WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Sep 10, 2023 – 09:00 AM EDT

PDB ID	:	4H8S
Title	:	Crystal structure of human APPL2BARPH domain
Authors	:	Martin, J.L.; King, G.J.
Deposited on	:	2012-09-23
Resolution	:	3.50 Å(reported)

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

|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
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)	:	2.35.1

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 3.50 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.
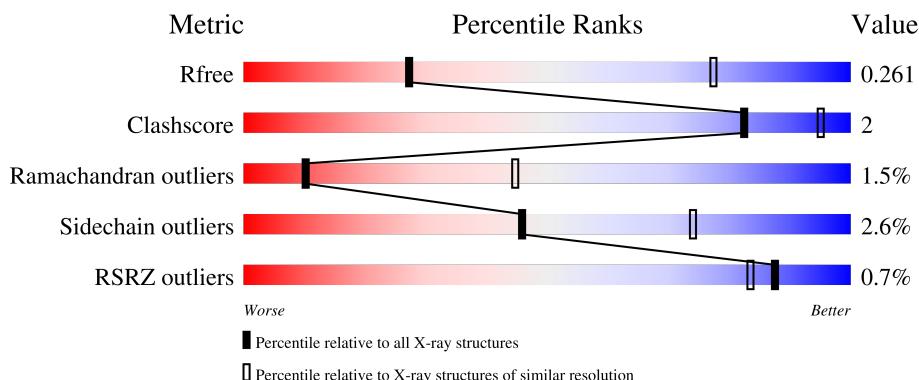
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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	407	86% 6% 7%
1	B	407	.% 84% 7% · 8%
1	C	407	84% 9% · 6%
1	D	407	.% 84% 7% · 8%
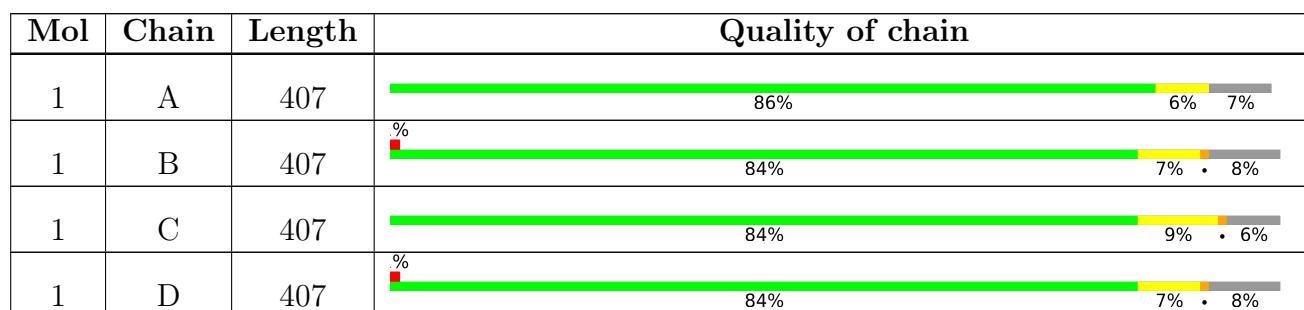
2 Entry composition ⓘ

There is only 1 type of molecule in this entry. The entry contains 23866 atoms, of which 11908 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 DCC-interacting protein 13-beta.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	378	Total	C	H	N	O	S	0	0	0
			5982	1880	2982	514	585	21			
1	B	374	Total	C	H	N	O	S	0	0	0
			5926	1859	2959	509	578	21			
1	C	382	Total	C	H	N	O	S	0	0	0
			6053	1905	3017	519	591	21			
1	D	373	Total	C	H	N	O	S	0	0	0
			5905	1850	2950	508	576	21			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MET	-	expression tag	UNP Q8NEU8
A	-21	HIS	-	expression tag	UNP Q8NEU8
A	-20	HIS	-	expression tag	UNP Q8NEU8
A	-19	HIS	-	expression tag	UNP Q8NEU8
A	-18	HIS	-	expression tag	UNP Q8NEU8
A	-17	HIS	-	expression tag	UNP Q8NEU8
A	-16	HIS	-	expression tag	UNP Q8NEU8
A	-15	SER	-	expression tag	UNP Q8NEU8
A	-14	SER	-	expression tag	UNP Q8NEU8
A	-13	GLY	-	expression tag	UNP Q8NEU8
A	-12	VAL	-	expression tag	UNP Q8NEU8
A	-11	ASP	-	expression tag	UNP Q8NEU8
A	-10	LEU	-	expression tag	UNP Q8NEU8
A	-9	GLY	-	expression tag	UNP Q8NEU8
A	-8	THR	-	expression tag	UNP Q8NEU8
A	-7	GLU	-	expression tag	UNP Q8NEU8
A	-6	ASN	-	expression tag	UNP Q8NEU8
A	-5	LEU	-	expression tag	UNP Q8NEU8
A	-4	TYR	-	expression tag	UNP Q8NEU8
A	-3	PHE	-	expression tag	UNP Q8NEU8
A	-2	GLN	-	expression tag	UNP Q8NEU8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	expression tag	UNP Q8NEU8
A	0	ASN	-	expression tag	UNP Q8NEU8
A	1	ALA	-	expression tag	UNP Q8NEU8
B	-22	MET	-	expression tag	UNP Q8NEU8
B	-21	HIS	-	expression tag	UNP Q8NEU8
B	-20	HIS	-	expression tag	UNP Q8NEU8
B	-19	HIS	-	expression tag	UNP Q8NEU8
B	-18	HIS	-	expression tag	UNP Q8NEU8
B	-17	HIS	-	expression tag	UNP Q8NEU8
B	-16	HIS	-	expression tag	UNP Q8NEU8
B	-15	SER	-	expression tag	UNP Q8NEU8
B	-14	SER	-	expression tag	UNP Q8NEU8
B	-13	GLY	-	expression tag	UNP Q8NEU8
B	-12	VAL	-	expression tag	UNP Q8NEU8
B	-11	ASP	-	expression tag	UNP Q8NEU8
B	-10	LEU	-	expression tag	UNP Q8NEU8
B	-9	GLY	-	expression tag	UNP Q8NEU8
B	-8	THR	-	expression tag	UNP Q8NEU8
B	-7	GLU	-	expression tag	UNP Q8NEU8
B	-6	ASN	-	expression tag	UNP Q8NEU8
B	-5	LEU	-	expression tag	UNP Q8NEU8
B	-4	TYR	-	expression tag	UNP Q8NEU8
B	-3	PHE	-	expression tag	UNP Q8NEU8
B	-2	GLN	-	expression tag	UNP Q8NEU8
B	-1	SER	-	expression tag	UNP Q8NEU8
B	0	ASN	-	expression tag	UNP Q8NEU8
B	1	ALA	-	expression tag	UNP Q8NEU8
C	-22	MET	-	expression tag	UNP Q8NEU8
C	-21	HIS	-	expression tag	UNP Q8NEU8
C	-20	HIS	-	expression tag	UNP Q8NEU8
C	-19	HIS	-	expression tag	UNP Q8NEU8
C	-18	HIS	-	expression tag	UNP Q8NEU8
C	-17	HIS	-	expression tag	UNP Q8NEU8
C	-16	HIS	-	expression tag	UNP Q8NEU8
C	-15	SER	-	expression tag	UNP Q8NEU8
C	-14	SER	-	expression tag	UNP Q8NEU8
C	-13	GLY	-	expression tag	UNP Q8NEU8
C	-12	VAL	-	expression tag	UNP Q8NEU8
C	-11	ASP	-	expression tag	UNP Q8NEU8
C	-10	LEU	-	expression tag	UNP Q8NEU8
C	-9	GLY	-	expression tag	UNP Q8NEU8
C	-8	THR	-	expression tag	UNP Q8NEU8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-7	GLU	-	expression tag	UNP Q8NEU8
C	-6	ASN	-	expression tag	UNP Q8NEU8
C	-5	LEU	-	expression tag	UNP Q8NEU8
C	-4	TYR	-	expression tag	UNP Q8NEU8
C	-3	PHE	-	expression tag	UNP Q8NEU8
C	-2	GLN	-	expression tag	UNP Q8NEU8
C	-1	SER	-	expression tag	UNP Q8NEU8
C	0	ASN	-	expression tag	UNP Q8NEU8
C	1	ALA	-	expression tag	UNP Q8NEU8
D	-22	MET	-	expression tag	UNP Q8NEU8
D	-21	HIS	-	expression tag	UNP Q8NEU8
D	-20	HIS	-	expression tag	UNP Q8NEU8
D	-19	HIS	-	expression tag	UNP Q8NEU8
D	-18	HIS	-	expression tag	UNP Q8NEU8
D	-17	HIS	-	expression tag	UNP Q8NEU8
D	-16	HIS	-	expression tag	UNP Q8NEU8
D	-15	SER	-	expression tag	UNP Q8NEU8
D	-14	SER	-	expression tag	UNP Q8NEU8
D	-13	GLY	-	expression tag	UNP Q8NEU8
D	-12	VAL	-	expression tag	UNP Q8NEU8
D	-11	ASP	-	expression tag	UNP Q8NEU8
D	-10	LEU	-	expression tag	UNP Q8NEU8
D	-9	GLY	-	expression tag	UNP Q8NEU8
D	-8	THR	-	expression tag	UNP Q8NEU8
D	-7	GLU	-	expression tag	UNP Q8NEU8
D	-6	ASN	-	expression tag	UNP Q8NEU8
D	-5	LEU	-	expression tag	UNP Q8NEU8
D	-4	TYR	-	expression tag	UNP Q8NEU8
D	-3	PHE	-	expression tag	UNP Q8NEU8
D	-2	GLN	-	expression tag	UNP Q8NEU8
D	-1	SER	-	expression tag	UNP Q8NEU8
D	0	ASN	-	expression tag	UNP Q8NEU8
D	1	ALA	-	expression tag	UNP Q8NEU8

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: DCC-interacting protein 13-beta
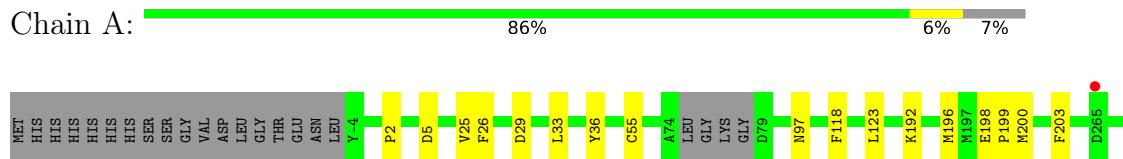
Chain A:

• Molecule 1: DCC-interacting protein 13-beta
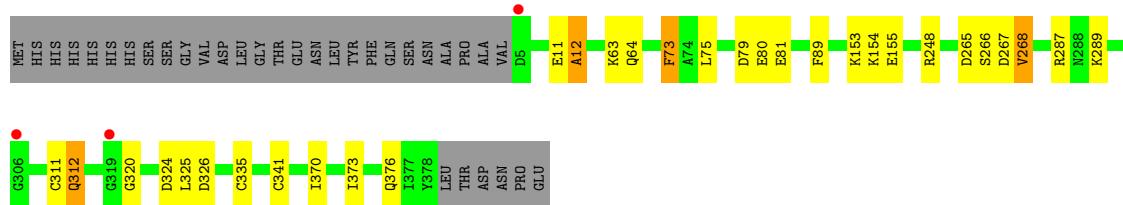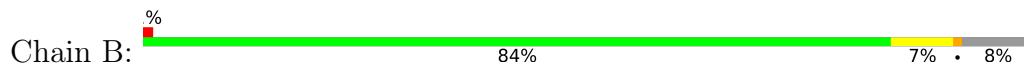
Chain B:

• Molecule 1: DCC-interacting protein 13-beta

Chain C:

• Molecule 1: DCC-interacting protein 13-beta

Chain D:
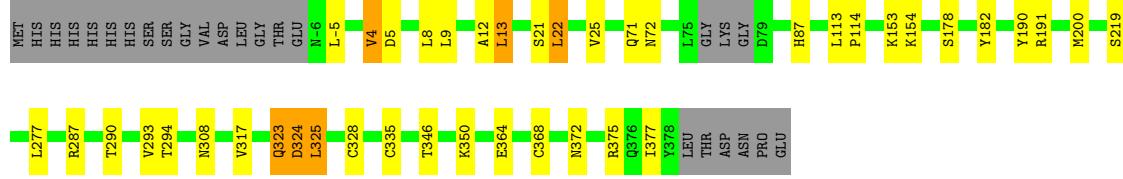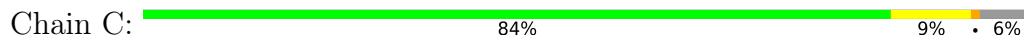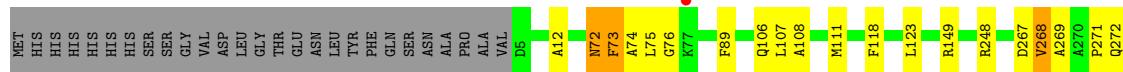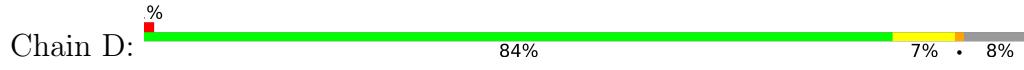
4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	97.96Å 208.01Å 218.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.95 – 3.50 46.95 – 3.50	Depositor EDS
% Data completeness (in resolution range)	95.4 (46.95-3.50) 94.4 (46.95-3.50)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.84 (at 3.48Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1031)	Depositor
R, R_{free}	0.209 , 0.256 0.221 , 0.261	Depositor DCC
R_{free} test set	2810 reflections (5.15%)	wwPDB-VP
Wilson B-factor (Å^2)	97.7	Xtriage
Anisotropy	0.357	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 90.3	EDS
L-test for twinning[2]	$< |L| > = 0.46, < L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.025 for -h,l,k	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	23866	wwPDB-VP
Average B, all atoms (Å^2)	119.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.33% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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)

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	0.29	0/3043	0.55	0/4100
1	B	0.28	0/3009	0.55	1/4052 (0.0%)
1	C	0.28	0/3080	0.51	0/4151
1	D	0.28	0/2996	0.55	1/4034 (0.0%)
All	All	0.28	0/12128	0.54	2/16337 (0.0%)

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	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	248	ARG	NE-CZ-NH1	5.65	123.12	120.30
1	B	248	ARG	NE-CZ-NH1	5.07	122.84	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	280	LYS	Peptide
1	B	12	ALA	Peptide

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	3000	2982	2990	15	0
1	B	2967	2959	2964	16	0
1	C	3036	3017	3027	20	0
1	D	2955	2950	2955	14	0
All	All	11958	11908	11936	59	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 (59) 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:C:372:ASN:OD1	1:C:375:ARG:NH2	2.19	0.76
1:C:8:LEU:CB	1:C:9:LEU:HA	2.17	0.75
1:A:280:LYS:HA	1:A:281:ALA:CB	2.27	0.65
1:A:324:ASP:HB3	1:A:325:LEU:HA	1.77	0.64
1:C:8:LEU:HB2	1:C:9:LEU:HA	1.80	0.63
1:D:106:GLN:O	1:D:108:ALA:N	2.33	0.61
1:A:280:LYS:HA	1:A:281:ALA:HB2	1.81	0.61
1:C:368:CYS:O	1:C:372:ASN:ND2	2.34	0.61
1:C:8:LEU:HB3	1:C:9:LEU:HA	1.84	0.59
1:D:287:ARG:NH1	1:D:335:CYS:SG	2.76	0.59
1:A:36:TYR:OH	1:B:64:GLN:O	2.12	0.59
1:C:287:ARG:NH1	1:C:335:CYS:SG	2.78	0.56
1:B:265:ASP:HA	1:B:266:SER:CB	2.36	0.56
1:C:290:THR:OG1	1:C:294:THR:OG1	2.24	0.56
1:D:271:PRO:HA	1:D:272:GLN:HB2	1.90	0.54
1:A:287:ARG:NH1	1:A:336:GLU:OE2	2.40	0.53
1:C:8:LEU:CB	1:C:9:LEU:CA	2.89	0.51
1:D:267:ASP:N	1:D:267:ASP:OD1	2.42	0.51
1:B:11:GLU:HA	1:B:12:ALA:HB2	1.91	0.51
1:A:55:CYS:O	1:A:97:ASN:ND2	2.45	0.49
1:B:265:ASP:HA	1:B:266:SER:HB3	1.95	0.49
1:A:346:THR:HB	1:A:347:PRO:HD2	1.94	0.49
1:B:79:ASP:O	1:B:81:GLU:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:8:LEU:HB3	1:C:9:LEU:CA	2.44	0.48
1:C:71:GLN:HB2	1:C:72:ASN:HA	1.96	0.47
1:A:200:MET:HB3	1:B:89:PHE:CD2	2.51	0.46
1:A:29:ASP:HB2	1:B:75:LEU:HD12	1.97	0.46
1:A:324:ASP:CB	1:A:325:LEU:HA	2.43	0.45
1:C:178:SER:O	1:C:182:TYR:CD1	2.70	0.45
1:D:118:PHE:CE1	1:D:123:LEU:HD21	2.52	0.45
1:C:200:MET:HB3	1:D:89:PHE:CD2	2.52	0.44
1:D:75:LEU:HG	1:D:76:GLY:CA	2.48	0.44
1:D:75:LEU:HG	1:D:76:GLY:HA2	1.99	0.44
1:B:311:CYS:O	1:B:312:GLN:C	2.56	0.44
1:C:324:ASP:O	1:C:325:LEU:CB	2.65	0.44
1:C:25:VAL:HG12	1:D:75:LEU:HB2	1.99	0.44
1:D:284:LEU:HD21	1:D:366:TRP:CE2	2.53	0.44
1:B:73:PHE:CD1	1:B:73:PHE:N	2.85	0.44
1:C:4:VAL:HG21	1:C:190:TYR:CZ	2.53	0.44
1:C:153:LYS:HA	1:C:154:LYS:HA	1.83	0.43
1:B:324:ASP:CB	1:B:325:LEU:HA	2.48	0.43
1:B:267:ASP:OD1	1:B:268:VAL:N	2.51	0.43
1:B:153:LYS:HA	1:B:154:LYS:HA	1.83	0.43
1:D:268:VAL:O	1:D:269:ALA:HB3	2.19	0.42
1:A:280:LYS:CA	1:A:281:ALA:CB	2.96	0.42
1:C:8:LEU:HD13	1:C:12:ALA:N	2.33	0.42
1:A:33:LEU:CD1	1:A:192:LYS:HD3	2.50	0.42
1:A:198:GLU:N	1:A:199:PRO:CD	2.82	0.42
1:B:376:GLN:OE1	1:B:376:GLN:N	2.52	0.42
1:C:113:LEU:HB3	1:C:114:PRO:HD3	2.00	0.42
1:A:118:PHE:CE1	1:A:123:LEU:HD21	2.54	0.42
1:D:74:ALA:N	1:D:75:LEU:HA	2.35	0.42
1:C:323:GLN:HG3	1:C:324:ASP:HB3	2.02	0.41
1:B:370:ILE:HA	1:B:373:ILE:HG22	2.02	0.41
1:D:73:PHE:CD2	1:D:73:PHE:N	2.86	0.41
1:D:353:ILE:HD12	1:D:353:ILE:N	2.36	0.41
1:A:5:ASP:CG	1:B:75:LEU:HD23	2.41	0.41
1:B:287:ARG:NH1	1:B:335:CYS:SG	2.94	0.41
1:C:21:SER:O	1:C:22:LEU:CB	2.68	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	374/407 (92%)	346 (92%)	23 (6%)	5 (1%)	12	48
1	B	372/407 (91%)	344 (92%)	24 (6%)	4 (1%)	14	52
1	C	378/407 (93%)	346 (92%)	24 (6%)	8 (2%)	7	38
1	D	371/407 (91%)	336 (91%)	29 (8%)	6 (2%)	9	43
All	All	1495/1628 (92%)	1372 (92%)	100 (7%)	23 (2%)	10	45

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	281	ALA
1	C	5	ASP
1	C	22	LEU
1	C	293	VAL
1	C	325	LEU
1	D	72	ASN
1	D	323	GLN
1	A	326	ASP
1	B	289	LYS
1	C	350	LYS
1	A	2	PRO
1	A	324	ASP
1	B	80	GLU
1	D	12	ALA
1	D	107	LEU
1	D	268	VAL
1	D	279	GLN
1	B	312	GLN
1	C	13	LEU
1	C	219	SER
1	A	312	GLN
1	B	320	GLY
1	C	4	VAL

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	330/355 (93%)	324 (98%)	6 (2%)	59	81
1	B	326/355 (92%)	320 (98%)	6 (2%)	59	81
1	C	334/355 (94%)	321 (96%)	13 (4%)	32	64
1	D	325/355 (92%)	316 (97%)	9 (3%)	43	72
All	All	1315/1420 (93%)	1281 (97%)	34 (3%)	46	74

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	VAL
1	A	26	PHE
1	A	196	MET
1	A	203	PHE
1	A	324	ASP
1	A	339	ARG
1	B	63	LYS
1	B	73	PHE
1	B	155	GLU
1	B	268	VAL
1	B	326	ASP
1	B	341	CYS
1	C	-5	LEU
1	C	13	LEU
1	C	87	HIS
1	C	191	ARG
1	C	277	LEU
1	C	308	ASN
1	C	317	VAL
1	C	323	GLN
1	C	324	ASP
1	C	328	CYS
1	C	346	THR
1	C	364	GLU

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Mol	Chain	Res	Type
1	C	377	ILE
1	D	72	ASN
1	D	73	PHE
1	D	111	MET
1	D	149	ARG
1	D	280	LYS
1	D	283	TYR
1	D	299	ARG
1	D	308	ASN
1	D	341	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6   Fit of model and data (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	378/407 (92%)	-0.19	2 (0%) 91	88	76, 116, 170, 296	0
1	B	374/407 (91%)	-0.16	3 (0%) 86	81	79, 121, 203, 274	0
1	C	382/407 (93%)	-0.19	0 100	100	80, 122, 181, 278	0
1	D	373/407 (91%)	-0.15	5 (1%) 77	71	69, 124, 203, 334	0
All	All	1507/1628 (92%)	-0.17	10 (0%) 87	83	69, 121, 190, 334	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	307	GLY	3.2
1	A	265	ASP	3.0
1	A	292	LEU	2.9
1	B	319	GLY	2.9
1	D	305	GLN	2.7
1	B	5	ASP	2.6
1	D	279	GLN	2.4
1	D	278	ILE	2.3
1	D	77	LYS	2.1
1	B	306	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 ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.