



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:33 AM GMT

PDB ID : 3P8C
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
<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

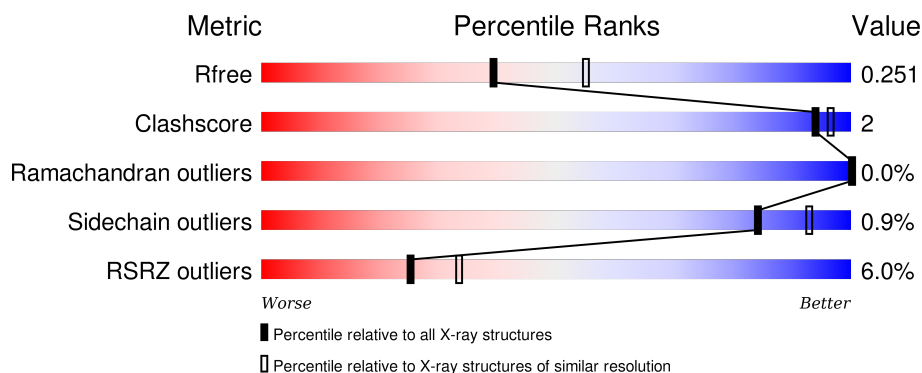
1 Overall quality at a glance i

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}	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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

Mol	Chain	Length	Quality of chain
1	A	1253	<div> <div>6%</div> <div> <div></div> <div>88%</div> <div>5%</div> <div>6%</div> </div> </div>
2	B	1128	<div> <div>5%</div> <div> <div></div> <div>91%</div> <div>5%</div> <div>.</div> </div> </div>
3	D	279	<div> <div>9%</div> <div> <div></div> <div>69%</div> <div>.</div> <div>27%</div> </div> </div>
4	E	75	<div> <div>3%</div> <div> <div></div> <div>76%</div> <div>9%</div> <div>15%</div> </div> </div>
5	F	159	<div> <div>2%</div> <div> <div></div> <div>96%</div> <div>.</div> <div>.</div> </div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	CL	B	1130	-	-	-	X
7	CL	B	1131	-	-	-	X
8	GOL	A	1259	-	-	-	X
8	GOL	A	1261	-	-	-	X

2 Entry composition [i](#)

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			

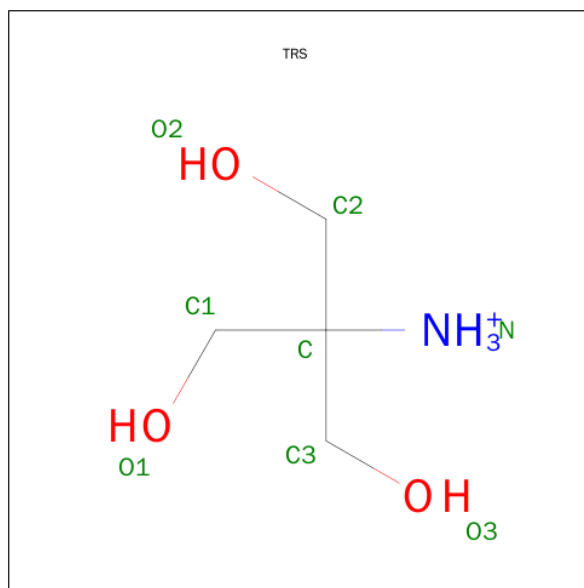
- Molecule 5 is a protein called Abl interactor 2.

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	3	Total	Cl	0	0
			3	3		
7	A	4	Total	Cl	0	0
			4	4		

- 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	B	1	Total	C	O	0	0
			6	3	3		

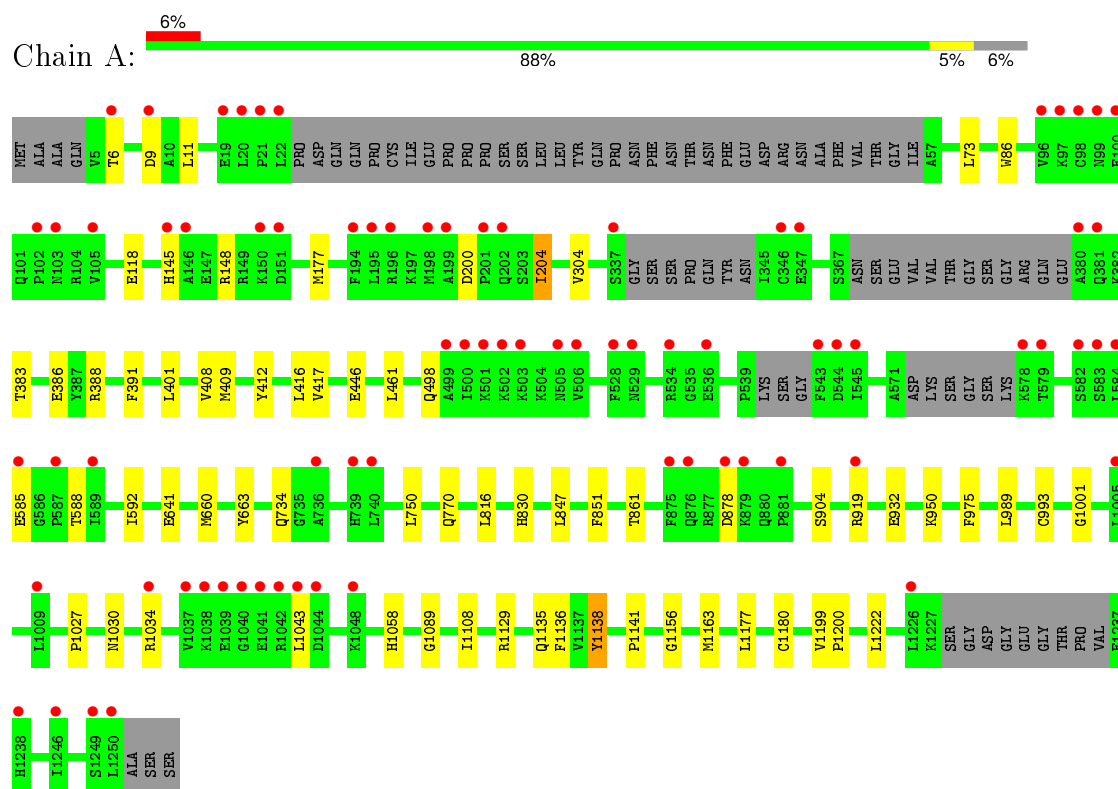
- Molecule 9 is water.

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

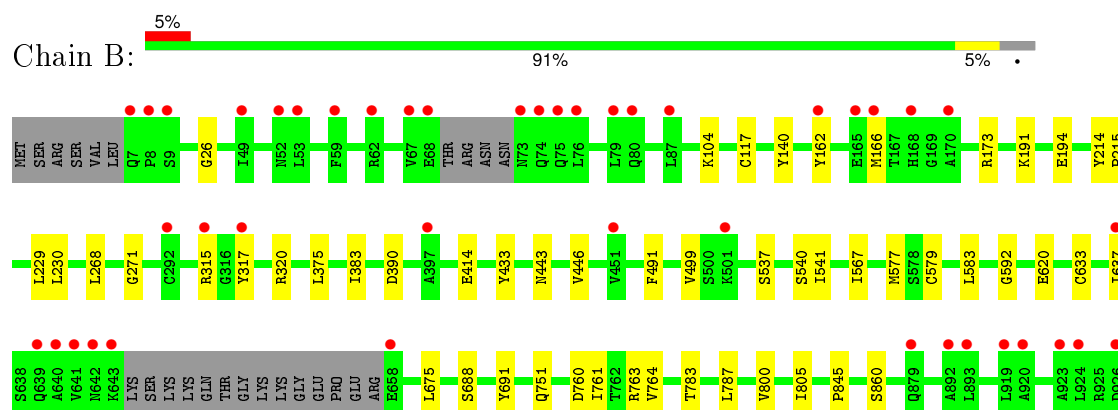
3 Residue-property plots [i](#)

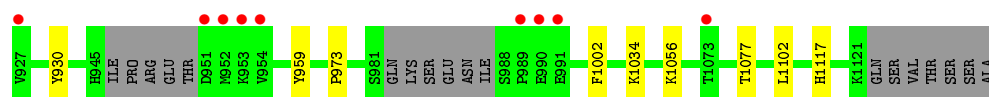
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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

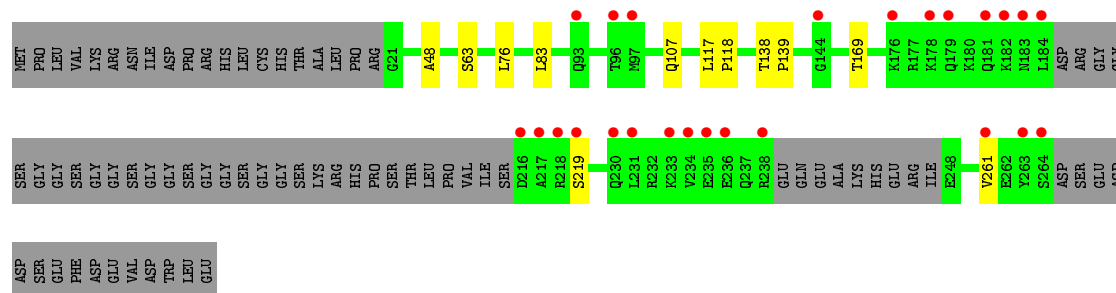


• Molecule 2: Nck-associated protein 1

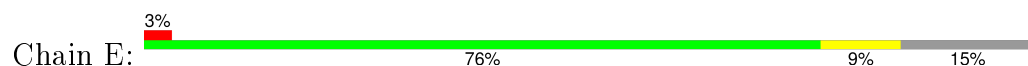




- Molecule 3: Wiskott-Aldrich syndrome protein family member 1



- 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) 86.9 (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 0.204 , 0.251	Depositor DCC
R_{free} test set	7135 reflections (5.01%)	DCC
Wilson B-factor (Å ²)	31.7	Xtriage
Anisotropy	0.150	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 27.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 142454 reflections (0.001%)	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, 0.375 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, TRS, 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	0.35	0/9960	0.46	0/13440
2	B	0.34	0/8956	0.47	0/12108
3	D	0.34	0/1713	0.46	0/2301
4	E	0.32	0/548	0.46	0/735
5	F	0.30	0/1270	0.46	0/1716
All	All	0.34	0/22447	0.46	0/30300

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	9753	0	9748	42	0
2	B	8782	0	8827	32	0
3	D	1690	0	1698	8	0
4	E	541	0	541	6	0
5	F	1255	0	1273	3	0
6	A	8	0	12	2	0
7	A	4	0	0	0	0
7	B	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	79	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 (79) 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:HD2	1.45	0.82
1:A:660:MET:CE	2:B:1117:HIS:CD2	2.71	0.73
1:A:660:MET:HE3	2:B:1117:HIS:CD2	2.23	0.72
1:A:498:GLN:HE22	1:A:585:GLU:HG3	1.58	0.67
1:A:660:MET:HE1	2:B:1117:HIS:CD2	2.35	0.60
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
1:A:145:HIS:HB3	1:A:148:ARG:HB3	1.86	0.58
1:A:641[B]:GLU:CD	1:A:641[B]:GLU:H	2.07	0.57
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
4:E:40:ASP:O	4:E:44:ARG:HG2	2.07	0.54
2:B:375:LEU:HB3	2:B:537:SER:HB3	1.89	0.54
8:A:1261:GOL:H31	4:E:59:ARG:HD3	1.90	0.53
2:B:577:MET:HE1	2:B:592:GLY:HA2	1.90	0.52
1:A:408:VAL:HG12	1:A:409:MET:HE1	1.91	0.52
2:B:104:LYS:HG3	2:B:140:TYR:CE1	2.45	0.51
2:B:633[B]:CYS:O	2:B:637:ILE:HG12	2.11	0.51
4:E:61:ILE:HD11	5:F:90:ILE:HG12	1.93	0.51
2:B:383:ILE:HG22	2:B:541:ILE:HG21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:760:ASP:OD2	2:B:763:ARG:HD2	2.13	0.48
2:B:1034[B]:LYS:HB2	2:B:1034[B]:LYS:HE3	1.71	0.48
1:A:446[A]:GLU:H	1:A:446[A]:GLU:CD	2.18	0.48
2:B:577:MET:CE	2:B:592:GLY:HA2	2.44	0.47
3:D:83:LEU:HD21	4:E:68:VAL:HG13	1.95	0.47
1:A:1129:ARG:HH21	1:A:1177:LEU:HB3	1.79	0.47
1:A:1108[A]:ILE:C	1:A:1108[A]:ILE:HD12	2.35	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: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:975:PHE:CD1	6:A:1254:TRS:H32	2.52	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:86:TRP:CH2	1:A:118:GLU:HB3	2.53	0.44
2:B:191:LYS:O	2:B:194:GLU:HG2	2.18	0.44
2:B:320:ARG:HA	2:B:320:ARG:HD3	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:1030:ASN:HB2	1:A:1058:HIS:CE1	2.54	0.43
1:A:200:ASP:O	1:A:204:ILE:HD12	2.19	0.43
2:B:117:CYS:HB3	2:B:499:VAL:HG12	1.99	0.43
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
2:B:1056:LYS:HG2	2:B:1102:LEU:HD21	2.01	0.43
1:A:1163:MET:HA	1:A:1222:LEU:HD13	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
1:A:412:TYR:CZ	1:A:416:LEU:HD11	2.54	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
1:A:660:MET:HA	1:A:660:MET:CE	2.49	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:139:LYS:HA	5:F:140:PRO:HD3	1.89	0.41
3:D:48:ALA:HB2	4:E:36:LEU:HD21	2.03	0.41
2:B:783:THR:O	2:B:787:LEU:HG	2.20	0.41
1:A:388:ARG:O	1:A:391:PHE:HB3	2.21	0.41
1:A:660:MET:HE2	1:A:663:TYR:CD2	2.56	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
2:B:26:GLY:HA3	2:B:583:LEU:HD12	2.02	0.41
1:A:830[B]:HIS:CG	1:A:830[B]:HIS:O	2.73	0.41
2:B:214:TYR:HB3	2:B:215:PRO:HD3	2.02	0.40
2:B:162:TYR:O	2:B:166:MET:HG2	2.21	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

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	1175/1253 (94%)	1150 (98%)	24 (2%)	1 (0%)	56	68
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%)	88	95
2	B	992/1021 (97%)	980 (99%)	12 (1%)	78	89
3	D	192/252 (76%)	191 (100%)	1 (0%)	92	97
4	E	59/67 (88%)	59 (100%)	0	100	100
5	F	138/140 (99%)	138 (100%)	0	100	100
All	All	2461/2611 (94%)	2440 (99%)	21 (1%)	84	93

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LEU
1	A	73	LEU
1	A	177	MET
1	A	204	ILE
1	A	734	GLN
1	A	878	ASP
1	A	904	SER
1	A	1138	TYR
2	B	173	ARG
2	B	268	LEU
2	B	315	ARG
2	B	390	ASP
2	B	433	TYR
2	B	491	PHE
2	B	688	SER
2	B	764	VAL
2	B	860	SER
2	B	930	TYR
2	B	1002	PHE
2	B	1077	THR
3	D	63	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	324	HIS
1	A	596	HIS
1	A	882	ASN
2	B	766	ASN
2	B	774	GLN
2	B	889	GLN
2	B	1038	GLN
2	B	1117	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 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	$\# Z > 2$
6	TRS	A	1254	-	7,7,7	0.95	1 (14%)	9,9,9	0.47	0
8	GOL	A	1259	-	5,5,5	0.32	0	5,5,5	0.25	0
8	GOL	A	1260	-	5,5,5	0.32	0	5,5,5	0.22	0
8	GOL	A	1261	-	5,5,5	0.31	0	5,5,5	0.30	0
8	GOL	B	1132	-	5,5,5	0.29	0	5,5,5	0.22	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
6	TRS	A	1254	-	-	0/9/9/9	0/0/0/0
8	GOL	A	1259	-	-	0/4/4/4	0/0/0/0
8	GOL	A	1260	-	-	0/4/4/4	0/0/0/0
8	GOL	A	1261	-	-	0/4/4/4	0/0/0/0
8	GOL	B	1132	-	-	0/4/4/4	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1254	TRS	C-N	-2.42	1.47	1.50

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1254	TRS	2	0
8	A	1261	GOL	1	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	78 (6%) 22 29	2, 12, 46, 99	0
2	B	1086/1128 (96%)	0.08	52 (4%) 34 43	2, 11, 41, 74	0
3	D	204/279 (73%)	0.61	25 (12%) 5 8	5, 27, 92, 110	0
4	E	64/75 (85%)	0.04	2 (3%) 52 62	3, 17, 55, 66	0
5	F	156/159 (98%)	-0.01	3 (1%) 70 76	10, 21, 40, 55	0
All	All	2685/2894 (92%)	0.15	160 (5%) 25 33	2, 13, 48, 110	0

All (160) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	234	VAL	8.3
3	D	184	LEU	7.6
3	D	181	GLN	6.9
1	A	198	MET	6.2
1	A	380	ALA	5.9
3	D	178	LYS	5.5
1	A	1040	GLY	5.3
3	D	217	ALA	5.3
1	A	528	PHE	5.3
3	D	261	VAL	5.1
3	D	219	SER	4.9
3	D	183	ASN	4.9
2	B	170	ALA	4.8
1	A	1250	LEU	4.8
2	B	642	ASN	4.7
3	D	182	LYS	4.7
1	A	503	LYS	4.6
1	A	1042	ARG	4.6
3	D	179	GLN	4.6
1	A	1249	SER	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	150	LYS	4.5
2	B	8	PRO	4.5
1	A	98	CYS	4.4
2	B	641	VAL	4.4
1	A	381	GLN	4.3
2	B	643	LYS	4.3
3	D	264	SER	4.1
1	A	194	PHE	4.1
2	B	892	ALA	4.1
2	B	74	GLN	4.0
1	A	337	SER	4.0
1	A	578	LYS	3.9
5	F	155	VAL	3.8
1	A	100	GLU	3.8
2	B	927	VAL	3.7
2	B	67	VAL	3.7
2	B	954	VAL	3.7
1	A	97	LYS	3.7
1	A	1043	LEU	3.7
2	B	62	ARG	3.7
2	B	7	GLN	3.5
1	A	582	SER	3.5
2	B	315	ARG	3.5
1	A	1044	ASP	3.4
2	B	952	MET	3.4
3	D	176	LYS	3.4
1	A	202	GLN	3.4
2	B	9	SER	3.4
3	D	238	ARG	3.4
1	A	875	PHE	3.4
1	A	587	PRO	3.4
1	A	584	LEU	3.3
2	B	166	MET	3.3
1	A	585	GLU	3.3
3	D	96	THR	3.3
1	A	500	ILE	3.2
2	B	80	GLN	3.2
1	A	96	VAL	3.2
1	A	589	ILE	3.1
3	D	231	LEU	3.1
4	E	73	THR	3.1
2	B	168	HIS	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	19	GLU	3.0
1	A	1238	HIS	3.0
2	B	951	ASP	3.0
1	A	99	ASN	3.0
3	D	235	GLU	3.0
5	F	2	ALA	3.0
1	A	22	LEU	3.0
1	A	346	CYS	2.9
1	A	102	PRO	2.9
1	A	506	VAL	2.8
2	B	73	ASN	2.8
2	B	79	LEU	2.8
1	A	739	HIS	2.8
3	D	216	ASP	2.8
2	B	49	ILE	2.8
2	B	637	ILE	2.7
2	B	162	TYR	2.7
1	A	1009	LEU	2.7
2	B	317	TYR	2.7
2	B	953	LYS	2.7
3	D	233	LYS	2.7
3	D	218	ARG	2.7
1	A	543	PHE	2.7
1	A	1039	GLU	2.6
1	A	583	SER	2.6
2	B	59	PHE	2.6
3	D	236	GLU	2.6
1	A	879	LYS	2.6
2	B	923	ALA	2.6
1	A	505	ASN	2.6
4	E	70	LYS	2.6
1	A	9	ASP	2.6
2	B	87	LEU	2.6
1	A	876	GLN	2.6
2	B	640	ALA	2.6
1	A	146	ALA	2.5
1	A	529	ASN	2.5
2	B	924	LEU	2.5
1	A	1048	LYS	2.5
2	B	451	VAL	2.5
1	A	151	ASP	2.5
1	A	105	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	145	HIS	2.5
1	A	502	LYS	2.5
1	A	736	ALA	2.5
1	A	199	ALA	2.5
2	B	639	GLN	2.4
1	A	195	LEU	2.4
3	D	263	TYR	2.4
1	A	347	GLU	2.4
1	A	536	GLU	2.4
2	B	879	GLN	2.4
2	B	920	ALA	2.4
2	B	990	GLU	2.4
1	A	881	PRO	2.4
3	D	144	GLY	2.4
1	A	1037	VAL	2.3
3	D	93	GLN	2.3
1	A	21	PRO	2.3
2	B	989	PRO	2.3
1	A	579	THR	2.3
3	D	230	GLN	2.3
2	B	52	ASN	2.3
2	B	926[A]	ASP	2.3
2	B	53	LEU	2.3
2	B	68	GLU	2.3
2	B	165	GLU	2.3
2	B	658	GLU	2.2
1	A	501	LYS	2.2
1	A	201	PRO	2.2
1	A	1038	LYS	2.2
2	B	75	GLN	2.2
1	A	6	THR	2.2
2	B	76	LEU	2.2
2	B	1073	THR	2.2
1	A	196	ARG	2.1
1	A	1226	LEU	2.1
1	A	1041	GLU	2.1
3	D	97	MET	2.1
1	A	740	LEU	2.1
2	B	919	LEU	2.1
1	A	499	ALA	2.1
1	A	544[A]	ASP	2.1
1	A	545	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	103	ASN	2.1
2	B	991	GLU	2.1
1	A	534	ARG	2.1
2	B	893	LEU	2.0
2	B	501	LYS	2.0
1	A	919[A]	ARG	2.0
5	F	17	ARG	2.0
1	A	878	ASP	2.0
1	A	20	LEU	2.0
2	B	397	ALA	2.0
2	B	292	CYS	2.0
1	A	1034	ARG	2.0
1	A	1246	ILE	2.0
1	A	1005	LEU	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
8	GOL	A	1261	6/6	0.79	0.38	18.51	72,75,81,84	0
7	CL	B	1130	1/1	0.87	0.36	17.97	77,77,77,77	0
7	CL	B	1131	1/1	0.96	0.46	7.71	55,55,55,55	0
8	GOL	A	1259	6/6	0.84	0.29	6.63	63,71,82,83	0
6	TRS	A	1254	8/8	0.60	0.25	-	67,83,93,94	0
8	GOL	B	1132	6/6	0.59	0.27	-	62,68,75,91	0
8	GOL	A	1260	6/6	0.93	0.14	-	82,88,89,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
7	CL	A	1257	1/1	0.90	0.46	-	103,103,103,103	0
7	CL	A	1255	1/1	0.77	0.74	-	86,86,86,86	0
7	CL	A	1258	1/1	0.89	0.32	-	89,89,89,89	0
7	CL	A	1256	1/1	0.75	0.50	-	93,93,93,93	0
7	CL	B	1129	1/1	0.81	0.36	-	94,94,94,94	0

6.5 Other polymers [i](#)

There are no such residues in this entry.