



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 04:38 PM GMT

PDB ID : 3P8C  
Title : Structure and Control of the Actin Regulatory WAVE Complex  
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Deposited on : 2010-10-13  
Resolution : 2.29 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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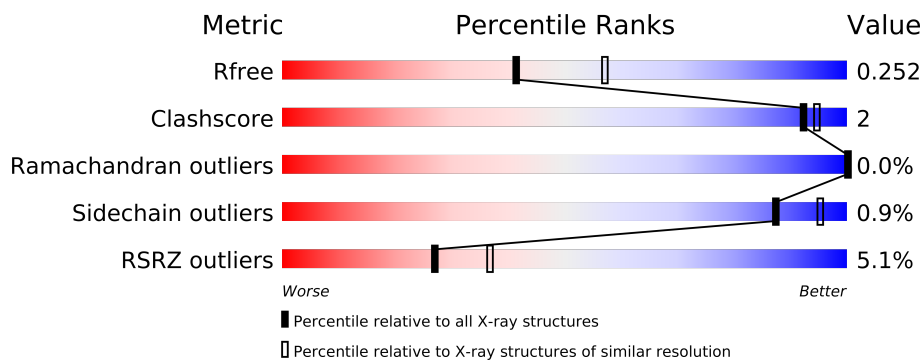
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

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))
$R_{free}$	66092	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	1253	
2	B	1128	
3	D	279	
4	E	75	
5	F	159	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
6	TRS	A	1254	-	X
7	CL	A	1255	-	X
7	CL	A	1256	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
7	CL	A	1257	-	X
7	CL	A	1258	-	X
7	CL	B	1129	-	X
7	CL	B	1130	-	X
7	CL	B	1131	-	X
8	GOL	A	1259	-	X
8	GOL	A	1260	-	X
8	GOL	A	1261	-	X
8	GOL	B	1132	-	X

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 23017 atoms, of which 0 are hydrogen and 0 are deuterium.

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			

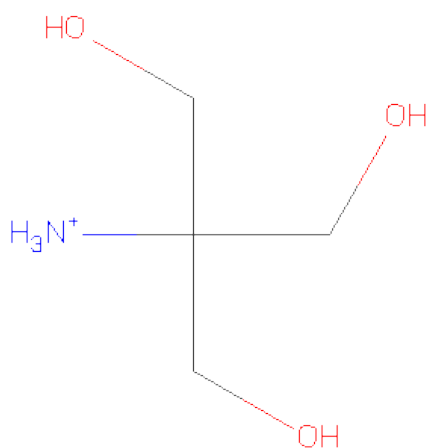
- Molecule 5 is a protein called Abl interactor 2.

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:  $C_4H_{12}NO_3$ ).

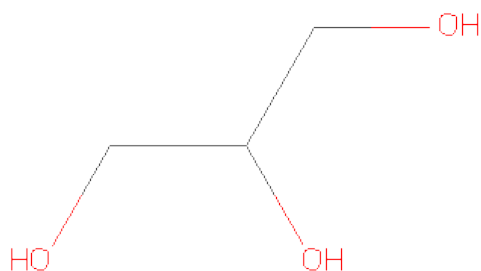


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			8	4	1	3		

- 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: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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.

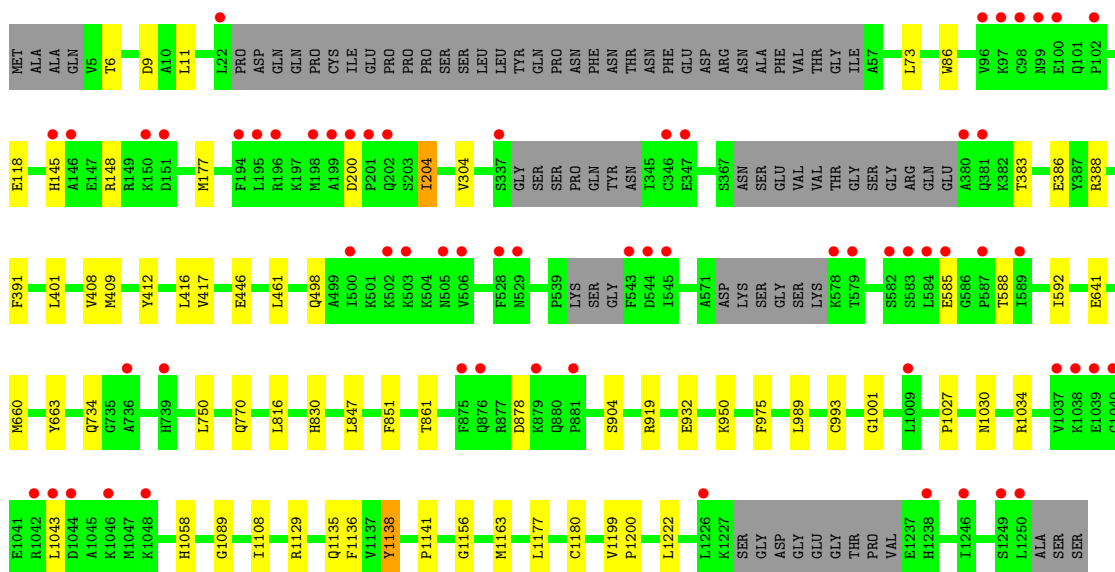
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	404	Total 404	O 404	0	0
9	B	426	Total 426	O 426	0	0
9	D	57	Total 57	O 57	0	0
9	E	12	Total 12	O 12	0	0
9	F	58	Total 58	O 58	0	0

### 3 Residue-property plots

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.

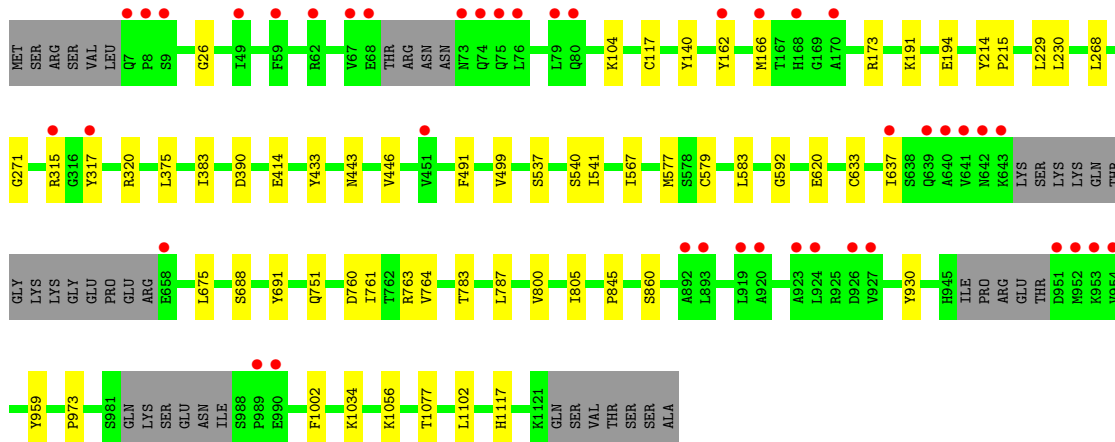
- Molecule 1: Cytoplasmic FMR1-interacting protein 1

Chain A: 



- Molecule 2: Nck-associated protein 1

Chain B: 



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



[illegible]

- Chain E:

MET  
 ALA  
 GLY  
 GLN  
 GLU  
 ASP  
 PRO  
 VAL  
 GLN  
 R10  
 L36  
 D40  
 R44  
 R59  
 R60  
 I61  
 E66  
 V68  
 T69  
 K70  
 T73  
 LEU  
 THR

- Chain F: 

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.57 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.188 , 0.237 0.206 , 0.252	Depositor DCC
$R_{free}$ test set	7136 reflections (5.01%)	DCC
Wilson B-factor (Å <sup>2</sup> )	31.7	Xtriage
Anisotropy	0.150	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 2.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	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 <sup>2</sup> )	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.*

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

## 5 Model quality

### 5.1 Standard geometry

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	79	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 2.

All (79) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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
2:B:760:ASP:OD2	2:B:763:ARG:HD2	2.13	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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%)	59	72
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%)	91	97
2	B	992/1021 (97%)	980 (99%)	12 (1%)	82	92
3	D	192/252 (76%)	191 (100%)	1 (0%)	94	98
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%)	87	95

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

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Mol	Chain	Res	Type
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 ⓘ

There are no RNA chains 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 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	0.96	1 (14%)	9,9,9	0.56	0
8	GOL	A	1259	-	5,5,5	0.31	0	5,5,5	0.30	0
8	GOL	A	1260	-	5,5,5	0.31	0	5,5,5	0.23	0
8	GOL	A	1261	-	5,5,5	0.30	0	5,5,5	0.34	0
8	GOL	B	1132	-	5,5,5	0.28	0	5,5,5	0.26	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	-2.48	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.

## 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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
1	A	1175/1253 (93%)	0.15	63 (5%)	25 34	2, 12, 46, 99	0
2	B	1086/1128 (96%)	0.07	42 (3%)	37 48	2, 11, 41, 74	0
3	D	204/279 (73%)	0.54	22 (10%)	6 10	5, 27, 92, 110	0
4	E	64/75 (85%)	0.05	2 (3%)	47 56	3, 17, 55, 66	0
5	F	156/159 (98%)	-0.03	3 (1%)	64 73	10, 21, 40, 55	0
All	All	2685/2894 (92%)	0.14	132 (4%)	27 39	2, 13, 48, 110	0

All (132) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	184	LEU	8.2
3	D	234	VAL	8.0
3	D	181	GLN	6.5
1	A	198	MET	6.2
1	A	528	PHE	5.9
3	D	178	LYS	5.9
1	A	380	ALA	5.8
1	A	1040	GLY	5.4
2	B	170	ALA	5.2
1	A	1250	LEU	5.2
3	D	182	LYS	4.8
1	A	98	CYS	4.8
1	A	1249	SER	4.7
1	A	150	LYS	4.7
1	A	578	LYS	4.6
1	A	503	LYS	4.5
1	A	1042	ARG	4.5
2	B	641	VAL	4.3
2	B	8	PRO	4.3
3	D	179	GLN	4.3

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Mol	Chain	Res	Type	RSRZ
3	D	183	ASN	4.2
2	B	74	GLN	4.1
1	A	337	SER	4.0
2	B	642	ASN	4.0
2	B	892	ALA	4.0
2	B	643	LYS	3.9
3	D	264	SER	3.9
2	B	67	VAL	3.9
3	D	261	VAL	3.8
2	B	952	MET	3.8
1	A	97	LYS	3.7
1	A	1043	LEU	3.7
3	D	219	SER	3.7
1	A	194	PHE	3.7
1	A	100	GLU	3.6
2	B	62	ARG	3.6
1	A	381	GLN	3.6
3	D	238	ARG	3.5
3	D	217	ALA	3.5
1	A	584	LEU	3.5
1	A	582	SER	3.5
2	B	451	VAL	3.5
3	D	231	LEU	3.4
1	A	202	GLN	3.4
2	B	927	VAL	3.4
5	F	155	VAL	3.3
1	A	739	HIS	3.3
3	D	176	LYS	3.3
2	B	7	GLN	3.3
1	A	1044	ASP	3.2
1	A	96	VAL	3.2
5	F	2	ALA	3.2
1	A	1238	HIS	3.2
1	A	875	PHE	3.1
1	A	346	CYS	3.1
1	A	587	PRO	3.0
2	B	951	ASP	3.0
2	B	59	PHE	3.0
4	E	73	THR	3.0
1	A	22	LEU	2.9
3	D	233	LYS	2.9
2	B	68	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
2	B	315	ARG	2.9
1	A	506	VAL	2.9
2	B	166	MET	2.9
2	B	80	GLN	2.9
2	B	954	VAL	2.9
1	A	505	ASN	2.8
1	A	99	ASN	2.8
1	A	881	PRO	2.8
2	B	79	LEU	2.8
2	B	162	TYR	2.8
2	B	9	SER	2.8
3	D	144	GLY	2.8
2	B	73	ASN	2.8
1	A	544[A]	ASP	2.8
1	A	146	ALA	2.7
1	A	543	PHE	2.7
1	A	199	ALA	2.7
3	D	96	THR	2.7
1	A	1246	ILE	2.7
1	A	585	GLU	2.6
3	D	235	GLU	2.6
1	A	879	LYS	2.6
1	A	102	PRO	2.6
2	B	637	ILE	2.6
1	A	583	SER	2.6
4	E	70	LYS	2.6
1	A	500	ILE	2.6
1	A	145	HIS	2.6
1	A	1009	LEU	2.6
2	B	75	GLN	2.5
5	F	135	ARG	2.5
1	A	579	THR	2.5
1	A	195	LEU	2.5
1	A	589	ILE	2.5
2	B	639	GLN	2.5
2	B	317	TYR	2.5
1	A	1039	GLU	2.4
3	D	236	GLU	2.4
2	B	920	ALA	2.4
2	B	953	LYS	2.4
1	A	1037	VAL	2.4
1	A	196	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	923	ALA	2.4
1	A	347	GLU	2.4
1	A	529	ASN	2.4
1	A	151	ASP	2.3
2	B	990	GLU	2.3
1	A	1046	LYS	2.3
2	B	168	HIS	2.3
3	D	97	MET	2.3
2	B	49	ILE	2.3
1	A	502	LYS	2.3
1	A	1038	LYS	2.3
2	B	76	LEU	2.3
2	B	640	ALA	2.3
2	B	924	LEU	2.3
2	B	926[A]	ASP	2.3
1	A	201	PRO	2.2
2	B	989	PRO	2.2
3	D	263	TYR	2.2
1	A	876	GLN	2.2
1	A	200	ASP	2.1
2	B	658	GLU	2.1
3	D	93	GLN	2.1
1	A	1048	LYS	2.1
1	A	545	ILE	2.1
1	A	736	ALA	2.1
1	A	1226	LEU	2.1
2	B	919	LEU	2.1
2	B	893	LEU	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 carbohydrates 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. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
7	CL	A	1255	1/1	0.71	21.79	86,86,86,86	0
8	GOL	A	1261	6/6	0.36	20.77	72,75,81,84	0
7	CL	B	1129	1/1	0.33	17.10	94,94,94,94	0
7	CL	A	1256	1/1	0.48	13.54	93,93,93,93	0
7	CL	B	1130	1/1	0.33	11.71	77,77,77,77	0
8	GOL	B	1132	6/6	0.26	9.73	62,68,75,91	0
7	CL	A	1257	1/1	0.41	9.60	103,103,103,103	0
7	CL	B	1131	1/1	0.46	8.02	55,55,55,55	0
8	GOL	A	1259	6/6	0.30	7.18	63,71,82,83	0
6	TRS	A	1254	8/8	0.25	4.77	67,83,93,94	0
7	CL	A	1258	1/1	0.27	2.96	89,89,89,89	0
8	GOL	A	1260	6/6	0.13	2.56	82,88,89,95	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.