



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 11:41 PM UTC

PDB ID : 5AEI / pdb_00005aei
Title : Designed Armadillo repeat protein YIIIM5AII in complex with peptide (KR)5
Authors : Hansen, S.; Tremmel, D.; Madhurantakam, C.; Reichen, C.; Mittl, P.; Plueckthun, A.
Deposited on : 2015-08-31
Resolution : 1.83 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

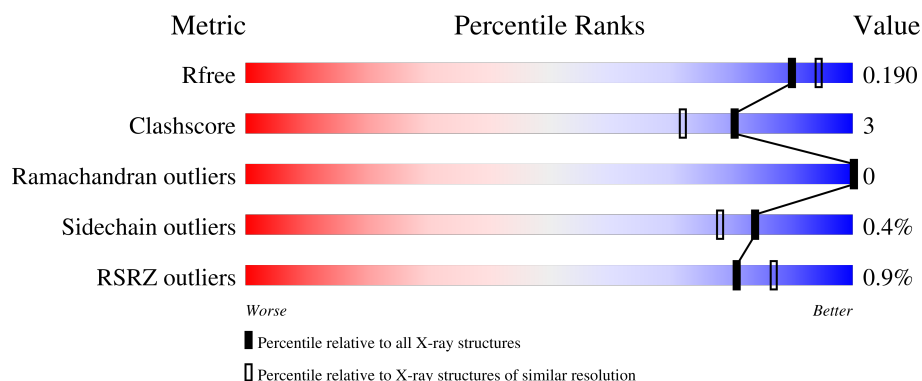
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.83 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	1296 (1.84-1.84)
Clashscore	190562	1329 (1.84-1.84)
Ramachandran outliers	187476	1318 (1.84-1.84)
Sidechain outliers	187428	1318 (1.84-1.84)
RSRZ outliers	180081	1296 (1.84-1.84)

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	286	 90% 7% .
1	B	286	 90% 8% .
1	C	286	 91% 7% ..
2	D	10	 80% 20%
2	E	10	 90% 10%

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Mol	Chain	Length	Quality of chain
2	F	10	 80%20%

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	ACT	C	1294	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7694 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 DESIGNED ARMADILLO REPEAT PROTEIN YIIM5AII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	281	Total	C	N	O	S	0	5	0
			2121	1321	361	438	1			
1	B	282	Total	C	N	O	S	0	10	0
			2167	1350	368	448	1			
1	C	282	Total	C	N	O	S	0	9	0
			2157	1341	367	448	1			

- Molecule 2 is a protein called KR5.

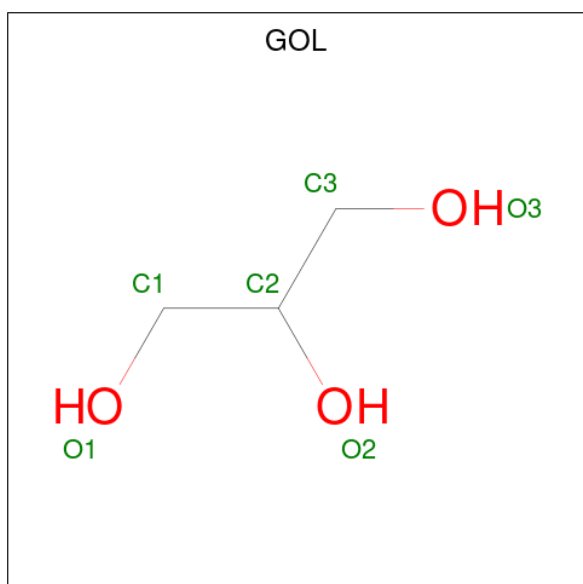
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	10	Total	C	N	O	0	0	0
			101	60	30	11			
2	E	10	Total	C	N	O	0	0	0
			101	60	30	11			
2	F	10	Total	C	N	O	0	0	0
			101	60	30	11			

- Molecule 3 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



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

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	3	Total	Ca	0	0
			3	3		
5	B	6	Total	Ca	0	0
			6	6		
5	C	4	Total	Ca	0	0
			4	4		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	300	Total	O	0	0
			300	300		
6	B	304	Total	O	0	0
			304	304		
6	C	253	Total	O	0	0
			253	253		
6	D	17	Total	O	0	0
			17	17		
6	E	20	Total	O	0	0
			20	20		
6	F	13	Total	O	0	0
			13	13		

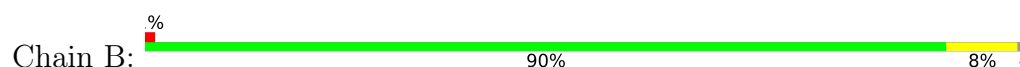
3 Residue-property plots [i](#)

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.

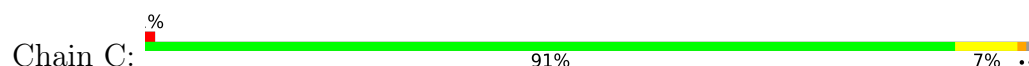
- Molecule 1: DESIGNED ARMADILLO REPEAT PROTEIN YIIIM5AII



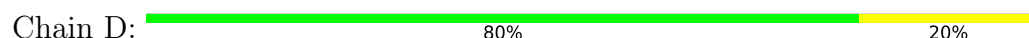
- Molecule 1: DESIGNED ARMADILLO REPEAT PROTEIN YIIIM5AII



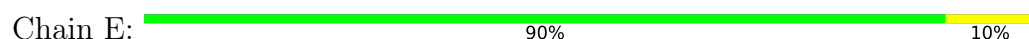
- Molecule 1: DESIGNED ARMADILLO REPEAT PROTEIN YIIIM5AII



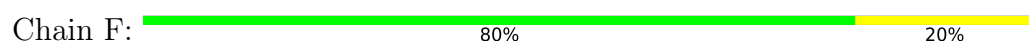
- Molecule 2: KR5

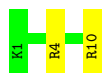


- Molecule 2: KR5



- Molecule 2: KR5





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	88.83Å 215.28Å 105.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	107.64 – 1.83 107.64 – 1.83	Depositor EDS
% Data completeness (in resolution range)	100.0 (107.64-1.83) 100.0 (107.64-1.83)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.15 (at 1.83Å)	Xtriage
Refinement program	REFMAC 5.8.0124	Depositor
R, R_{free}	0.149 , 0.179 0.161 , 0.190	Depositor DCC
R_{free} test set	4390 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	17.0	Xtriage
Anisotropy	0.329	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 43.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7694	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.06% 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: ACT, CA, GOL

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	1.59	11/2143 (0.5%)	1.19	4/2919 (0.1%)
1	B	1.54	17/2191 (0.8%)	1.15	2/2985 (0.1%)
1	C	1.57	20/2181 (0.9%)	1.14	4/2971 (0.1%)
2	D	1.65	0/100	1.51	1/122 (0.8%)
2	E	1.76	1/100 (1.0%)	1.51	0/122
2	F	1.74	1/100 (1.0%)	1.43	1/122 (0.8%)
All	All	1.57	50/6815 (0.7%)	1.17	12/9241 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	C	0	2
All	All	0	4

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	290	LEU	CA-C	7.45	1.63	1.52
1	A	204[A]	SER	C-N	7.39	1.44	1.33
1	A	204[B]	SER	C-N	7.39	1.44	1.33
1	A	204[C]	SER	C-N	7.39	1.44	1.33
1	A	126	GLY	C-O	7.17	1.30	1.23
1	C	201	TRP	CB-CG	-6.69	1.29	1.50
1	A	124	SER	C-O	6.63	1.32	1.24
1	B	17	VAL	CA-C	-6.11	1.44	1.52
1	B	205	ASN	CA-CB	5.92	1.62	1.53
1	B	258	ALA	CA-C	5.81	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	204[A]	SER	C-N	5.75	1.42	1.33
1	C	204[B]	SER	C-N	5.75	1.42	1.33
1	C	204[C]	SER	C-N	5.75	1.42	1.33
1	C	55	LEU	N-CA	-5.71	1.41	1.46
1	A	205	ASN	N-CA	5.70	1.53	1.46
1	B	145	LEU	N-CA	5.70	1.53	1.46
1	C	273	SER	CB-OG	-5.69	1.30	1.42
2	F	4	ARG	CZ-NH1	5.69	1.40	1.32
1	A	177	ASP	N-CA	5.67	1.53	1.46
1	C	264	ALA	CA-CB	-5.66	1.44	1.53
1	B	244	ALA	C-O	5.59	1.30	1.24
1	C	210	GLY	C-O	5.59	1.30	1.23
1	C	22	SER	CA-C	5.55	1.59	1.53
1	C	40	SER	C-O	-5.54	1.16	1.24
1	B	204[A]	SER	C-N	5.46	1.41	1.33
1	B	204[B]	SER	C-N	5.46	1.41	1.33
1	B	204[C]	SER	C-N	5.46	1.41	1.33
1	C	65	PRO	C-O	-5.43	1.17	1.24
1	C	201	TRP	N-CA	-5.41	1.40	1.46
1	B	114	GLU	C-O	5.40	1.30	1.24
1	C	192	ASN	N-CA	-5.37	1.39	1.46
1	A	259	VAL	CA-CB	-5.36	1.48	1.54
1	B	46	ILE	CA-CB	-5.34	1.48	1.54
1	C	116	LEU	C-O	5.28	1.30	1.24
1	B	13	LEU	N-CA	-5.27	1.41	1.46
1	C	204[A]	SER	C-O	5.20	1.30	1.24
1	C	204[B]	SER	C-O	5.20	1.30	1.24
1	C	204[C]	SER	C-O	5.20	1.30	1.24
1	B	214	ILE	CA-CB	-5.19	1.48	1.54
1	B	26	GLN	N-CA	5.16	1.52	1.46
1	B	85	ASN	N-CA	-5.14	1.40	1.46
2	E	10	ARG	CB-CG	-5.13	1.37	1.52
1	C	245	LEU	N-CA	5.13	1.52	1.46
1	C	148	SER	CA-C	5.12	1.58	1.53
1	C	119	LEU	C-O	-5.07	1.18	1.24
1	A	87	GLN	C-O	5.07	1.30	1.24
1	B	186	GLN	CA-C	5.07	1.59	1.52
1	B	201	TRP	CB-CG	-5.02	1.34	1.50
1	A	65	PRO	C-O	-5.01	1.18	1.24
1	B	96	ALA	CA-CB	-5.00	1.44	1.53

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	27	GLU	CB-CG-CD	-6.78	101.07	112.60
2	D	10	ARG	CB-CA-C	5.87	121.25	110.10
1	C	273	SER	CB-CA-C	-5.70	101.84	111.02
1	A	97	LEU	CA-C-N	-5.41	113.35	118.97
1	A	97	LEU	C-N-CA	-5.41	113.35	118.97
1	C	97	LEU	CA-C-N	-5.24	113.23	119.05
1	C	97	LEU	C-N-CA	-5.24	113.23	119.05
1	B	96	ALA	N-CA-C	5.19	118.88	112.54
1	C	96	ALA	N-CA-C	5.07	117.70	111.82
2	F	10	ARG	CB-CA-C	5.03	119.65	110.10
1	A	96	ALA	N-CA-C	5.02	117.64	111.82
1	B	147	SER	CA-CB-OG	-5.01	101.08	111.10

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	204[A]	SER	Mainchain
1	A	204[B]	SER	Mainchain
1	C	204[A]	SER	Mainchain
1	C	204[C]	SER	Mainchain

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	2121	0	2129	8	0
1	B	2167	0	2165	17	0
1	C	2157	0	2149	7	0
2	D	101	0	132	1	0
2	E	101	0	132	0	0
2	F	101	0	132	0	0
3	A	8	0	6	0	0
3	B	4	0	3	0	0
3	C	8	0	6	5	0
4	A	6	0	8	0	0
5	A	3	0	0	0	0
5	B	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	4	0	0	0	0
6	A	300	0	0	3	2
6	B	304	0	0	6	1
6	C	253	0	0	5	3
6	D	17	0	0	0	1
6	E	20	0	0	0	0
6	F	13	0	0	0	0
All	All	7694	0	6862	35	6

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 3.

All (35) 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:B:16:MET:CE	1:B:35:LEU:HG	2.05	0.86
1:B:16:MET:HE2	1:B:35:LEU:CD2	2.11	0.79
1:C:18:GLN:HG2	6:C:2009:HOH:O	1.90	0.72
1:B:204[B]:SER:HG	1:B:243[B]:TRP:CD1	2.11	0.69
1:B:144:GLN:HG3	6:B:2180:HOH:O	1.95	0.67
1:C:280:GLN:OE1	3:C:1294:ACT:H3	1.95	0.66
3:C:1294:ACT:H1	6:C:2240:HOH:O	1.98	0.62
1:B:16:MET:HE3	1:B:35:LEU:HG	1.81	0.62
1:B:16:MET:HE2	1:B:35:LEU:HG	1.82	0.60
1:C:12:GLU:HG3	1:C:16:MET:HE3	1.84	0.60
1:A:12:GLU:HG3	1:A:16:MET:HE3	1.85	0.59
1:B:19:GLN:HG2	6:B:2027:HOH:O	2.02	0.59
1:A:119[B]:LEU:HD11	1:A:133:VAL:HG13	1.85	0.58
1:A:194:GLN:HG2	6:A:2185:HOH:O	2.02	0.58
1:C:239:GLN:HE22	1:C:282:GLU:HG3	1.68	0.58
1:B:16:MET:HE2	1:B:35:LEU:HD21	1.86	0.57
1:B:16:MET:CE	1:B:35:LEU:CD2	2.82	0.56
1:B:170:GLU:HG2	6:B:2166:HOH:O	2.06	0.56
1:C:239:GLN:NE2	1:C:282:GLU:HG3	2.22	0.54
1:B:70[B]:LEU:HD12	6:B:2079:HOH:O	2.10	0.52
1:B:16:MET:HE2	1:B:35:LEU:CG	2.39	0.52
1:B:16:MET:CE	1:B:35:LEU:CG	2.85	0.51
1:C:280:GLN:OE1	3:C:1294:ACT:CH3	2.62	0.48
1:A:201:TRP:CE3	2:D:2:ARG:NH1	2.82	0.47
1:A:45:GLN:NE2	6:A:2033:HOH:O	2.32	0.47
1:A:204[C]:SER:OG	1:A:244:ALA:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:34:LYS:HG3	6:B:2031:HOH:O	2.16	0.46
3:C:1294:ACT:CH3	6:C:2251:HOH:O	2.64	0.45
1:B:204[B]:SER:OG	1:B:243[B]:TRP:CD1	2.69	0.44
1:B:16:MET:CE	1:B:35:LEU:HD23	2.48	0.43
3:C:1294:ACT:H3	6:C:2251:HOH:O	2.17	0.43
1:A:186:GLN:NE2	6:A:2215:HOH:O	2.50	0.42
1:A:28:LEU:C	1:A:28:LEU:HD23	2.46	0.41
1:B:19:GLN:CG	6:B:2027:HOH:O	2.65	0.41
1:C:34:LYS:HG3	6:C:2027:HOH:O	2.22	0.40

All (6) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:2087:HOH:O	6:C:2090:HOH:O[4_555]	1.78	0.42
6:C:2086:HOH:O	6:C:2086:HOH:O[4_555]	1.79	0.41
6:C:2071:HOH:O	6:C:2071:HOH:O[3_555]	1.81	0.39
6:D:2009:HOH:O	6:D:2016:HOH:O[3_554]	2.10	0.10
6:A:2050:HOH:O	6:B:2036:HOH:O[6_554]	2.18	0.02
6:A:2079:HOH:O	6:A:2182:HOH:O[3_554]	2.18	0.02

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	285/286 (100%)	285 (100%)	0	0	100	100
1	B	291/286 (102%)	291 (100%)	0	0	100	100
1	C	290/286 (101%)	290 (100%)	0	0	100	100
2	D	8/10 (80%)	8 (100%)	0	0	100	100
2	E	8/10 (80%)	8 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	8/10 (80%)	8 (100%)	0	0	100	100
All	All	890/888 (100%)	890 (100%)	0	0	100	100

There are no Ramachandran outliers to report.

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	227/224 (101%)	225 (99%)	2 (1%)	70	60
1	B	233/224 (104%)	233 (100%)	0	100	100
1	C	232/224 (104%)	231 (100%)	1 (0%)	84	78
2	D	10/10 (100%)	10 (100%)	0	100	100
2	E	10/10 (100%)	10 (100%)	0	100	100
2	F	10/10 (100%)	10 (100%)	0	100	100
All	All	722/702 (103%)	719 (100%)	3 (0%)	84	78

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	194	GLN
1	A	291	GLN
1	C	273	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	228	GLN
1	B	110	GLN
1	B	194	GLN
1	B	211	ASN
1	C	21	ASN

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Mol	Chain	Res	Type
1	C	110	GLN
1	C	113	GLN
1	C	152	GLN
1	C	194	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 13 are monoatomic - leaving 6 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	$\# Z > 2$
3	ACT	C	1294	-	3,3,3	1.36	1 (33%)	3,3,3	0.79	0
3	ACT	C	1293	5	3,3,3	0.90	0	3,3,3	0.81	0
4	GOL	A	1294	-	5,5,5	0.56	0	5,5,5	0.68	0
3	ACT	B	1293	-	3,3,3	1.06	0	3,3,3	1.08	0
3	ACT	A	1293	-	3,3,3	1.18	0	3,3,3	0.27	0
3	ACT	A	1292	5	3,3,3	0.72	0	3,3,3	0.65	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
4	GOL	A	1294	-	-	2/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1294	ACT	O-C	2.25	1.32	1.22

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1294	GOL	O1-C1-C2-C3
4	A	1294	GOL	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1294	ACT	5	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	281/286 (98%)	-0.45	4 (1%) 73 81	5, 15, 38, 65	5 (1%)
1	B	282/286 (98%)	-0.48	2 (0%) 84 90	6, 16, 35, 73	10 (3%)
1	C	282/286 (98%)	-0.50	2 (0%) 84 90	6, 17, 35, 71	9 (3%)
2	D	10/10 (100%)	-0.52	0 100 100	16, 22, 26, 28	0
2	E	10/10 (100%)	-0.56	0 100 100	16, 22, 26, 29	0
2	F	10/10 (100%)	-0.64	0 100 100	16, 21, 27, 34	0
All	All	875/888 (98%)	-0.48	8 (0%) 81 87	5, 16, 36, 73	24 (2%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	292	SER	3.5
1	B	11	SER	3.4
1	A	291	GLN	3.3
1	B	292	SER	2.8
1	A	11	SER	2.6
1	A	201	TRP	2.4
1	C	11	SER	2.3
1	A	272	GLN	2.1

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 oligosaccharides 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
3	ACT	C	1294	4/4	0.74	0.17	17,34,34,39	0
3	ACT	A	1293	4/4	0.76	0.21	51,55,57,58	0
5	CA	C	1298	1/1	0.89	0.11	40,40,40,40	0
4	GOL	A	1294	6/6	0.90	0.11	26,29,34,35	0
3	ACT	B	1293	4/4	0.90	0.11	22,26,27,32	0
3	ACT	A	1292	4/4	0.97	0.06	18,18,19,19	0
3	ACT	C	1293	4/4	0.98	0.05	16,19,20,22	0
5	CA	C	1296	1/1	0.99	0.02	21,21,21,21	0
5	CA	C	1297	1/1	0.99	0.02	14,14,14,14	0
5	CA	A	1297	1/1	0.99	0.04	19,19,19,19	0
5	CA	B	1295	1/1	1.00	0.02	14,14,14,14	0
5	CA	B	1296	1/1	1.00	0.03	13,13,13,13	0
5	CA	B	1297	1/1	1.00	0.04	14,14,14,14	0
5	CA	B	1298	1/1	1.00	0.02	13,13,13,13	0
5	CA	B	1299	1/1	1.00	0.03	13,13,13,13	0
5	CA	C	1295	1/1	1.00	0.03	12,12,12,12	1
5	CA	A	1296	1/1	1.00	0.03	14,14,14,14	0
5	CA	A	1295	1/1	1.00	0.03	12,12,12,12	0
5	CA	B	1294	1/1	1.00	0.04	12,12,12,12	0

6.5 Other polymers [i](#)

There are no such residues in this entry.