



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 09:41 PM UTC

PDB ID : 6QEV / pdb_00006qev
Title : EngBF DARPin Fusion 4b B6
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Deposited on : 2019-01-08
Resolution : 2.70 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

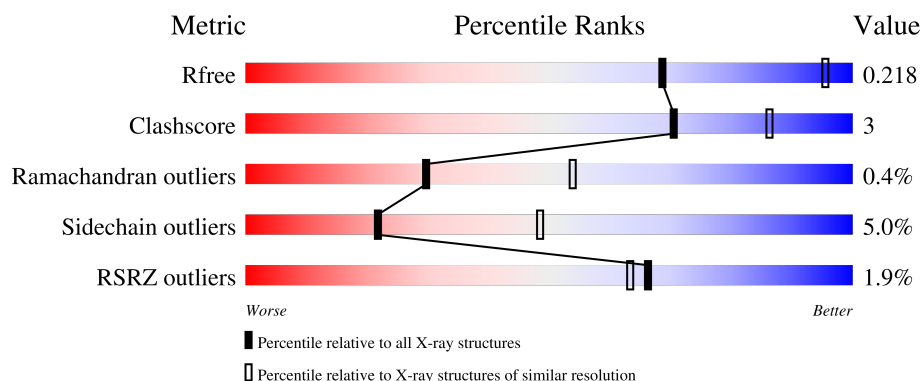
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	B	1357	2% 84% 14% ..
2	D	15	33% 80% 20%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10968 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 PEGA domain-containing protein,PEGA domain-containing protein,EngBF DARPin fusion B6 complex.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	1346	Total	C	N	O	S	0	0	0
			10328	6434	1767	2099	28			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	334	GLY	-	expression tag	UNP A0A414FD23
B	335	PRO	-	expression tag	UNP A0A414FD23
B	336	LEU	-	expression tag	UNP A0A414FD23
B	337	GLY	-	expression tag	UNP A0A414FD23
B	338	SER	-	expression tag	UNP A0A414FD23
B	339	MET	-	expression tag	UNP A0A414FD23
B	342	CYS	SER	conflict	UNP A0A414FD23
B	1309	ARG	GLN	conflict	UNP A0A414FD23

- Molecule 2 is a protein called PRO-LYS-SER-ILE-ARG-ILE-GLY-PRO-GLY-GLN-ALA-PHE-TYR-ALA-DPR.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	15	Total	C	N	O	0	0	0
			113	75	20	18			

- Molecule 3 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	4	Total	Mn	0	0
			4	4		

- Molecule 4 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



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

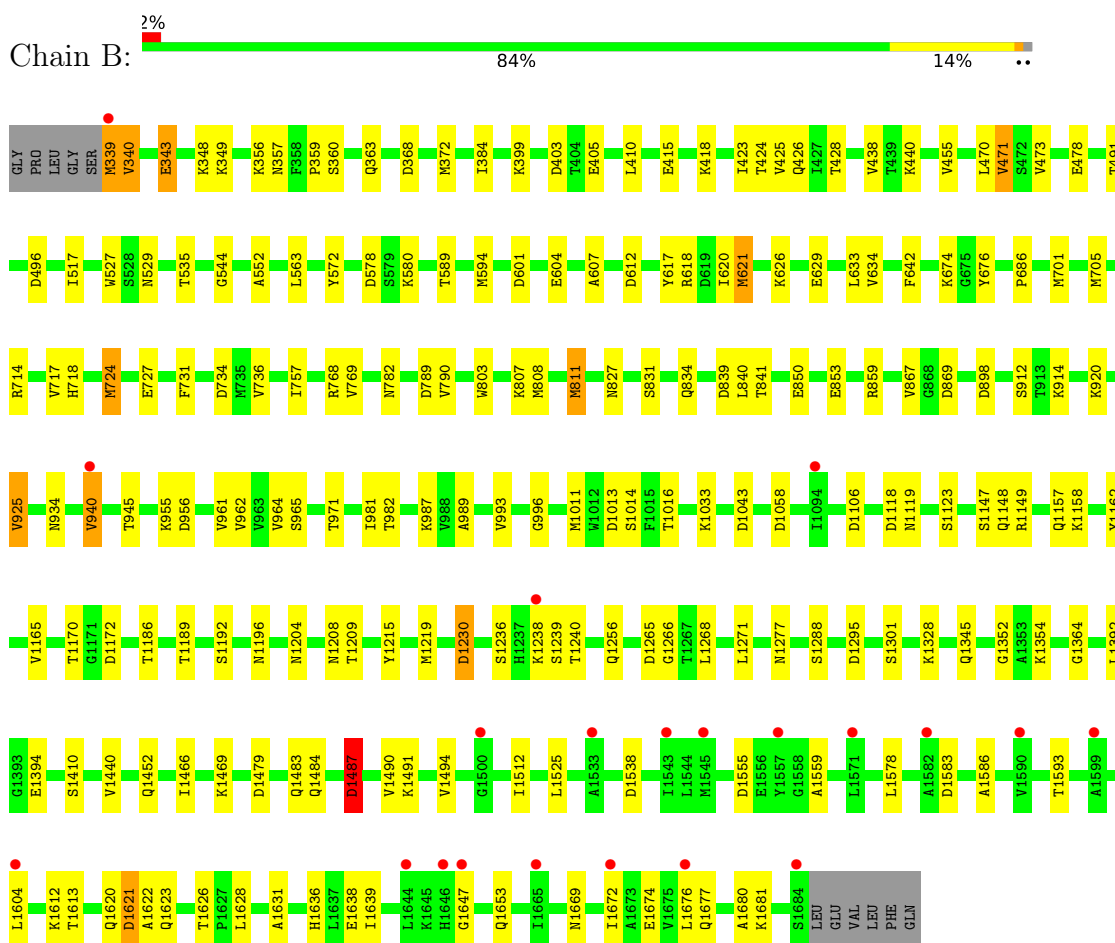
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	498	Total	O	0	0
			498	498		
5	D	1	Total	O	0	0
			1	1		

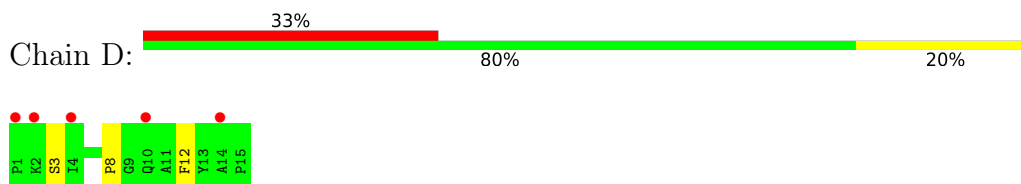
3 Residue-property plots

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: PEGA domain-containing protein, PEGA domain-containing protein, EngBF DARPin fusion B6 complex



- Molecule 2: PRO-LYS-SER-ILE-ARG-ILE-GLY-PRO-GLY-GLN-ALA-PHE-TYR-ALA-DP R



4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	194.77Å 194.77Å 123.71Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.69 – 2.70 48.69 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.69-2.70) 99.9 (48.69-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.16 (at 2.69Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.176 , 0.218 0.179 , 0.218	Depositor DCC
R_{free} test set	3658 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	68.6	Xtriage
Anisotropy	0.133	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 50.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.020 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10968	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.27% 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: MN, MPD, DPR

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	B	0.87	4/10528 (0.0%)	1.38	64/14282 (0.4%)
2	D	0.89	0/109	1.40	2/145 (1.4%)
All	All	0.87	4/10637 (0.0%)	1.38	66/14427 (0.5%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	621	MET	SD-CE	-7.53	1.60	1.79
1	B	811	MET	SD-CE	-6.11	1.64	1.79
1	B	572	TYR	CA-C	5.86	1.55	1.52
1	B	940	VAL	CA-C	5.24	1.59	1.52

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1555	ASP	CA-CB-CG	7.09	119.69	112.60
1	B	1230	ASP	CA-CB-CG	6.82	119.42	112.60
2	D	3	SER	CA-C-N	6.79	129.37	120.60
2	D	3	SER	C-N-CA	6.79	129.37	120.60
1	B	1295	ASP	CA-C-N	6.62	130.23	120.90
1	B	1295	ASP	C-N-CA	6.62	130.23	120.90
1	B	1013	ASP	CA-CB-CG	6.60	119.20	112.60
1	B	1240	THR	CA-C-N	6.60	130.49	121.05
1	B	1240	THR	C-N-CA	6.60	130.49	121.05
1	B	1058	ASP	CA-CB-CG	6.40	119.00	112.60
1	B	1265	ASP	CA-CB-CG	6.30	118.90	112.60
1	B	840	LEU	CA-C-N	6.22	128.90	120.38
1	B	840	LEU	C-N-CA	6.22	128.90	120.38
1	B	956	ASP	CA-CB-CG	6.08	118.68	112.60
1	B	529	ASN	CA-CB-CG	6.00	118.60	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1106	ASP	CA-C-N	5.96	129.37	120.31
1	B	1106	ASP	C-N-CA	5.96	129.37	120.31
1	B	607	ALA	N-CA-C	5.92	118.54	110.55
1	B	850	GLU	CB-CG-CD	5.92	122.66	112.60
1	B	1621	ASP	CA-CB-CG	5.91	118.51	112.60
1	B	578	ASP	CA-CB-CG	5.81	118.41	112.60
1	B	496	ASP	N-CA-C	5.71	118.97	110.52
1	B	1240	THR	N-CA-C	-5.71	105.98	113.17
1	B	544	GLY	CA-C-N	5.68	128.36	120.29
1	B	544	GLY	C-N-CA	5.68	128.36	120.29
1	B	925	VAL	CA-C-N	5.66	130.39	122.36
1	B	925	VAL	C-N-CA	5.66	130.39	122.36
1	B	415	GLU	CA-C-N	5.64	128.11	120.38
1	B	415	GLU	C-N-CA	5.64	128.11	120.38
1	B	1593	THR	N-CA-C	-5.63	102.82	110.36
1	B	1208	ASN	CA-CB-CG	5.62	118.22	112.60
1	B	859	ARG	N-CA-C	5.60	120.11	112.88
1	B	1043	ASP	CA-C-N	5.58	128.53	120.38
1	B	1043	ASP	C-N-CA	5.58	128.53	120.38
1	B	368	ASP	CA-CB-CG	5.56	118.16	112.60
1	B	853	GLU	CA-C-N	5.50	127.60	120.56
1	B	853	GLU	C-N-CA	5.50	127.60	120.56
1	B	1487	ASP	CA-CB-CG	5.48	118.08	112.60
1	B	789	ASP	CA-C-N	5.47	131.82	121.97
1	B	789	ASP	C-N-CA	5.47	131.82	121.97
1	B	1680	ALA	CA-C-N	5.44	127.83	120.38
1	B	1680	ALA	C-N-CA	5.44	127.83	120.38
1	B	1538	ASP	CA-CB-CG	5.42	118.02	112.60
1	B	601	ASP	CA-CB-CG	5.38	117.98	112.60
1	B	782	ASN	CA-CB-CG	5.37	117.97	112.60
1	B	934	ASN	CA-CB-CG	5.36	117.96	112.60
1	B	811	MET	CA-C-N	5.33	127.39	120.56
1	B	811	MET	C-N-CA	5.33	127.39	120.56
1	B	898	ASP	CA-CB-CG	5.33	117.92	112.60
1	B	1118	ASP	CA-CB-CG	5.32	117.92	112.60
1	B	1209	THR	N-CA-C	-5.31	105.39	111.07
1	B	734	ASP	CA-CB-CG	5.26	117.86	112.60
1	B	803	TRP	CA-C-N	5.26	127.32	120.28
1	B	803	TRP	C-N-CA	5.26	127.32	120.28
1	B	589	THR	N-CA-C	-5.22	105.65	112.23
1	B	612	ASP	CA-C-N	5.22	125.77	119.98
1	B	612	ASP	C-N-CA	5.22	125.77	119.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	343	GLU	CB-CG-CD	5.16	121.37	112.60
1	B	724	MET	N-CA-CB	-5.16	101.93	111.53
1	B	642	PHE	CA-C-N	5.12	127.85	120.11
1	B	642	PHE	C-N-CA	5.12	127.85	120.11
1	B	1622	ALA	N-CA-C	-5.09	105.92	111.82
1	B	853	GLU	N-CA-C	-5.05	105.85	111.36
1	B	1265	ASP	N-CA-C	-5.03	103.04	110.48
1	B	1631	ALA	CA-C-N	5.00	127.24	120.44
1	B	1631	ALA	C-N-CA	5.00	127.24	120.44

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	B	10328	0	9899	69	0
2	D	113	0	116	2	0
3	B	4	0	0	0	0
4	B	24	0	42	3	0
5	B	498	0	0	1	0
5	D	1	0	0	0	0
All	All	10968	0	10057	69	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 3.

All (69) 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:768:ARG:HD2	1:B:811:MET:HE1	1.38	1.05
1:B:470:LEU:HD22	1:B:594:MET:HE2	1.67	0.74
1:B:1583:ASP:HB3	1:B:1586:ALA:HB2	1.76	0.66
1:B:405:GLU:HG3	1:B:428:THR:HG22	1.78	0.63
1:B:1636:HIS:HB3	1:B:1639:ILE:HD13	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:348:LYS:H	4:B:1707:MPD:H31	1.67	0.60
1:B:1638:GLU:H	1:B:1638:GLU:CD	2.10	0.59
1:B:1149:ARG:HH12	1:B:1230:ASP:HA	1.68	0.59
1:B:618:ARG:HA	1:B:621:MET:HG2	1.85	0.58
1:B:1165:VAL:HG11	1:B:1219:MET:HE2	1.87	0.57
1:B:471:VAL:HG13	1:B:517:ILE:HD11	1.87	0.56
1:B:727:GLU:HG2	5:B:2114:HOH:O	2.06	0.56
1:B:1364:GLY:HA2	1:B:1392:LEU:HD13	1.86	0.56
1:B:473:VAL:HG13	1:B:517:ILE:HD12	1.89	0.55
1:B:839:ASP:OD1	1:B:841:THR:HB	2.07	0.54
1:B:724:MET:HB2	1:B:757:ILE:HG13	1.88	0.54
1:B:348:LYS:HB2	4:B:1707:MPD:HM3	1.89	0.54
1:B:1638:GLU:HG2	1:B:1639:ILE:HD12	1.89	0.53
1:B:1669:ASN:HB3	1:B:1672:ILE:HD13	1.89	0.53
1:B:1189:THR:HB	1:B:1345:GLN:HB3	1.90	0.52
1:B:808:MET:HA	1:B:811:MET:HE2	1.92	0.51
1:B:869:ASP:O	1:B:996:GLY:HA3	2.10	0.51
1:B:827:ASN:HB3	1:B:831:SER:HB2	1.92	0.51
1:B:1277:ASN:OD1	4:B:1705:MPD:H12	2.11	0.51
1:B:343:GLU:HG2	1:B:356:LYS:HE3	1.92	0.50
1:B:617:TYR:HD2	1:B:621:MET:HE3	1.77	0.50
1:B:1623:GLN:HE22	2:D:12:PHE:H	1.60	0.49
1:B:339:MET:HG2	1:B:340:VAL:H	1.77	0.49
1:B:552:ALA:HB1	1:B:563:LEU:HD11	1.93	0.49
1:B:1172:ASP:H	1:B:1238:LYS:HE3	1.78	0.49
1:B:686:PRO:HD3	1:B:724:MET:HG3	1.93	0.49
1:B:384:ILE:HD11	1:B:423:ILE:HD11	1.94	0.49
1:B:1620:GLN:HG2	1:B:1626:THR:HG22	1.95	0.48
1:B:1301:SER:HB3	1:B:1328:LYS:HB2	1.96	0.47
1:B:626:LYS:O	1:B:629:GLU:HG2	2.14	0.47
1:B:1192:SER:HB3	1:B:1215:TYR:HB3	1.97	0.47
1:B:1268:LEU:HD11	1:B:1271:LEU:HB2	1.97	0.46
1:B:1677:GLN:HG2	1:B:1681:LYS:HE3	1.96	0.46
1:B:491:THR:HG22	1:B:867:VAL:HG11	1.98	0.46
1:B:633:LEU:HD22	1:B:714:ARG:HD3	1.96	0.46
1:B:807:LYS:O	1:B:811:MET:HG3	2.16	0.45
1:B:633:LEU:CD2	1:B:714:ARG:HD3	2.47	0.45
1:B:962:VAL:HA	1:B:982:THR:O	2.16	0.45
1:B:425:VAL:HG22	1:B:438:VAL:HG22	1.98	0.45
1:B:964:VAL:HG12	1:B:981:ILE:HG12	1.97	0.44
1:B:1119:ASN:O	1:B:1148:GLN:HG3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:359:PRO:HD3	1:B:410:LEU:HD21	1.98	0.44
1:B:981:ILE:HB	1:B:989:ALA:HB3	1.98	0.44
1:B:955:LYS:HG2	1:B:961:VAL:HG22	1.99	0.44
1:B:1219:MET:HG3	1:B:1345:GLN:HB2	1.99	0.44
1:B:925:VAL:HG21	1:B:945:THR:HG21	2.00	0.44
1:B:1578:LEU:HD13	1:B:1613:THR:HG21	2.00	0.43
1:B:676:TYR:CD1	1:B:717:VAL:HB	2.54	0.43
1:B:1559:ALA:HB2	2:D:8:PRO:HB3	2.01	0.43
1:B:1352:GLY:HA2	1:B:1512:ILE:HG13	2.01	0.42
1:B:1328:LYS:HG3	1:B:1440:VAL:HG22	2.01	0.42
1:B:724:MET:HE3	1:B:731:PHE:CE2	2.55	0.42
1:B:1162:TYR:HA	1:B:1219:MET:O	2.19	0.42
1:B:372:MET:SD	1:B:471:VAL:HG22	2.60	0.42
1:B:1487:ASP:O	1:B:1491:LYS:HG2	2.20	0.42
1:B:527:TRP:HB3	1:B:620:ILE:HD12	2.02	0.42
1:B:718:HIS:CD2	1:B:718:HIS:C	2.98	0.42
1:B:1196:ASN:HB3	1:B:1204:ASN:HA	2.02	0.41
1:B:424:THR:HB	1:B:440:LYS:HB3	2.02	0.41
1:B:634:VAL:HA	1:B:914:LYS:HG3	2.03	0.41
1:B:1490:VAL:O	1:B:1494:VAL:HG23	2.20	0.41
1:B:1157:GLN:HE21	1:B:1256:GLN:HE22	1.68	0.41
1:B:617:TYR:CE2	1:B:621:MET:HB3	2.55	0.41
1:B:701:MET:O	1:B:705:MET:HG3	2.22	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	B	1344/1357 (99%)	1278 (95%)	61 (4%)	5 (0%)	30 54
2	D	13/15 (87%)	12 (92%)	1 (8%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1357/1372 (99%)	1290 (95%)	62 (5%)	5 (0%)	30 54

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	790	VAL
1	B	940	VAL
1	B	1469	LYS
1	B	1266	GLY
1	B	1647	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	B	1095/1104 (99%)	1040 (95%)	55 (5%)	22 48
2	D	10/10 (100%)	10 (100%)	0	100 100
All	All	1105/1114 (99%)	1050 (95%)	55 (5%)	22 48

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	339	MET
1	B	340	VAL
1	B	349	LYS
1	B	357	ASN
1	B	360	SER
1	B	363	GLN
1	B	399	LYS
1	B	403	ASP
1	B	418	LYS
1	B	426	GLN
1	B	455	VAL
1	B	471	VAL
1	B	478	GLU

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Mol	Chain	Res	Type
1	B	535	THR
1	B	580	LYS
1	B	604	GLU
1	B	674	LYS
1	B	736	VAL
1	B	769	VAL
1	B	834	GLN
1	B	912	SER
1	B	920	LYS
1	B	965	SER
1	B	971	THR
1	B	987	LYS
1	B	993	VAL
1	B	1011	MET
1	B	1014	SER
1	B	1016	THR
1	B	1033	LYS
1	B	1123	SER
1	B	1147	SER
1	B	1158	LYS
1	B	1170	THR
1	B	1186	THR
1	B	1236	SER
1	B	1239	SER
1	B	1288	SER
1	B	1354	LYS
1	B	1394	GLU
1	B	1410	SER
1	B	1452	GLN
1	B	1466	ILE
1	B	1479	ASP
1	B	1483	GLN
1	B	1484	GLN
1	B	1487	ASP
1	B	1525	LEU
1	B	1604	LEU
1	B	1612	LYS
1	B	1621	ASP
1	B	1628	LEU
1	B	1653	GLN
1	B	1674	GLU
1	B	1676	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	357	ASN
1	B	437	ASN
1	B	444	ASN
1	B	498	ASN
1	B	702	ASN
1	B	782	ASN
1	B	827	ASN
1	B	835	HIS
1	B	905	ASN
1	B	936	ASN
1	B	1093	GLN
1	B	1119	ASN
1	B	1157	GLN
1	B	1217	GLN
1	B	1228	ASN
1	B	1375	GLN
1	B	1452	GLN
1	B	1484	GLN
1	B	1486	GLN
1	B	1547	ASN
1	B	1636	HIS
1	B	1667	ASN
1	B	1669	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 4 are monoatomic - leaving 3 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	MPD	B	1707	-	7,7,7	0.60	0	9,10,10	0.55	0
4	MPD	B	1706	-	7,7,7	0.90	1 (14%)	9,10,10	0.37	0
4	MPD	B	1705	-	7,7,7	0.84	0	9,10,10	0.45	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	MPD	B	1707	-	-	3/5/5/5	-
4	MPD	B	1706	-	-	2/5/5/5	-
4	MPD	B	1705	-	-	2/5/5/5	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1706	MPD	C3-C2	2.14	1.60	1.54

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1707	MPD	C2-C3-C4-O4
4	B	1706	MPD	O2-C2-C3-C4
4	B	1705	MPD	C1-C2-C3-C4
4	B	1705	MPD	CM-C2-C3-C4
4	B	1706	MPD	C1-C2-C3-C4
4	B	1707	MPD	C1-C2-C3-C4
4	B	1707	MPD	CM-C2-C3-C4

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1707	MPD	2	0
4	B	1705	MPD	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	B	1346/1357 (99%)	-0.07	21 (1%) 70 68	45, 66, 111, 144	0
2	D	14/15 (93%)	2.10	5 (35%) 1 0	106, 119, 146, 151	0
All	All	1360/1372 (99%)	-0.05	26 (1%) 66 63	45, 67, 113, 151	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	1	PRO	6.2
2	D	4	ILE	5.4
1	B	1094	ILE	3.5
2	D	2	LYS	3.4
1	B	339	MET	3.2
1	B	1684	SER	3.2
1	B	1545	MET	3.0
1	B	1533	ALA	2.9
1	B	1557	TYR	2.9
1	B	1672	ILE	2.8
1	B	1604	LEU	2.6
2	D	14	ALA	2.5
1	B	1543	ILE	2.2
1	B	1647	GLY	2.2
1	B	1644	LEU	2.2
1	B	1599	ALA	2.2
1	B	1665	ILE	2.2
2	D	10	GLN	2.2
1	B	1571	LEU	2.2
1	B	940	VAL	2.2
1	B	1590	VAL	2.1
1	B	1676	LEU	2.0
1	B	1238	LYS	2.0
1	B	1582	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	1646	HIS	2.0
1	B	1500	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
2	DPR	D	15	7/8	0.59	0.30	138,140,145,145	0

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	MPD	B	1707	8/8	0.78	0.31	97,101,102,105	0
4	MPD	B	1706	8/8	0.79	0.32	90,99,107,109	0
4	MPD	B	1705	8/8	0.82	0.25	50,54,79,83	0
3	MN	B	1702	1/1	0.98	0.10	80,80,80,80	0
3	MN	B	1701	1/1	0.99	0.02	71,71,71,71	0
3	MN	B	1703	1/1	0.99	0.03	85,85,85,85	0
3	MN	B	1704	1/1	0.99	0.03	85,85,85,85	0

6.5 Other polymers [i](#)

There are no such residues in this entry.