B:213:VAL:CB	2:B:258:MET:HE1	2.48	0.44
2:B:191:LYS:O	2:B:194:GLU:HG2	2.18	0.44
2:B:320:ARG:HD3	2:B:320:ARG:HA	1.76	0.44
1:A:1200:PRO:HB2	9:A:1364:HOH:O	2.17	0.44
2:B:540:SER:HB2	2:B:579:CYS:HB3	2.00	0.43
1:A:6:THR:HG23	1:A:9:ASP:HB2	2.01	0.43
1:A:200:ASP:O	1:A:204:ILE:HD12	2.19	0.43
1:A:1030:ASN:HB2	1:A:1058:HIS:CE1	2.54	0.43
2:B:117:CYS:HB3	2:B:499:VAL:HG12	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:169:THR:HG23	3:D:261:VAL:HG21	1.99	0.43
1:A:401:LEU:HD21	1:A:461:LEU:HB3	2.01	0.43
1:A:1163:MET:HA	1:A:1222:LEU:HD13	2.01	0.43
2:B:1056:LYS:HG2	2:B:1102:LEU:HD21	2.01	0.43
1:A:1136:PHE:HA	1:A:1180:CYS:SG	2.59	0.42
2:B:229:LEU:HG	2:B:230:LEU:HG	2.01	0.42
3:D:69:LEU:HD23	5:F:86:MET:HE3	2.00	0.42
1:A:307:LEU:HD23	1:A:311:MET:HE3	2.01	0.42
1:A:412:TYR:CZ	1:A:416:LEU:HD11	2.54	0.42
2:B:442:LEU:HD11	2:B:516:MET:HE1	2.00	0.42
2:B:443:ASN:HA	2:B:446:VAL:HG12	2.01	0.42
1:A:1135:GLN:HA	1:A:1138:TYR:CE2	2.55	0.42
3:D:76:LEU:HD13	4:E:65:GLU:HG2	2.02	0.42
2:B:800:VAL:HG22	2:B:805:ILE:HB	2.02	0.41
1:A:975:PHE:HD1	6:A:1254:TRS:H32	1.84	0.41
2:B:414:GLU:HG2	2:B:691:TYR:OH	2.20	0.41
1:A:1001:GLY:HA3	1:A:1156:GLY:O	2.21	0.41
5:F:139:LYS:HA	5:F:140:PRO:HD3	1.89	0.41
2:B:783:THR:O	2:B:787:LEU:HG	2.20	0.41
3:D:48:ALA:HB2	4:E:36:LEU:HD21	2.03	0.41
1:A:388:ARG:O	1:A:391:PHE:HB3	2.21	0.41
1:A:950:LYS:CG	1:A:1108[A]:ILE:HG12	2.51	0.41
1:A:1141:PRO:HD2	1:A:1199:VAL:HG13	2.03	0.41
1:A:830[B]:HIS:CG	1:A:830[B]:HIS:O	2.73	0.41
2:B:26:GLY:HA3	2:B:583:LEU:HD12	2.02	0.41
2:B:162:TYR:O	2:B:166:MET:HG2	2.21	0.40
2:B:214:TYR:HB3	2:B:215:PRO:HD3	2.02	0.40
3:D:138:THR:HB	3:D:139:PRO:HD3	2.03	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	1175/1253 (94%)	1150 (98%)	24 (2%)	1 (0%)	48	60
2	B	1086/1128 (96%)	1066 (98%)	20 (2%)	0	100	100
3	D	199/279 (71%)	193 (97%)	6 (3%)	0	100	100
4	E	63/75 (84%)	63 (100%)	0	0	100	100
5	F	155/159 (98%)	154 (99%)	1 (1%)	0	100	100
All	All	2678/2894 (92%)	2626 (98%)	51 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1089	GLY

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%)	1072 (99%)	8 (1%)	76	87
2	B	992/1021 (97%)	979 (99%)	13 (1%)	61	77
3	D	192/252 (76%)	191 (100%)	1 (0%)	81	90
4	E	59/67 (88%)	58 (98%)	1 (2%)	53	72
5	F	138/140 (99%)	138 (100%)	0	100	100
All	All	2461/2611 (94%)	2438 (99%)	23 (1%)	70	84

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LEU
1	A	73	LEU
1	A	204	ILE
1	A	345	ILE
1	A	549	ARG
1	A	734	GLN
1	A	747	GLU

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Mol	Chain	Res	Type
1	A	904	SER
2	B	173	ARG
2	B	232	LEU
2	B	268	LEU
2	B	272	ILE
2	B	315	ARG
2	B	390	ASP
2	B	675	LEU
2	B	688	SER
2	B	764	VAL
2	B	860	SER
2	B	912	VAL
2	B	953	LYS
2	B	1077	THR
3	D	63	SER
4	E	57	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	251	ASN
1	A	312	GLN
1	A	474	HIS
1	A	498	GLN
1	A	512	GLN
1	A	614	GLN
1	A	701	GLN
1	A	709	GLN
1	A	882	ASN
1	A	1070	GLN
1	A	1243	GLN
2	B	89	ASN
2	B	589	HIS
2	B	751	GLN
2	B	774	GLN
2	B	779	HIS
2	B	889	GLN
2	B	1037	ASN
2	B	1038	GLN
2	B	1117	HIS
3	D	107	GLN
3	D	110	GLN

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Mol	Chain	Res	Type
3	D	122	GLN
3	D	230	GLN

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 12 ligands modelled in this entry, 7 are monoatomic - leaving 5 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	1261	-	5,5,5	0.35	0	5,5,5	0.33	0
8	GOL	A	1259	-	5,5,5	0.36	0	5,5,5	0.29	0
8	GOL	A	1260	-	5,5,5	0.35	0	5,5,5	0.29	0
6	TRS	A	1254	-	7,7,7	0.32	0	9,9,9	0.39	0
8	GOL	B	1132	-	5,5,5	0.32	0	5,5,5	0.23	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	1261	-	-	0/4/4/4	-
8	GOL	A	1259	-	-	2/4/4/4	-
8	GOL	A	1260	-	-	2/4/4/4	-
6	TRS	A	1254	-	-	4/9/9/9	-
8	GOL	B	1132	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1254	TRS	C1-C-C3-O3
6	A	1254	TRS	N-C-C3-O3
8	A	1259	GOL	O1-C1-C2-C3
8	A	1260	GOL	C1-C2-C3-O3
8	B	1132	GOL	O1-C1-C2-C3
8	B	1132	GOL	O1-C1-C2-O2
6	A	1254	TRS	C2-C-C3-O3
8	A	1260	GOL	O2-C2-C3-O3
6	A	1254	TRS	C1-C-C2-O2
8	A	1259	GOL	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	1261	GOL	1	0
6	A	1254	TRS	2	0
8	B	1132	GOL	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å ²)	Q < 0.9
1	A	1175/1253 (93%)	-0.16	34 (2%)	53	56	1, 12, 46, 99	14 (1%)
2	B	1086/1128 (96%)	-0.27	18 (1%)	69	70	2, 11, 41, 74	10 (0%)
3	D	204/279 (73%)	0.49	21 (10%)	12	13	5, 27, 92, 110	1 (0%)
4	E	64/75 (85%)	-0.04	4 (6%)	26	28	3, 17, 55, 66	1 (1%)
5	F	156/159 (98%)	-0.09	2 (1%)	75	76	8, 21, 40, 55	1 (0%)
All	All	2685/2894 (92%)	-0.15	79 (2%)	53	56	1, 13, 48, 110	27 (1%)

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	184	LEU	6.9
1	A	875	PHE	6.0
3	D	217	ALA	6.0
3	D	234	VAL	5.8
1	A	57	ALA	4.5
3	D	220	VAL	4.4
5	F	155	VAL	4.0
1	A	539	PRO	3.8
1	A	194	PHE	3.6
1	A	22	LEU	3.6
2	B	8	PRO	3.6
2	B	67	VAL	3.5
2	B	317	TYR	3.5
1	A	337	SER	3.5
3	D	182	LYS	3.5
1	A	528	PHE	3.4
3	D	178	LYS	3.4
3	D	231	LEU	3.4
1	A	199	ALA	3.4
1	A	571	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
3	D	218	ARG	3.3
4	E	68	VAL	3.3
4	E	13[A]	HIS	3.3
1	A	380	ALA	3.2
3	D	219	SER	3.2
2	B	451	VAL	3.1
3	D	181	GLN	3.1
1	A	545	ILE	3.1
1	A	740	LEU	3.1
1	A	58	ARG	3.1
3	D	237	GLN	2.9
1	A	506	VAL	2.9
4	E	12	ILE	2.9
3	D	216	ASP	2.7
1	A	1250	LEU	2.7
1	A	585	GLU	2.6
1	A	543	PHE	2.6
1	A	1238	HIS	2.6
1	A	584	LEU	2.5
2	B	162	TYR	2.5
3	D	95	ILE	2.4
3	D	180	LYS	2.4
2	B	318	ASN	2.4
2	B	170	ALA	2.4
1	A	1246	ILE	2.4
1	A	198	MET	2.4
1	A	1249	SER	2.4
2	B	315	ARG	2.4
1	A	1237	GLU	2.4
4	E	70	LYS	2.3
1	A	879	LYS	2.3
2	B	319	LYS	2.3
1	A	346	CYS	2.3
1	A	505	ASN	2.3
3	D	249	ASN	2.3
3	D	97	MET	2.3
1	A	503	LYS	2.3
3	D	92	LEU	2.2
2	B	62	ARG	2.2
1	A	100	GLU	2.2
2	B	952	MET	2.2
2	B	52	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	739	HIS	2.1
2	B	884	PHE	2.1
1	A	98	CYS	2.1
3	D	22	ILE	2.1
1	A	150	LYS	2.0
1	A	582	SER	2.0
2	B	658	GLU	2.0
2	B	892	ALA	2.0
2	B	945	HIS	2.0
1	A	151	ASP	2.0
3	D	183	ASN	2.0
2	B	930	TYR	2.0
2	B	641	VAL	2.0
3	D	99	LYS	2.0
5	F	0	ALA	2.0
1	A	512	GLN	2.0
3	D	179	GLN	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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
6	TRS	A	1254	8/8	0.69	0.33	67,83,93,94	0
7	CL	A	1258	1/1	0.70	0.42	89,89,89,89	0
7	CL	B	1129	1/1	0.72	0.42	94,94,94,94	0
7	CL	A	1257	1/1	0.75	0.37	103,103,103,103	0
8	GOL	A	1259	6/6	0.80	0.27	63,71,82,83	0
7	CL	A	1255	1/1	0.81	0.47	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	GOL	B	1132	6/6	0.82	0.31	62,68,75,91	0
8	GOL	A	1261	6/6	0.86	0.31	72,75,81,84	0
8	GOL	A	1260	6/6	0.87	0.24	82,88,89,95	0
7	CL	A	1256	1/1	0.88	0.37	93,93,93,93	0
7	CL	B	1130	1/1	0.89	0.36	77,77,77,77	0
7	CL	B	1131	1/1	0.93	0.27	55,55,55,55	0

6.5 Other polymers [i](#)

There are no such residues in this entry.