



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:59 AM UTC

PDB ID : 5MFM / pdb_00005mfm
Title : Designed armadillo repeat protein peptide fusion YIIM6AII_GS11_(KR)5
Authors : Hansen, S.; Ernst, P.; Reichen, C.; Ewald, C.; Mittl, P.; Plueckthun, A.
Deposited on : 2016-11-18
Resolution : 2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

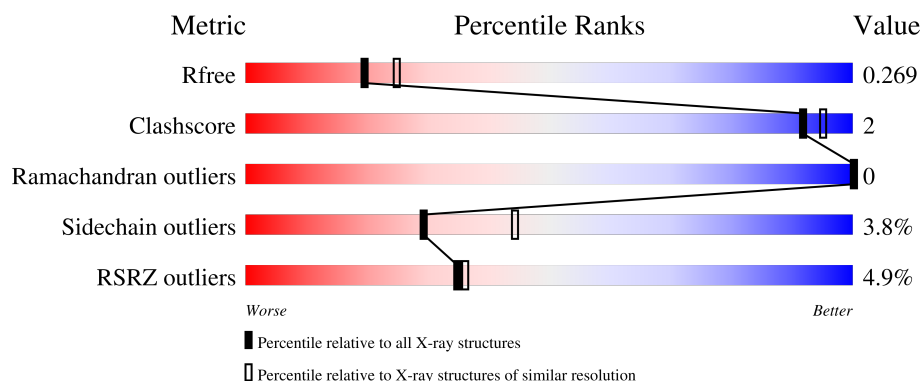
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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

Mol	Chain	Length	Quality of chain
1	A	348	2% 93% 8% • •
1	B	348	2% 92% 8% • •
1	D	348	4% 87% 8% •
1	E	348	5% 87% 8% •
1	F	348	5% 90% 6% •

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Mol	Chain	Length	Quality of chain
1	P	348	4% 9% 88%
1	Q	348	2% 10% 88%
2	C	350	5% 89% 7% 5%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 16466 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 YIIIM6AII_GS11_(KR)5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	335	Total	C	N	O	S	0	10	0
			2589	1610	467	511	1			
1	B	333	Total	C	N	O	S	0	10	0
			2579	1605	465	508	1			
1	D	333	Total	C	N	O	S	0	11	0
			2585	1608	466	510	1			
1	E	333	Total	C	N	O	S	0	10	0
			2579	1605	465	508	1			
1	F	334	Total	C	N	O	S	0	1	0
			2492	1552	438	501	1			
1	P	42	Total	C	N	O		0	0	0
			321	194	58	69				
1	Q	42	Total	C	N	O		0	0	0
			321	194	58	69				

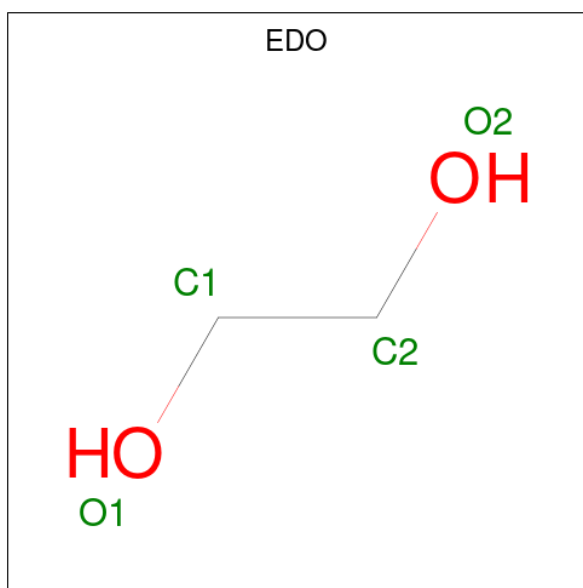
- Molecule 2 is a protein called Importin subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	334	Total	C	N	O	S	0	10	0
			2585	1608	466	510	1			

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	5	Total	Ca	0	0
			5	5		
3	B	4	Total	Ca	0	0
			4	4		
3	C	7	Total	Ca	0	0
			7	7		
3	D	7	Total	Ca	0	0
			7	7		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Mg	0	0
			2	2		
5	B	2	Total	Mg	0	0
			2	2		
5	C	2	Total	Mg	0	0
			2	2		
5	D	1	Total	Mg	0	0
			1	1		
5	E	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	F	1	Total	Mg	0	0
			1	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	73	Total	O	0	0
			73	73		
6	B	57	Total	O	0	0
			57	57		
6	C	62	Total	O	0	0
			62	62		
6	D	38	Total	O	0	0
			38	38		
6	E	55	Total	O	0	0
			55	55		
6	F	64	Total	O	0	0
			64	64		
6	P	3	Total	O	0	0
			3	3		
6	Q	6	Total	O	0	0
			6	6		

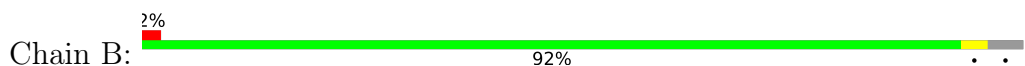
3 Residue-property plots [i](#)

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.

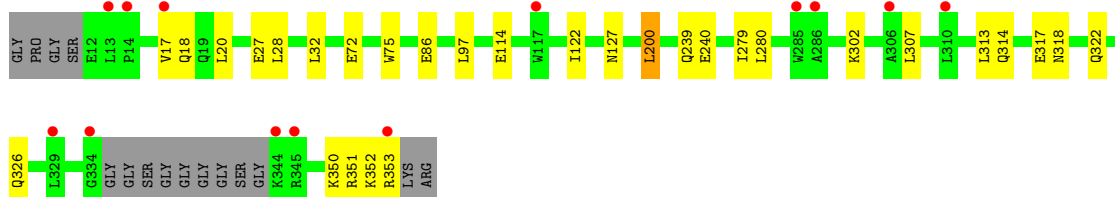
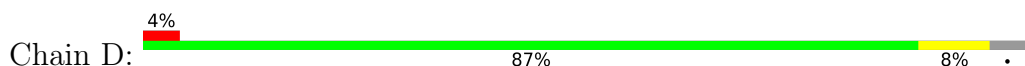
- Molecule 1: YIIIM6AII_GS11_(KR)5



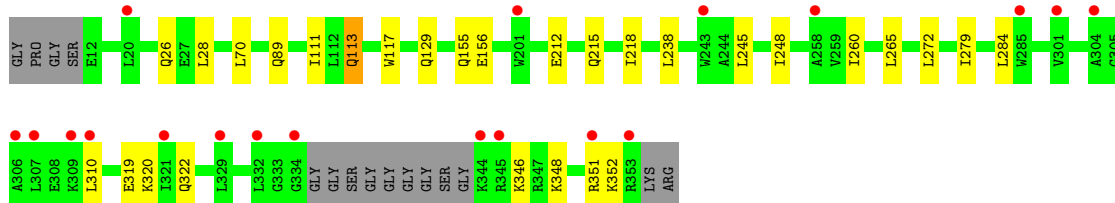
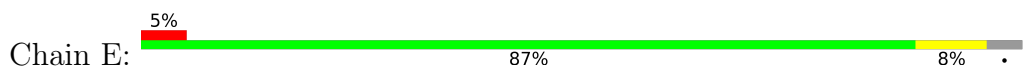
- Molecule 1: YIIIM6AII_GS11_(KR)5



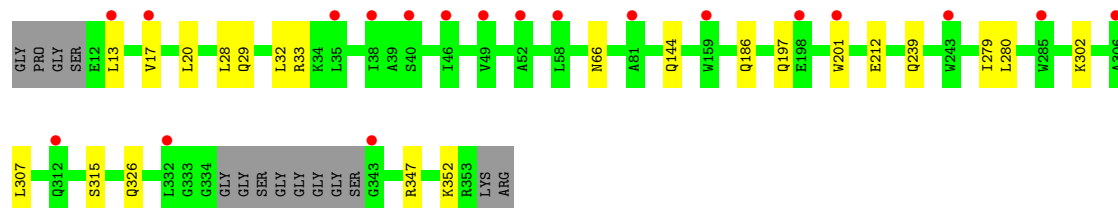
- Molecule 1: YIIIM6AII_GS11_(KR)5



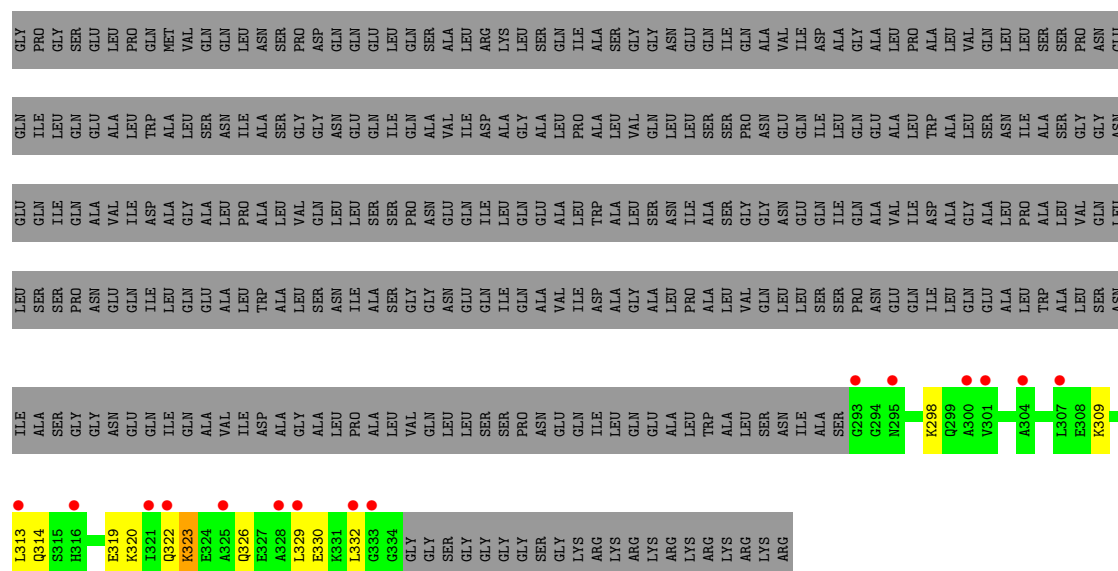
- Molecule 1: YIIIM6AII_GS11_(KR)5



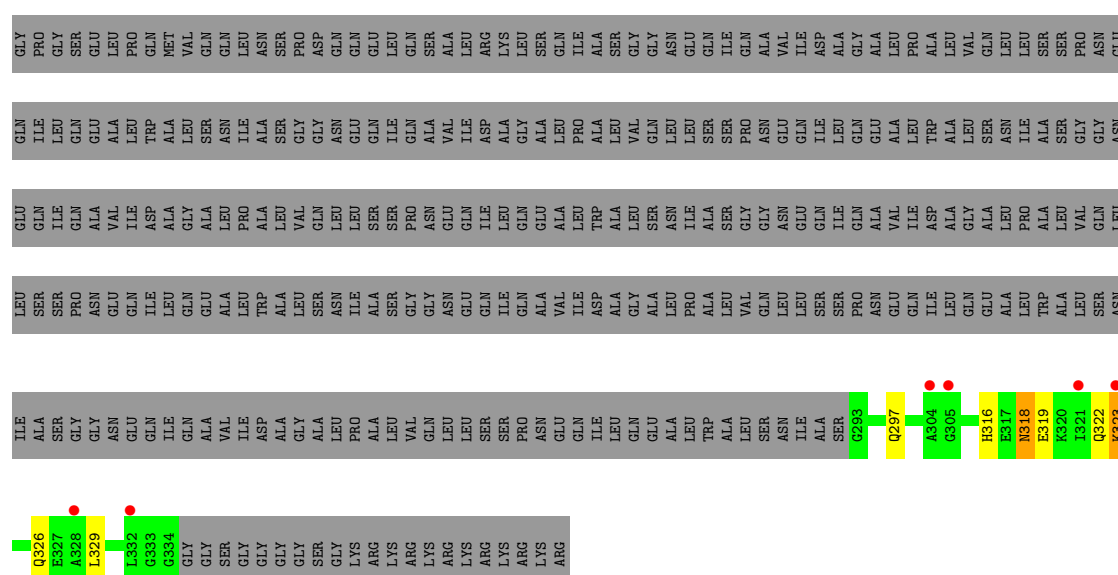
- Molecule 1: YIIIM6AII_GS11_(KR)5



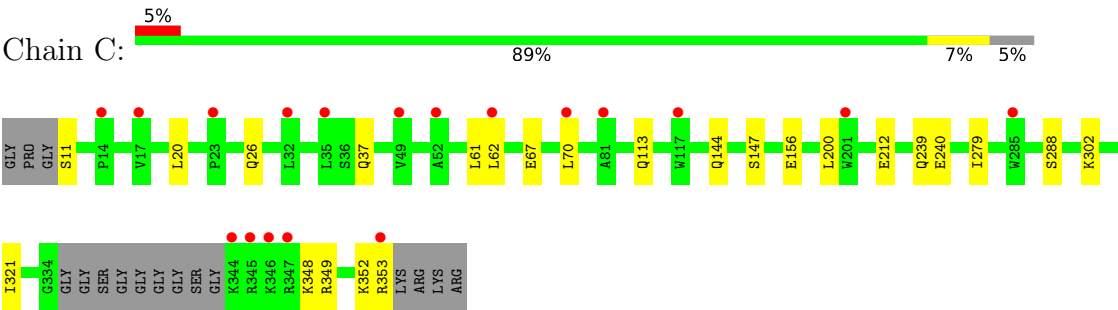
Chain P: 4% 9% 88%



Chain Q: 2% 10% .. 88%



● Molecule 2: Importin subunit alpha



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.76Å 89.39Å 123.85Å 90.00° 97.07° 90.00°	Depositor
Resolution (Å)	44.69 – 2.30 44.69 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.6 (44.69-2.30) 98.6 (44.69-2.30)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.68 (at 2.29Å)	Xtrriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.217 , 0.251 0.234 , 0.269	Depositor DCC
R_{free} test set	3887 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	48.5	Xtrriage
Anisotropy	0.212	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 62.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16466	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 22.67 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.4386e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: CA, MG, EDO

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	0.73	0/2613	1.35	0/3536
1	B	0.73	0/2603	1.36	0/3523
1	D	0.72	0/2609	1.36	0/3531
1	E	0.71	0/2603	1.37	0/3523
1	F	0.75	0/2517	1.39	0/3418
1	P	0.68	0/321	1.41	0/424
1	Q	0.77	0/321	1.47	0/424
2	C	0.73	0/2609	1.37	0/3531
All	All	0.73	0/16196	1.37	0/21910

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

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	2589	0	2658	6	0
1	B	2579	0	2650	4	0
1	D	2585	0	2654	13	0
1	E	2579	0	2650	13	0
1	F	2492	0	2531	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	P	321	0	318	3	0
1	Q	321	0	318	4	0
2	C	2585	0	2655	11	0
3	A	5	0	0	0	0
3	B	4	0	0	0	0
3	C	7	0	0	0	0
3	D	7	0	0	0	0
4	A	4	0	6	0	0
4	D	4	0	6	0	0
4	F	16	0	24	0	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
5	C	2	0	0	0	0
5	D	1	0	0	0	0
5	E	2	0	0	0	0
5	F	1	0	0	0	0
6	A	73	0	0	0	0
6	B	57	0	0	0	0
6	C	62	0	0	0	0
6	D	38	0	0	0	0
6	E	55	0	0	0	0
6	F	64	0	0	0	0
6	P	3	0	0	0	0
6	Q	6	0	0	0	0
All	All	16466	0	16470	53	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 (53) 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:D:352[A]:LYS:HB2	1:F:352:LYS:HB2	1.82	0.60
1:D:350[B]:LYS:HB2	1:F:352:LYS:HB2	1.83	0.60
1:E:113:GLN:HG2	1:E:156:GLU:HG3	1.86	0.57
1:D:32:LEU:HB3	1:D:72:GLU:HG2	1.87	0.55
2:C:302:LYS:HE3	1:Q:297:GLN:HG3	1.88	0.55
1:D:314:GLN:HE21	1:D:326:GLN:HG3	1.74	0.52
1:A:113:GLN:HG2	1:A:156:GLU:HG3	1.89	0.52
2:C:156:GLU:HA	2:C:349[B]:ARG:HH22	1.75	0.52
2:C:348[B]:LYS:HB2	1:E:352[B]:LYS:HB3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:302:LYS:HG2	1:D:307:LEU:HD13	1.92	0.51
2:C:26:GLN:HA	1:E:320:LYS:HG3	1.93	0.51
2:C:352[B]:LYS:HB3	1:E:348[B]:LYS:HB2	1.95	0.49
1:F:17:VAL:HA	1:F:20:LEU:HD12	1.95	0.49
1:F:29:GLN:HG3	1:F:33:ARG:HH22	1.77	0.49
1:Q:316:HIS:HD2	1:Q:318:ASN:H	1.61	0.48
2:C:37:GLN:HE22	2:C:353[B]:ARG:HG3	1.80	0.47
1:Q:323:LYS:HA	1:Q:326:GLN:HB3	1.97	0.47
1:D:75:TRP:HA	1:D:353[A]:ARG:HH11	1.80	0.46
1:Q:316:HIS:CD2	1:Q:318:ASN:H	2.33	0.46
2:C:113:GLN:HG3	2:C:156:GLU:HG3	1.98	0.46
2:C:200:LEU:HB3	2:C:240:GLU:HB3	1.98	0.46
1:P:323:LYS:HA	1:P:326:GLN:HB2	1.97	0.46
1:D:318:ASN:HD21	1:F:66:ASN:HD21	1.63	0.46
1:B:24:ASP:HB3	1:B:27:GLU:HG2	1.98	0.45
1:D:17:VAL:HA	1:D:20:LEU:HD12	1.98	0.45
1:B:16:MET:HE2	1:B:34:LYS:HD3	2.00	0.44
1:D:200:LEU:HB3	1:D:240:GLU:HB3	1.98	0.44
1:A:311:GLU:HA	1:A:314:GLN:HE21	1.81	0.44
1:P:314:GLN:HA	1:P:322:GLN:CG	2.48	0.44
1:D:114:GLU:HG2	1:D:353[A]:ARG:HH12	1.81	0.43
1:F:239:GLN:HG3	1:F:279:ILE:HD13	1.98	0.43
1:E:89:GLN:HB2	1:E:129:GLN:HE21	1.84	0.43
2:C:239:GLN:HG3	2:C:279:ILE:HD13	2.01	0.43
1:E:70:LEU:HG	1:E:111:ILE:HD12	2.01	0.43
1:E:215:GLN:HA	1:E:218:ILE:HD12	2.01	0.43
1:A:197:GLN:HG2	1:A:240:GLU:HG3	2.01	0.42
1:D:97:LEU:HD21	1:D:122:ILE:HG21	2.00	0.42
1:E:155:GLN:HE22	1:E:351[A]:ARG:HH22	1.67	0.42
1:E:238:LEU:HD23	1:E:279:ILE:HD12	2.00	0.42
1:E:245:LEU:HA	1:E:248:ILE:HD12	2.02	0.42
1:B:155:GLN:HE21	1:B:155:GLN:HB3	1.72	0.42
1:D:239:GLN:HG3	1:D:279:ILE:HD13	2.01	0.42
2:C:348[B]:LYS:HD2	1:E:352[B]:LYS:HD2	2.01	0.41
1:A:200:LEU:HB3	1:A:240:GLU:HB3	2.02	0.41
1:F:197:GLN:HE21	1:F:201:TRP:HE1	1.69	0.41
1:P:298:LYS:HB3	1:P:332:LEU:HD23	2.02	0.41
1:A:239:GLN:HG3	1:A:279:ILE:HD13	2.02	0.41
2:C:20:LEU:HB3	2:C:61:LEU:HD11	2.02	0.41
1:E:117:TRP:HE1	1:E:351[A]:ARG:HB3	1.86	0.41
1:E:260:ILE:HG12	1:E:265:LEU:HD11	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:LEU:HG	1:B:111:ILE:HD12	2.03	0.40
1:A:70:LEU:HG	1:A:111:ILE:HD12	2.03	0.40
1:D:114:GLU:HG2	1:D:351[B]:ARG:HH12	1.86	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	339/348 (97%)	337 (99%)	2 (1%)	0	100	100
1	B	337/348 (97%)	335 (99%)	2 (1%)	0	100	100
1	D	338/348 (97%)	337 (100%)	1 (0%)	0	100	100
1	E	337/348 (97%)	333 (99%)	4 (1%)	0	100	100
1	F	331/348 (95%)	330 (100%)	1 (0%)	0	100	100
1	P	40/348 (12%)	35 (88%)	5 (12%)	0	100	100
1	Q	40/348 (12%)	35 (88%)	5 (12%)	0	100	100
2	C	338/350 (97%)	333 (98%)	5 (2%)	0	100	100
All	All	2100/2786 (75%)	2075 (99%)	25 (1%)	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	272/267 (102%)	267 (98%)	5 (2%)	51	70
1	B	271/267 (102%)	265 (98%)	6 (2%)	45	65
1	D	272/267 (102%)	262 (96%)	10 (4%)	30	45
1	E	271/267 (102%)	260 (96%)	11 (4%)	27	41
1	F	262/267 (98%)	250 (95%)	12 (5%)	24	36
1	P	32/267 (12%)	25 (78%)	7 (22%)	1	1
1	Q	32/267 (12%)	27 (84%)	5 (16%)	2	3
2	C	272/269 (101%)	263 (97%)	9 (3%)	33	50
All	All	1684/2138 (79%)	1619 (96%)	65 (4%)	29	43

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	113	GLN
1	A	344[A]	LYS
1	A	344[B]	LYS
1	A	352[A]	LYS
1	A	352[B]	LYS
1	B	12	GLU
1	B	28	LEU
1	B	113	GLN
1	B	155	GLN
1	B	280	LEU
1	B	307	LEU
2	C	11	SER
2	C	62	LEU
2	C	67	GLU
2	C	70	LEU
2	C	144	GLN
2	C	147	SER
2	C	212	GLU
2	C	288	SER
2	C	321	ILE
1	D	18	GLN
1	D	27	GLU
1	D	28	LEU
1	D	86	GLU
1	D	127	ASN
1	D	200	LEU
1	D	280	LEU

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Mol	Chain	Res	Type
1	D	313	LEU
1	D	317	GLU
1	D	322	GLN
1	E	26	GLN
1	E	28	LEU
1	E	113	GLN
1	E	212	GLU
1	E	272	LEU
1	E	284	LEU
1	E	310	LEU
1	E	319	GLU
1	E	322	GLN
1	E	346[A]	LYS
1	E	346[B]	LYS
1	F	13	LEU
1	F	28	LEU
1	F	32	LEU
1	F	144	GLN
1	F	186	GLN
1	F	212	GLU
1	F	280	LEU
1	F	302	LYS
1	F	307	LEU
1	F	315	SER
1	F	326	GLN
1	F	347	ARG
1	P	309	LYS
1	P	313	LEU
1	P	319	GLU
1	P	320	LYS
1	P	323	LYS
1	P	329	LEU
1	P	330	GLU
1	Q	318	ASN
1	Q	319	GLU
1	Q	322	GLN
1	Q	323	LYS
1	Q	329	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (71) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	85	ASN
1	A	144	GLN
1	A	236	GLN
1	A	270	GLN
1	A	295	ASN
1	A	299	GLN
1	A	314	GLN
1	B	21	ASN
1	B	25	GLN
1	B	47	GLN
1	B	66	ASN
1	B	113	GLN
1	B	186	GLN
1	B	194	GLN
1	B	314	GLN
1	B	318	ASN
2	C	19	GLN
2	C	37	GLN
2	C	45	GLN
2	C	47	GLN
2	C	66	ASN
2	C	110	GLN
2	C	169	ASN
2	C	239	GLN
2	C	322	GLN
2	C	326	GLN
1	D	19	GLN
1	D	26	GLN
1	D	29	GLN
1	D	37	GLN
1	D	68	GLN
1	D	71	GLN
1	D	89	GLN
1	D	102	GLN
1	D	110	GLN
1	D	127	ASN
1	D	152	GLN
1	D	169	ASN
1	D	211	ASN
1	D	236	GLN
1	D	278	GLN
1	D	281	GLN

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Mol	Chain	Res	Type
1	D	314	GLN
1	D	326	GLN
1	E	15	GLN
1	E	26	GLN
1	E	43	ASN
1	E	71	GLN
1	E	155	GLN
1	E	194	GLN
1	E	236	GLN
1	E	312	GLN
1	F	60	GLN
1	F	66	ASN
1	F	110	GLN
1	F	197	GLN
1	F	228	GLN
1	F	236	GLN
1	F	253	ASN
1	F	281	GLN
1	F	326	GLN
1	P	295	ASN
1	P	297	GLN
1	P	312	GLN
1	P	316	HIS
1	P	318	ASN
1	Q	316	HIS
1	Q	318	ASN
1	Q	322	GLN
1	Q	326	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 39 ligands modelled in this entry, 33 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	$\# Z > 2$
4	EDO	D	405	-	3,3,3	0.52	0	2,2,2	0.24	0
4	EDO	F	401	-	3,3,3	0.58	0	2,2,2	0.34	0
4	EDO	F	403	-	3,3,3	0.66	0	2,2,2	0.02	0
4	EDO	A	406	-	3,3,3	0.44	0	2,2,2	0.31	0
4	EDO	F	404	-	3,3,3	0.51	0	2,2,2	0.37	0
4	EDO	F	402	-	3,3,3	0.53	0	2,2,2	0.28	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	EDO	D	405	-	-	0/1/1/1	-
4	EDO	F	401	-	-	0/1/1/1	-
4	EDO	F	403	-	-	1/1/1/1	-
4	EDO	A	406	-	-	0/1/1/1	-
4	EDO	F	404	-	-	0/1/1/1	-
4	EDO	F	402	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	F	403	EDO	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

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	335/348 (96%)	0.17	6 (1%) 67 69	28, 56, 99, 120	11 (3%)
1	B	333/348 (95%)	0.39	6 (1%) 67 69	32, 66, 111, 129	10 (3%)
1	D	333/348 (95%)	0.52	13 (3%) 43 45	28, 74, 137, 158	11 (3%)
1	E	333/348 (95%)	0.47	19 (5%) 29 31	26, 67, 208, 223	10 (3%)
1	F	334/348 (95%)	0.44	19 (5%) 29 31	42, 68, 132, 188	11 (3%)
1	P	42/348 (12%)	1.72	15 (35%) 1 1	100, 155, 192, 196	16 (38%)
1	Q	42/348 (12%)	1.24	6 (14%) 6 7	70, 108, 145, 154	12 (28%)
2	C	334/350 (95%)	0.38	18 (5%) 31 33	27, 59, 140, 170	18 (5%)
All	All	2086/2786 (74%)	0.44	102 (4%) 35 36	26, 67, 145, 223	99 (4%)

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	344[A]	LYS	9.4
1	D	344[A]	LYS	6.6
1	A	344[A]	LYS	6.1
1	B	344[A]	LYS	6.1
1	E	345[A]	ARG	5.6
2	C	17	VAL	5.2
1	D	345[A]	ARG	4.9
1	P	301	VAL	4.8
1	E	306	ALA	4.7
1	P	329	LEU	4.6
1	B	345[A]	ARG	4.4
2	C	346[A]	LYS	4.4
1	E	258	ALA	4.3
2	C	344[A]	LYS	4.2
1	F	306	ALA	3.9
1	F	201	TRP	3.9

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Mol	Chain	Res	Type	RSRZ
1	P	332	LEU	3.8
2	C	81	ALA	3.7
2	C	201	TRP	3.6
1	A	345[A]	ARG	3.5
1	E	201	TRP	3.4
2	C	347[A]	ARG	3.4
1	D	13	LEU	3.3
1	P	321	ILE	3.3
1	F	40	SER	3.3
1	P	300	ALA	3.2
1	P	293	GLY	3.2
1	F	46	ILE	3.2
1	P	316	HIS	3.1
1	E	351[A]	ARG	3.1
2	C	345[A]	ARG	3.1
1	Q	328	ALA	3.1
1	F	13	LEU	3.1
1	D	334	GLY	2.9
1	P	304	ALA	2.9
1	E	307	LEU	2.8
2	C	62	LEU	2.8
1	Q	321	ILE	2.8
1	E	329	LEU	2.8
2	C	14	PRO	2.8
1	A	41	GLY	2.7
1	E	310	LEU	2.7
1	P	328	ALA	2.7
2	C	32	LEU	2.7
1	Q	304	ALA	2.7
1	F	312[A]	GLN	2.6
1	D	353[A]	ARG	2.6
1	Q	305	GLY	2.6
1	P	313	LEU	2.5
1	A	35	LEU	2.5
2	C	353[A]	ARG	2.5
1	F	52	ALA	2.5
1	P	333	GLY	2.5
1	D	17	VAL	2.4
1	F	17	VAL	2.4
1	F	58	LEU	2.4
1	F	35	LEU	2.4
1	Q	332	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	16	MET	2.4
1	E	353[A]	ARG	2.4
2	C	35	LEU	2.3
1	P	295	ASN	2.3
1	F	343	GLY	2.3
1	B	334	GLY	2.3
1	D	117	TRP	2.3
1	E	243	TRP	2.3
1	E	285	TRP	2.3
1	F	159	TRP	2.3
1	F	49	VAL	2.3
1	D	285	TRP	2.3
1	F	243	TRP	2.3
1	P	325	ALA	2.3
1	P	322	GLN	2.2
1	A	16	MET	2.2
2	C	23	PRO	2.2
1	A	75	TRP	2.2
1	D	310	LEU	2.2
1	E	20	LEU	2.2
2	C	117	TRP	2.2
2	C	285	TRP	2.2
1	E	321	ILE	2.2
1	F	38	ILE	2.2
1	E	301	VAL	2.2
1	D	14	PRO	2.2
1	Q	323	LYS	2.2
1	B	20	LEU	2.1
1	D	329	LEU	2.1
1	P	307	LEU	2.1
2	C	49	VAL	2.1
1	E	309	LYS	2.1
1	E	334	GLY	2.1
1	E	304	ALA	2.1
1	F	81	ALA	2.1
2	C	70	LEU	2.1
1	D	286	ALA	2.1
1	E	332	LEU	2.1
1	D	306	ALA	2.0
1	F	198	GLU	2.0
2	C	52	ALA	2.0
1	F	285	TRP	2.0

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Mol	Chain	Res	Type	RSRZ
1	F	332	LEU	2.0
1	B	14	PRO	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 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
4	EDO	A	406	4/4	0.62	0.17	96,96,97,97	0
4	EDO	F	404	4/4	0.72	0.15	110,111,111,111	0
4	EDO	D	405	4/4	0.73	0.18	95,95,95,95	0
3	CA	C	409	1/1	0.79	0.08	125,125,125,125	0
4	EDO	F	402	4/4	0.80	0.13	59,59,59,60	0
3	CA	C	404	1/1	0.81	0.09	123,123,123,123	0
4	EDO	F	403	4/4	0.82	0.14	50,51,52,52	0
3	CA	D	404	1/1	0.84	0.09	109,109,109,109	0
3	CA	B	402	1/1	0.85	0.08	80,80,80,80	0
3	CA	D	409	1/1	0.85	0.08	100,100,100,100	0
4	EDO	F	401	4/4	0.85	0.12	63,63,63,63	0
5	MG	C	405	1/1	0.86	0.10	79,79,79,79	0
3	CA	D	407	1/1	0.87	0.14	86,86,86,86	0
3	CA	D	402	1/1	0.89	0.09	74,74,74,74	0
3	CA	C	401	1/1	0.90	0.14	67,67,67,67	0
5	MG	B	406	1/1	0.91	0.10	70,70,70,70	0
3	CA	A	403	1/1	0.91	0.11	74,74,74,74	0
5	MG	D	406	1/1	0.92	0.10	77,77,77,77	0
5	MG	C	406	1/1	0.93	0.10	52,52,52,52	0
3	CA	D	408	1/1	0.93	0.08	62,62,62,62	0
3	CA	A	404	1/1	0.94	0.04	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CA	B	403	1/1	0.94	0.09	117,117,117,117	0
5	MG	A	408	1/1	0.94	0.12	55,55,55,55	0
5	MG	B	405	1/1	0.94	0.09	62,62,62,62	0
3	CA	C	408	1/1	0.95	0.05	93,93,93,93	0
3	CA	D	403	1/1	0.95	0.06	56,56,56,56	0
5	MG	E	401	1/1	0.95	0.08	62,62,62,62	0
5	MG	F	405	1/1	0.95	0.05	68,68,68,68	0
3	CA	C	403	1/1	0.96	0.06	53,53,53,53	0
3	CA	A	401	1/1	0.96	0.04	55,55,55,55	0
3	CA	A	402	1/1	0.96	0.06	56,56,56,56	0
3	CA	B	404	1/1	0.96	0.15	105,105,105,105	0
3	CA	D	401	1/1	0.96	0.07	71,71,71,71	0
5	MG	A	407	1/1	0.96	0.06	58,58,58,58	0
3	CA	A	405	1/1	0.96	0.06	113,113,113,113	0
3	CA	B	401	1/1	0.97	0.04	61,61,61,61	0
3	CA	C	402	1/1	0.98	0.07	60,60,60,60	0
5	MG	E	402	1/1	0.98	0.05	56,56,56,56	0
3	CA	C	407	1/1	0.98	0.03	50,50,50,50	0

6.5 Other polymers [i](#)

There are no such residues in this entry.