Full wwPDB X-ray Structure Validation Report (i)

Jun 11, 2024 – 11:04 PM EDT

PDB ID	:	6NDZ
Title	:	Designed repeat protein in complex with Fz8
Authors	:	Miao, Y.; Jude, K.M.; Garcia, K.C.
Deposited on	:	2018-12-14
Resolution	:	2.26 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 (i) 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 (i)) were used in the production of this report:

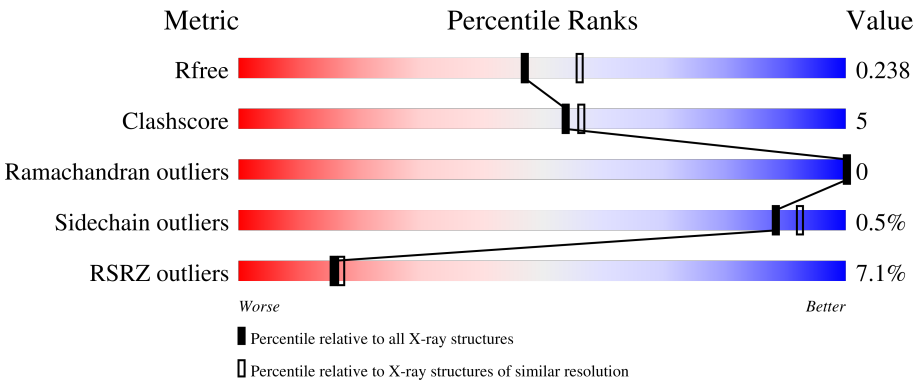
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.26 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}	130704	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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 <=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	125	% 87% 10% • •
1	C	125	2% 85% 10% • •
1	E	125	2% 86% 10% •
2	B	200	85% 10% 5%
2	D	200	10% 80% 15% 5%

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Mol	Chain	Length	Quality of chain
2	F	200	20% 84% 11% 6%

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
3	MPD	B	203	-	X	-	-
4	ACT	C	201	-	-	X	-
5	ACY	A	205	-	-	X	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 7282 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 Frizzled-8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	122	983	623	168	177	15	0	0	0
1	C	120	964	612	163	174	15	0	0	0
1	E	120	964	612	163	174	15	0	0	0

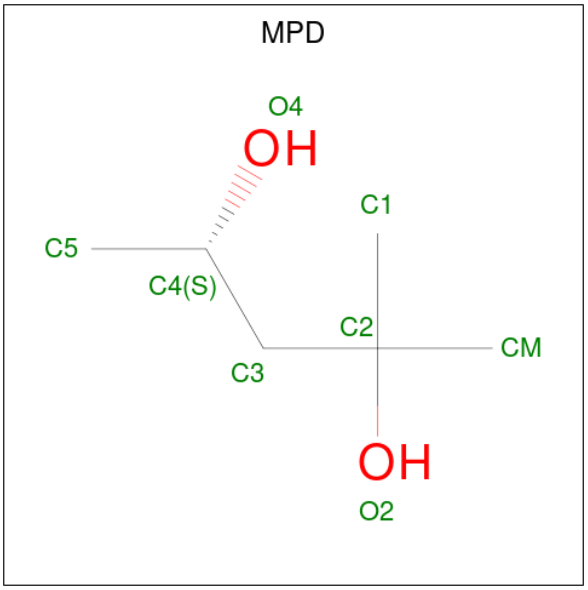
There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	22	GLN	ASN	engineered mutation	UNP Q9H461
A	124	HIS	-	expression tag	UNP Q9H461
A	125	HIS	-	expression tag	UNP Q9H461
A	126	HIS	-	expression tag	UNP Q9H461
A	127	HIS	-	expression tag	UNP Q9H461
A	128	HIS	-	expression tag	UNP Q9H461
A	129	HIS	-	expression tag	UNP Q9H461
C	22	GLN	ASN	engineered mutation	UNP Q9H461
C	124	HIS	-	expression tag	UNP Q9H461
C	125	HIS	-	expression tag	UNP Q9H461
C	126	HIS	-	expression tag	UNP Q9H461
C	127	HIS	-	expression tag	UNP Q9H461
C	128	HIS	-	expression tag	UNP Q9H461
C	129	HIS	-	expression tag	UNP Q9H461
E	22	GLN	ASN	engineered mutation	UNP Q9H461
E	124	HIS	-	expression tag	UNP Q9H461
E	125	HIS	-	expression tag	UNP Q9H461
E	126	HIS	-	expression tag	UNP Q9H461
E	127	HIS	-	expression tag	UNP Q9H461
E	128	HIS	-	expression tag	UNP Q9H461
E	129	HIS	-	expression tag	UNP Q9H461

- Molecule 2 is a protein called Designed repeat binding protein.

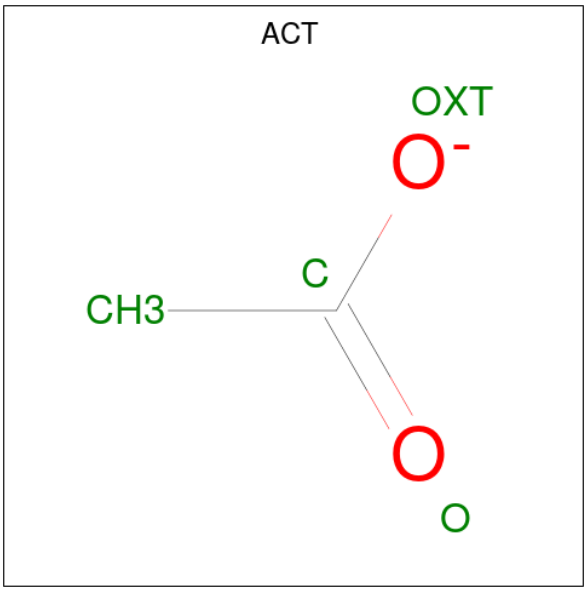
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	190	1371	851	252	263	5	0	0	0
			Total	C	N	O	S			
2	D	190	1367	848	251	263	5	0	0	0
			Total	C	N	O	S			
2	F	189	1362	846	250	261	5	0	0	0

- Molecule 3 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



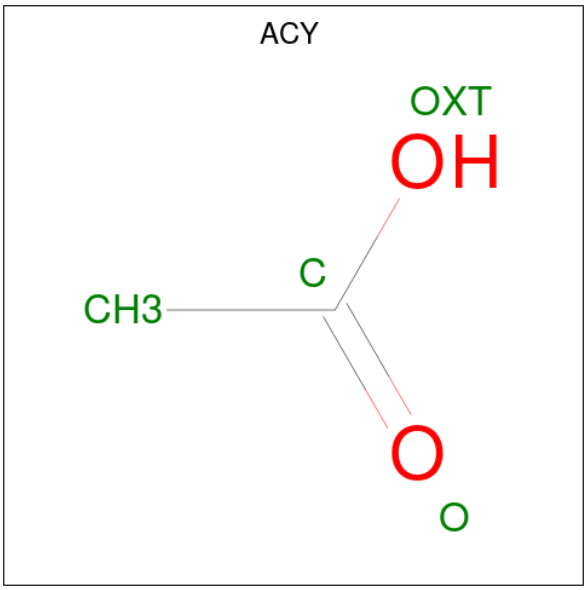
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	8	6	2	0	0
			Total	C	O		
3	B	1	8	6	2	0	0
			Total	C	O		
3	B	1	8	6	2	0	0
			Total	C	O		
3	B	1	8	6	2	0	0

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O		0	0
			4	2	2			
4	A	1	Total	C	O		0	0
			4	2	2			
4	A	1	Total	C	O		0	0
			4	2	2			
4	C	1	Total	C	O		0	0
			4	2	2			

- Molecule 5 is ACETIC ACID (three-letter code: ACY) (formula: $C_2H_4O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	A	1	4	2	2	0	0
			Total	C	O		
5	F	1	4	2	2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	59	59	59	0	0
			Total	O		
6	B	47	47	47	0	0
			Total	O		
6	C	39	39	39	0	0
			Total	O		
6	D	9	9	9	0	0
			Total	O		
6	E	42	42	42	0	0
			Total	O		
6	F	19	19	19	0	0

3 Residue-property plots (i)

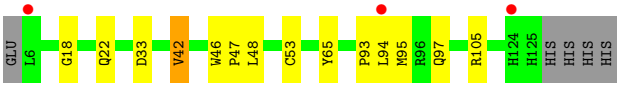
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Frizzled-8

Chain A:

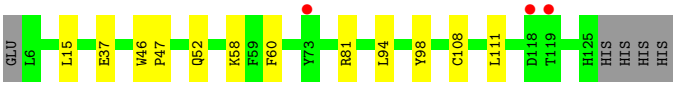
• Molecule 1: Frizzled-8

Chain C:



• Molecule 1: Frizzled-8

Chain E:

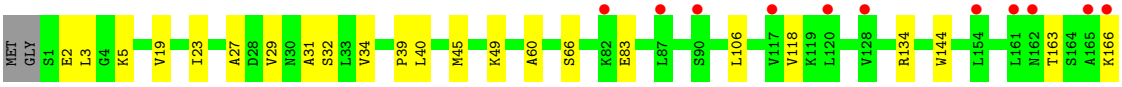


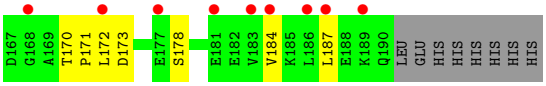
• Molecule 2: Designed repeat binding protein

Chain B:

• Molecule 2: Designed repeat binding protein

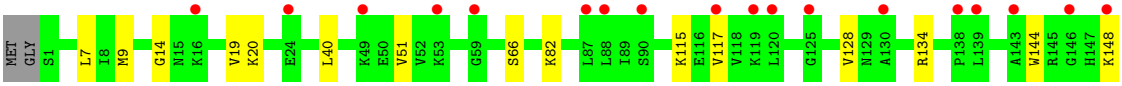
Chain D:

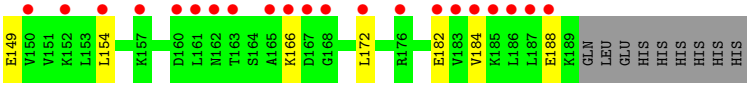




• Molecule 2: Designed repeat binding protein

Chain F:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	79.93Å 109.02Å 114.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.78 – 2.26 42.78 – 2.26	Depositor EDS
% Data completeness (in resolution range)	94.2 (42.78-2.26) 94.2 (42.78-2.26)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.07 (at 2.27Å)	Xtriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, R_{free}	0.212 , 0.238 0.212 , 0.238	Depositor DCC
R_{free} test set	1998 reflections (4.49%)	wwPDB-VP
Wilson B-factor (Å^2)	54.6	Xtriage
Anisotropy	0.320	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 46.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.018 for -h,l,k	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7282	wwPDB-VP
Average B, all atoms (Å^2)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.21% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MPD, ACT, ACY

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	0.27	0/1014	0.47	0/1378
1	C	0.26	0/994	0.46	0/1351
1	E	0.27	0/994	0.46	0/1351
2	B	0.24	0/1385	0.42	0/1868
2	D	0.25	0/1381	0.45	0/1864
2	F	0.26	0/1376	0.43	0/1856
All	All	0.26	0/7144	0.45	0/9668

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	983	0	922	12	0
1	C	964	0	907	9	0
1	E	964	0	907	8	0
2	B	1371	0	1429	14	0
2	D	1367	0	1418	21	0
2	F	1362	0	1421	17	0
3	A	8	0	14	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	24	0	42	2	0
4	A	12	0	9	1	0
4	C	4	0	3	2	0
5	A	4	0	3	2	0
5	F	4	0	3	0	0
6	A	59	0	0	1	0
6	B	47	0	0	1	0
6	C	39	0	0	0	0
6	D	9	0	0	1	0
6	E	42	0	0	0	0
6	F	19	0	0	1	0
All	All	7282	0	7078	75	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 5.

All (75) 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:125:HIS:HE1	2:D:34:VAL:HA	1.54	0.72
1:A:114:GLN:NE2	1:A:123:ASP:OD2	2.23	0.71
2:B:152:LYS:HB3	2:B:186:LEU:HD21	1.77	0.67
2:F:134:ARG:HB3	2:F:166:LYS:HB2	1.81	0.63
2:D:66:SER:OG	6:D:201:HOH:O	2.16	0.61
3:B:201:MPD:O4	3:B:201:MPD:O2	2.17	0.59
2:B:134:ARG:HB3	2:B:166:LYS:HB2	1.85	0.59
2:D:134:ARG:HE	2:D:166:LYS:HG2	1.68	0.59
2:F:115:LYS:HD3	2:F:149:GLU:HG3	1.84	0.58
2:D:134:ARG:HB3	2:D:166:LYS:HB2	1.85	0.58
1:C:18:GLY:HA2	4:C:201:ACT:H2	1.86	0.57
2:B:176:ARG:NH1	6:B:302:HOH:O	2.38	0.56
1:E:52:GLN:HG3	2:F:144:TRP:HH2	1.71	0.56
2:F:148:LYS:HD3	2:F:182:GLU:HB3	1.87	0.56
3:A:201:MPD:HO2	3:A:201:MPD:HO4	1.53	0.55
2:B:73:LEU:HD11	2:B:85:VAL:HG13	1.88	0.54
2:D:134:ARG:HH21	2:D:166:LYS:HG2	1.71	0.54
2:D:106:LEU:HD11	2:D:118:VAL:HG13	1.90	0.54
1:A:20:GLY:H	5:A:205:ACY:H2	1.74	0.53
1:C:53:CYS:HB3	1:C:94:LEU:HD12	1.89	0.53
1:A:125:HIS:O	1:A:126:HIS:ND1	2.42	0.53
1:A:5:GLU:N	6:A:304:HOH:O	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:GLU:OE2	2:B:145:ARG:NH2	2.41	0.53
2:B:134:ARG:HE	2:B:166:LYS:HG2	1.74	0.53
2:D:172:LEU:HD13	2:D:187:LEU:HB2	1.91	0.52
2:D:49:LYS:HD2	2:D:83:GLU:HB3	1.91	0.52
1:C:93:PRO:O	1:C:97:GLN:HG3	2.10	0.52
3:A:201:MPD:O4	3:A:201:MPD:O2	2.26	0.51
2:F:134:ARG:HH21	2:F:166:LYS:HG2	1.76	0.51
1:A:125:HIS:CE1	2:D:34:VAL:HA	2.40	0.50
2:F:134:ARG:HE	2:F:166:LYS:HG2	1.76	0.50
2:B:17:ASP:H	3:B:202:MPD:C1	2.24	0.50
1:E:15:LEU:O	1:E:58:LYS:HE3	2.13	0.49
2:F:14:GLY:HA2	2:F:51:VAL:HG21	1.95	0.48
2:D:172:LEU:HD11	2:D:184:VAL:HG13	1.96	0.48
2:F:66:SER:OG	6:F:301:HOH:O	2.20	0.48
2:B:134:ARG:HH21	2:B:166:LYS:HG2	1.80	0.46
2:B:119:LYS:HB2	2:B:153:LEU:HD21	1.97	0.46
2:D:170:THR:OG1	2:D:173:ASP:OD1	2.31	0.46
1:E:37:GLU:HG2	2:F:9:MET:SD	2.55	0.46
1:A:125:HIS:HB3	2:D:32:SER:OG	2.16	0.46
1:C:46:TRP:N	1:C:47:PRO:HD2	2.31	0.45
2:D:40:LEU:HD23	2:D:40:LEU:HA	1.87	0.45
1:A:95:MET:HG2	2:B:100:ALA:HB1	1.98	0.45
2:F:82:LYS:HB3	2:F:117:VAL:HG22	1.98	0.45
5:A:205:ACY:C	1:C:105:ARG:HH21	2.30	0.44
1:E:94:LEU:O	1:E:98:TYR:HD1	2.01	0.44
1:C:33:ASP:OD1	2:D:5:LYS:NZ	2.48	0.44
1:C:22:GLN:HG2	4:C:201:ACT:H1	1.99	0.43
2:D:31:ALA:O	2:D:39:PRO:HD3	2.18	0.43
1:A:6:LEU:HD21	4:A:202:ACT:O	2.18	0.43
2:B:184:VAL:O	2:B:188:GLU:HG3	2.18	0.43
1:C:42:VAL:HG23	1:C:65:TYR:CD2	2.54	0.43
2:F:128:VAL:HG13	2:F:154:LEU:HD22	2.01	0.43
2:F:7:LEU:HD11	2:F:19:VAL:HG13	2.00	0.43
2:B:47:GLY:HA2	2:B:84:VAL:HG21	2.00	0.42
2:F:172:LEU:HD11	2:F:184:VAL:HG13	2.01	0.42
2:B:14:GLY:HA2	2:B:51:VAL:HG21	2.01	0.42
1:E:60:PHE:HE1	1:E:111:LEU:HD11	1.84	0.42
2:D:144:TRP:CZ3	2:D:178:SER:HB3	2.55	0.42
2:D:163:THR:O	2:D:171:PRO:HD3	2.19	0.42
2:F:184:VAL:O	2:F:188:GLU:HG3	2.20	0.42
1:A:39:GLY:HA2	1:A:42:VAL:HG12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:166:LYS:HD2	2:F:166:LYS:HA	1.93	0.41
1:C:48:LEU:HD11	1:C:95:MET:SD	2.61	0.41
2:D:29:VAL:HG22	2:D:60:ALA:HB2	2.03	0.41
1:A:46:TRP:CG	1:A:47:PRO:HD3	2.56	0.41
2:D:2:GLU:HG3	2:D:3:LEU:N	2.34	0.41
1:E:46:TRP:CG	1:E:47:PRO:HD3	2.56	0.41
1:E:81:ARG:HG3	1:E:108:CYS:HB3	2.02	0.41
2:B:172:LEU:HD13	2:B:187:LEU:HB2	2.01	0.41
2:F:40:LEU:HD23	2:F:40:LEU:HA	1.92	0.41
2:D:3:LEU:HG	2:D:27:ALA:HA	2.02	0.40
2:D:19:VAL:O	2:D:23:ILE:HG13	2.21	0.40
1:E:52:GLN:HG3	2:F:144:TRP:CH2	2.53	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	120/125 (96%)	118 (98%)	2 (2%)	0	100	100
1	C	118/125 (94%)	117 (99%)	1 (1%)	0	100	100
1	E	118/125 (94%)	116 (98%)	2 (2%)	0	100	100
2	B	188/200 (94%)	182 (97%)	6 (3%)	0	100	100
2	D	188/200 (94%)	182 (97%)	6 (3%)	0	100	100
2	F	187/200 (94%)	179 (96%)	8 (4%)	0	100	100
All	All	919/975 (94%)	894 (97%)	25 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	109/113 (96%)	108 (99%)	1 (1%)	78	86
1	C	107/113 (95%)	106 (99%)	1 (1%)	78	86
1	E	107/113 (95%)	107 (100%)	0	100	100
2	B	140/149 (94%)	140 (100%)	0	100	100
2	D	139/149 (93%)	138 (99%)	1 (1%)	84	90
2	F	139/149 (93%)	138 (99%)	1 (1%)	84	90
All	All	741/786 (94%)	737 (100%)	4 (0%)	88	92

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	C	42	VAL
2	D	45	MET
2	F	20	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	114	GLN
1	A	125	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

10 ligands are modelled in this entry.

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	$\#\|Z\| > 2$
4	ACT	A	203	-	3,3,3	1.30	0	3,3,3	1.38	0
4	ACT	A	204	-	3,3,3	1.29	0	3,3,3	1.39	0
3	MPD	B	201	-	7,7,7	0.27	0	9,10,10	0.18	0
3	MPD	A	201	-	7,7,7	0.29	0	9,10,10	0.20	0
3	MPD	B	203	-	7,7,7	0.34	0	9,10,10	7.57	6 (66%)
4	ACT	A	202	-	3,3,3	1.29	0	3,3,3	1.33	0
5	ACY	A	205	-	3,3,3	1.44	0	3,3,3	1.68	1 (33%)
3	MPD	B	202	-	7,7,7	0.25	0	9,10,10	0.27	0
5	ACY	F	201	-	3,3,3	1.47	0	3,3,3	1.71	1 (33%)
4	ACT	C	201	-	3,3,3	1.21	0	3,3,3	1.38	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
3	MPD	B	203	-	-	3/5/5/5	-
3	MPD	A	201	-	-	0/5/5/5	-
3	MPD	B	202	-	-	0/5/5/5	-
3	MPD	B	201	-	-	1/5/5/5	-

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	203	MPD	CM-C2-C1	15.09	142.02	110.57
3	B	203	MPD	O2-C2-CM	-11.65	70.70	108.08
3	B	203	MPD	O2-C2-C1	-11.38	71.55	108.08
3	B	203	MPD	O2-C2-C3	2.94	120.84	109.80
3	B	203	MPD	CM-C2-C3	-2.63	97.71	109.96
3	B	203	MPD	C1-C2-C3	-2.59	97.88	109.96
5	F	201	ACY	O-C-CH3	-2.36	113.15	122.33
5	A	205	ACY	O-C-CH3	-2.32	113.29	122.33

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	201	MPD	O2-C2-C3-C4
3	B	203	MPD	CM-C2-C3-C4
3	B	203	MPD	C2-C3-C4-C5
3	B	203	MPD	C2-C3-C4-O4

There are no ring outliers.

6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	201	MPD	1	0
3	A	201	MPD	2	0
4	A	202	ACT	1	0
5	A	205	ACY	2	0
3	B	202	MPD	1	0
4	C	201	ACT	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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	122/125 (97%)	0.04	1 (0%)	86	87	38, 50, 103, 155	0
1	C	120/125 (96%)	0.13	3 (2%)	57	60	41, 56, 102, 139	0
1	E	120/125 (96%)	0.27	3 (2%)	57	60	47, 59, 95, 155	0
2	B	190/200 (95%)	0.18	0	100	100	39, 54, 100, 132	0
2	D	190/200 (95%)	0.70	20 (10%)	6	6	51, 86, 133, 168	0
2	F	189/200 (94%)	1.07	39 (20%)	1	1	50, 88, 147, 176	0
All	All	931/975 (95%)	0.46	66 (7%)	16	17	38, 65, 133, 176	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	187	LEU	7.2
2	F	183	VAL	6.4
2	F	172	LEU	5.6
2	F	161	LEU	5.5
2	F	154	LEU	4.7
2	F	166	LYS	4.6
1	E	119	THR	4.6
2	F	186	LEU	4.5
2	D	168	GLY	4.4
2	D	187	LEU	4.3
2	D	120	LEU	4.3
1	E	118	ASP	4.2
2	F	182	GLU	4.0
2	D	183	VAL	3.9
2	F	120	LEU	3.9
2	F	185	LYS	3.9
2	D	128	VAL	3.9
2	F	162	ASN	3.7
2	D	154	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
2	F	150	VAL	3.5
2	F	160	ASP	3.3
2	F	176	ARG	3.2
2	D	189	LYS	3.2
2	F	165	ALA	3.2
2	F	139	LEU	3.1
2	D	172	LEU	3.1
2	F	87	LEU	3.0
2	F	188	GLU	3.0
2	F	152	LYS	3.0
2	F	53	LYS	2.9
2	F	16	LYS	2.9
2	D	165	ALA	2.9
2	D	184	VAL	2.8
2	F	143	ALA	2.7
2	F	117	VAL	2.7
2	D	186	LEU	2.6
2	D	87	LEU	2.6
2	F	167	ASP	2.6
2	F	163	THR	2.5
2	F	59	GLY	2.5
1	C	124	HIS	2.5
2	F	184	VAL	2.5
2	D	117	VAL	2.5
2	F	168	GLY	2.5
2	F	24	GLU	2.5
2	F	148	LYS	2.5
1	C	6	LEU	2.4
2	D	181	GLU	2.4
2	F	90	SER	2.3
2	F	157	LYS	2.3
1	A	125	HIS	2.3
2	F	88	LEU	2.3
2	D	166	LYS	2.3
2	D	161	LEU	2.2
2	D	177	GLU	2.2
1	C	94	LEU	2.2
2	F	49	LYS	2.1
2	F	119	LYS	2.1
2	F	138	PRO	2.1
2	F	125	GLY	2.1
2	D	162	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
2	F	130	ALA	2.1
1	E	73	TYR	2.1
2	D	90	SER	2.0
2	D	82	LYS	2.0
2	F	146	GLY	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 monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	ACY	A	205	4/4	0.35	0.42	83,96,97,101	0
3	MPD	B	201	8/8	0.51	0.33	69,81,86,88	0
5	ACY	F	201	4/4	0.59	0.39	76,81,82,85	0
3	MPD	A	201	8/8	0.67	0.39	104,108,117,122	0
3	MPD	B	203	8/8	0.67	0.30	97,101,105,106	0
3	MPD	B	202	8/8	0.70	0.19	73,80,85,89	0
4	ACT	C	201	4/4	0.86	0.40	84,86,88,95	0
4	ACT	A	202	4/4	0.88	0.27	68,76,76,78	0
4	ACT	A	204	4/4	0.91	0.30	81,84,86,90	0
4	ACT	A	203	4/4	0.91	0.19	84,89,89,92	0

6.5 Other polymers (i)

There are no such residues in this entry.