



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:04 PM UTC

PDB ID : 3H5R / pdb_00003h5r
Title : Crystal structure of E. coli MccB + Succinimide
Authors : Regni, C.A.; Roush, R.F.; Miller, D.; Nourse, A.; Walsh, C.T.; Schulman, B.A.
Deposited on : 2009-04-22
Resolution : 2.10 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

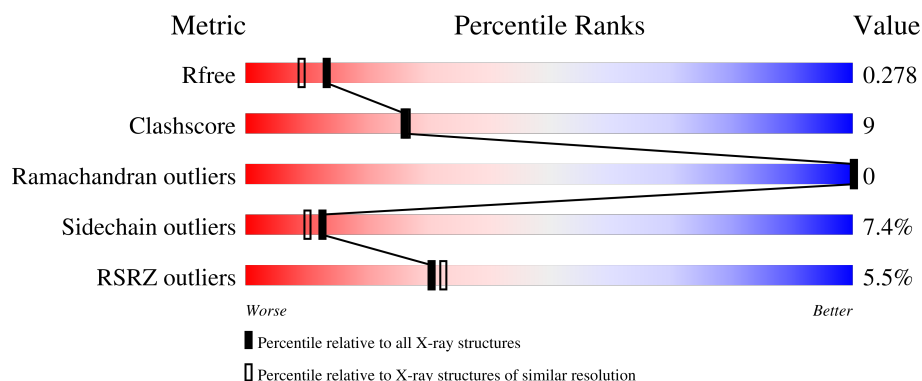
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	353	6% 82% 14% ..
1	B	353	5% 79% 14% 5%
1	C	353	3% 76% 19% ..
1	D	353	4% 69% 23% 6%
2	E	7	57% 57% 29% 14%

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Mol	Chain	Length	Quality of chain
2	F	7	43% 57% 14% 29%
2	G	7	14% 14% 86%
2	H	7	14% 86%

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
2	SNN	F	77	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10712 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 MccB protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	340	Total	C	N	O	S	0	0	0
			2599	1659	449	480	11			
1	B	334	Total	C	N	O	S	0	0	0
			2551	1636	427	477	11			
1	C	343	Total	C	N	O	S	0	0	0
			2621	1675	446	489	11			
1	D	333	Total	C	N	O	S	0	0	0
			2546	1627	434	474	11			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP Q47506
A	-1	SER	-	expression tag	UNP Q47506
A	0	HIS	-	expression tag	UNP Q47506
B	-2	GLY	-	expression tag	UNP Q47506
B	-1	SER	-	expression tag	UNP Q47506
B	0	HIS	-	expression tag	UNP Q47506
C	-2	GLY	-	expression tag	UNP Q47506
C	-1	SER	-	expression tag	UNP Q47506
C	0	HIS	-	expression tag	UNP Q47506
D	-2	GLY	-	expression tag	UNP Q47506
D	-1	SER	-	expression tag	UNP Q47506
D	0	HIS	-	expression tag	UNP Q47506

- Molecule 2 is a protein called Microcin C7 analog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	7	Total	C	N	O	S	0	0	0
			51	28	12	10	1			
2	F	7	Total	C	N	O	S	0	0	0
			51	28	12	10	1			

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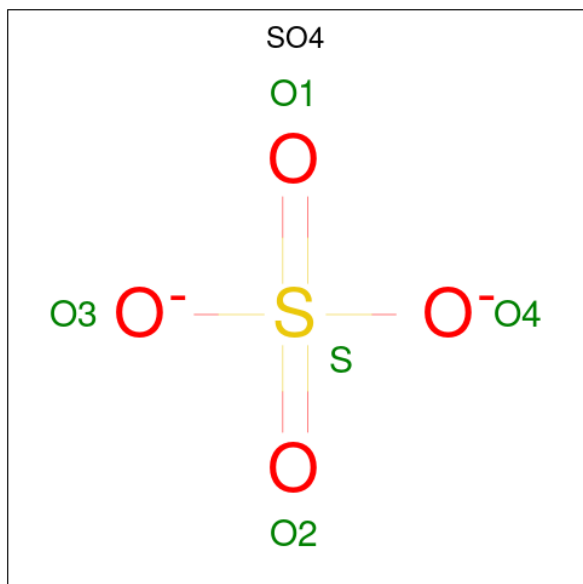
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	1	Total	C	N	O	S	0	0	0
			8	5	1	1	1			
2	H	1	Total	C	N	O	S	0	0	0
			8	5	1	1	1			

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		
3	B	1	Total	Zn	0	0
			1	1		
3	C	1	Total	Zn	0	0
			1	1		
3	D	1	Total	Zn	0	0
			1	1		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		

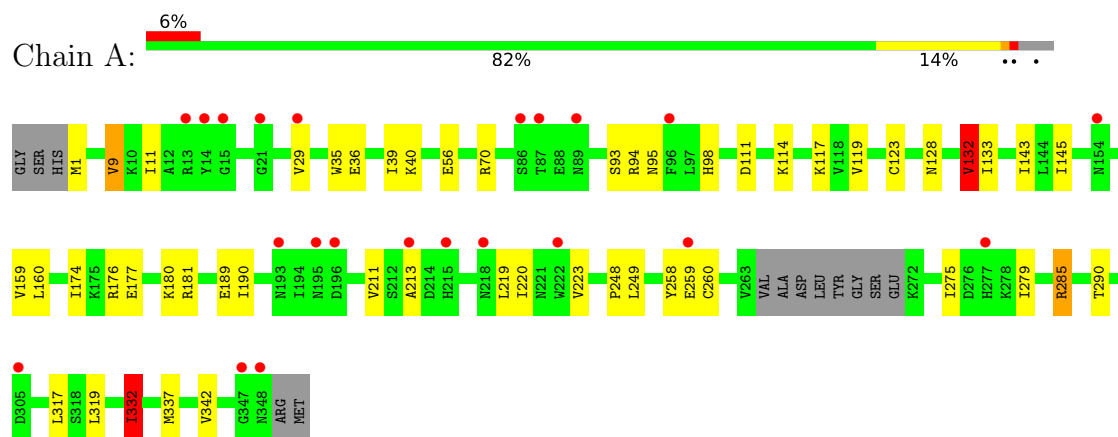
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	82	Total 82	O 82	0	0
5	B	70	Total 70	O 70	0	0
5	C	69	Total 69	O 69	0	0
5	D	38	Total 38	O 38	0	0
5	E	1	Total 1	O 1	0	0
5	F	3	Total 3	O 3	0	0

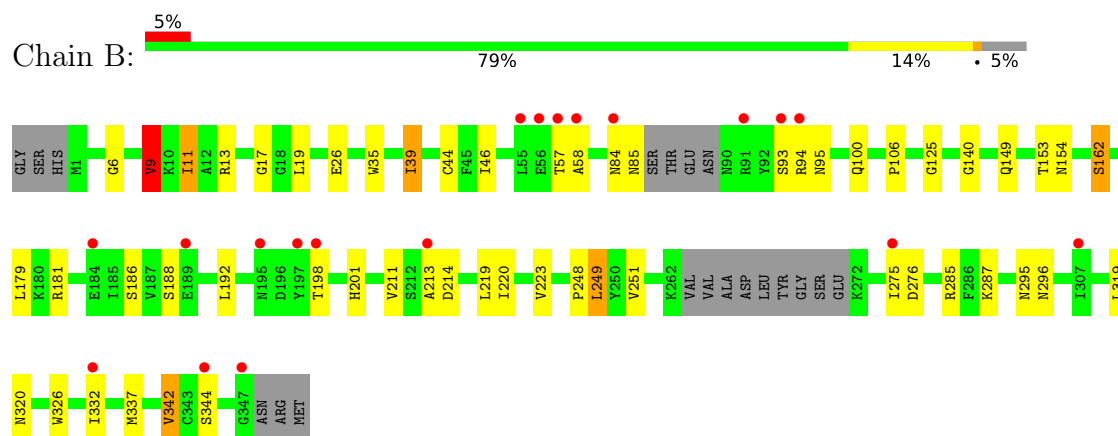
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

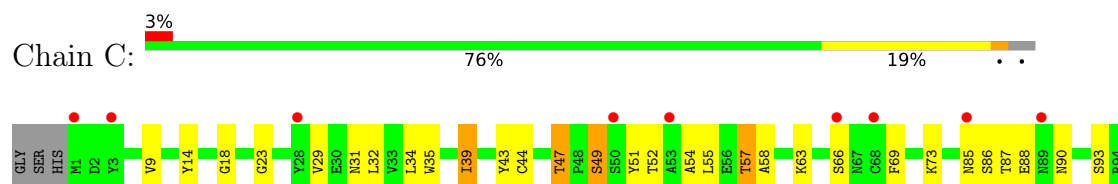
• Molecule 1: MccB protein

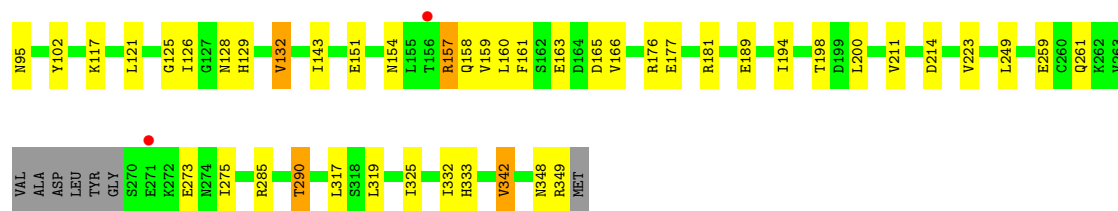


• Molecule 1: MccB protein

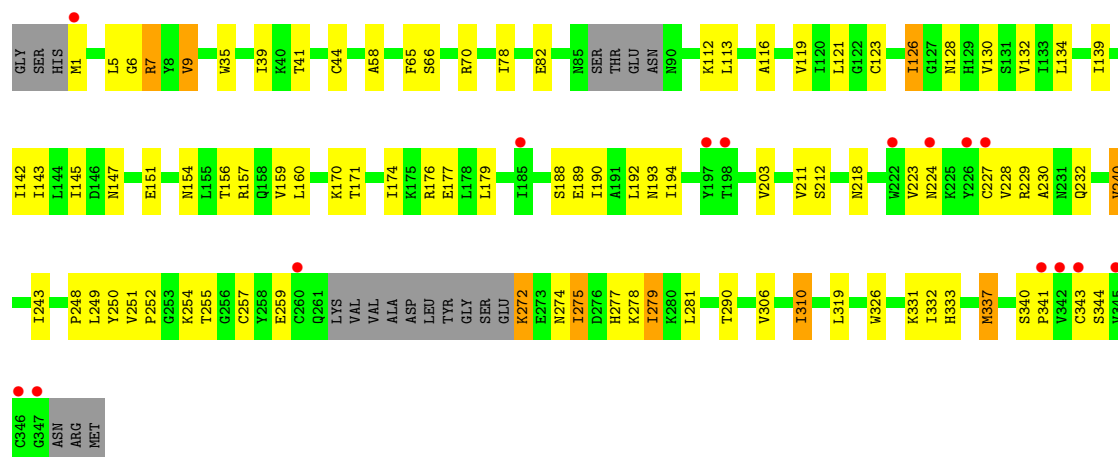


• Molecule 1: MccB protein





● Molecule 1: MccB protein



● Molecule 2: Microcin C7 analog



● Molecule 2: Microcin C7 analog



● Molecule 2: Microcin C7 analog



● Molecule 2: Microcin C7 analog



WT1	ARG
	THR
	GLY
	ASN
	ALA
	SNN

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	55.93Å 137.97Å 80.13Å 90.00° 92.10° 90.00°	Depositor
Resolution (Å)	27.95 – 2.10 27.95 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (27.95-2.10) 99.8 (27.95-2.10)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.35 (at 2.08Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.194 , 0.250 0.237 , 0.278	Depositor DCC
R_{free} test set	3598 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	37.6	Xtriage
Anisotropy	0.258	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 36.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.034 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10712	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.34% 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: ZN, SNN, SO4

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	0.84	1/2653 (0.0%)	1.04	3/3607 (0.1%)
1	B	0.87	0/2603	1.03	7/3540 (0.2%)
1	C	0.81	0/2675	0.95	0/3637
1	D	0.94	8/2598 (0.3%)	0.99	2/3534 (0.1%)
2	E	0.58	0/42	0.81	0/54
2	F	0.60	0/42	1.05	0/54
2	G	0.73	0/7	0.79	0/7
2	H	0.76	0/7	0.29	0/7
All	All	0.86	9/10627 (0.1%)	1.00	12/14440 (0.1%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	272	LYS	N-CA	11.77	1.68	1.46
1	D	250	TYR	C-N	11.15	1.45	1.33
1	D	229	ARG	C-N	8.17	1.44	1.33
1	D	250	TYR	C-O	7.62	1.33	1.24
1	D	230	ALA	CA-C	7.56	1.64	1.52
1	A	9	VAL	CA-CB	6.71	1.62	1.54
1	D	272	LYS	CA-CB	5.62	1.64	1.53
1	D	251	VAL	CA-C	-5.54	1.48	1.52
1	D	252	PRO	C-O	5.20	1.30	1.24

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	250	TYR	CA-C-N	-7.54	116.29	122.85
1	D	250	TYR	C-N-CA	-7.54	116.29	122.85
1	A	132	VAL	CB-CA-C	-6.59	103.13	112.22
1	B	249	LEU	N-CA-C	-6.24	97.54	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	93	SER	N-CA-C	6.13	118.75	111.33
1	A	332	ILE	CB-CA-C	-5.93	101.79	110.62
1	A	132	VAL	N-CA-CB	5.49	118.82	110.58
1	B	140	GLY	N-CA-C	5.35	119.61	112.77
1	B	251	VAL	CA-C-N	5.32	125.62	119.93
1	B	251	VAL	C-N-CA	5.32	125.62	119.93
1	B	9	VAL	N-CA-CB	5.10	117.24	110.26
1	B	95	ASN	N-CA-C	-5.08	105.93	111.82

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	2599	0	2526	45	0
1	B	2551	0	2480	37	0
1	C	2621	0	2551	59	0
1	D	2546	0	2471	72	0
2	E	51	0	42	3	0
2	F	51	0	42	9	0
2	G	8	0	8	0	0
2	H	8	0	8	5	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	B	5	0	0	0	0
4	C	5	0	0	0	0
5	A	82	0	0	11	0
5	B	70	0	0	7	0
5	C	69	0	0	10	0
5	D	38	0	0	2	0
5	E	1	0	0	0	0
5	F	3	0	0	0	0
All	All	10712	0	10128	193	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 9.

All (193) 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:272:LYS:N	1:D:272:LYS:CA	1.68	1.52
1:C:157:ARG:HD3	1:C:290:THR:HG23	1.31	1.09
1:D:333:HIS:HD2	2:H:71:MET:HE1	1.17	1.06
1:C:157:ARG:HD3	1:C:290:THR:CG2	1.85	1.04
1:A:181:ARG:CZ	5:A:402:HOH:O	2.11	0.97
1:D:333:HIS:CD2	2:H:71:MET:HE1	2.01	0.94
1:D:171:THR:CG2	1:D:189:GLU:HB3	2.00	0.92
1:A:332:ILE:HG13	1:B:332:ILE:HG13	1.52	0.90
1:D:248:PRO:HG3	1:D:337:MET:HE2	1.58	0.85
1:B:186:SER:HB2	5:D:364:HOH:O	1.76	0.84
1:D:157:ARG:NH2	5:D:385:HOH:O	2.11	0.84
1:D:171:THR:HG21	1:D:189:GLU:HB3	1.59	0.82
1:C:157:ARG:NH1	5:C:408:HOH:O	2.12	0.82
1:C:55:LEU:HA	5:C:392:HOH:O	1.79	0.80
1:A:285:ARG:HD3	1:B:46:ILE:HG23	1.61	0.79
1:B:214:ASP:HA	2:F:77:SNN:CA	2.12	0.78
1:C:177:GLU:OE1	1:C:181:ARG:NH2	2.18	0.76
1:A:290:THR:OG1	1:B:94:ARG:CB	2.35	0.75
1:A:159:VAL:O	1:B:181:ARG:NH1	2.20	0.74
1:A:248:PRO:HG3	1:A:337:MET:HE1	1.69	0.74
1:A:117:LYS:HE3	1:A:143:ILE:HD11	1.69	0.72
1:D:171:THR:HG22	1:D:189:GLU:OE1	1.90	0.72
1:C:47:THR:HB	5:C:364:HOH:O	1.89	0.72
1:C:157:ARG:HD3	1:C:290:THR:HG21	1.72	0.72
1:D:248:PRO:HG3	1:D:337:MET:CE	2.21	0.71
1:A:176:ARG:NH1	1:A:177:GLU:OE2	2.25	0.70
1:B:211:VAL:HG21	1:B:223:VAL:HG11	1.76	0.68
1:B:214:ASP:HA	2:F:77:SNN:N	2.08	0.68
1:C:157:ARG:NH2	5:C:362:HOH:O	2.27	0.67
1:C:157:ARG:CD	1:C:290:THR:HG23	2.18	0.67
1:C:58:ALA:HB3	5:C:392:HOH:O	1.94	0.67
1:D:132:VAL:HG11	1:D:160:LEU:HD21	1.76	0.67
1:C:285:ARG:HG2	1:D:7:ARG:HD2	1.77	0.66
1:D:113:LEU:HA	1:D:310:ILE:HD11	1.77	0.66
1:A:117:LYS:HE3	1:A:143:ILE:CD1	2.25	0.65
1:A:94:ARG:O	5:A:384:HOH:O	2.13	0.65
1:C:39:ILE:HD11	1:D:278:LYS:HB3	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:128:ASN:O	1:C:132:VAL:HG23	1.98	0.64
1:A:213:ALA:HB3	1:A:219:LEU:HD21	1.80	0.64
1:A:248:PRO:HG3	1:A:337:MET:CE	2.26	0.64
1:A:119:VAL:HG13	1:A:145:ILE:HD12	1.80	0.63
1:A:145:ILE:HG12	1:A:190:ILE:HB	1.81	0.63
1:A:211:VAL:HG21	1:A:223:VAL:HG11	1.81	0.62
1:D:333:HIS:HD2	2:H:71:MET:CE	2.04	0.62
1:C:333:HIS:NE2	5:C:400:HOH:O	2.19	0.62
1:D:272:LYS:N	1:D:272:LYS:C	2.56	0.62
1:C:132:VAL:HG22	1:C:160:LEU:HD11	1.83	0.61
1:A:258:TYR:HA	1:A:337:MET:HE1	1.82	0.61
1:D:227:CYS:HB3	1:D:232:GLN:O	2.01	0.60
1:D:147:ASN:HB3	1:D:193:ASN:ND2	2.16	0.60
1:D:248:PRO:CG	1:D:337:MET:HE2	2.31	0.60
1:B:213:ALA:HB3	1:B:219:LEU:HD22	1.85	0.58
1:C:332:ILE:HD11	1:D:332:ILE:HG13	1.85	0.58
1:D:6:GLY:O	1:D:9:VAL:HG13	2.04	0.57
1:A:181:ARG:NE	5:A:402:HOH:O	2.29	0.57
1:D:333:HIS:CD2	2:H:71:MET:CE	2.85	0.57
1:D:116:ALA:HB2	1:D:310:ILE:HD13	1.87	0.56
1:A:258:TYR:HA	1:A:337:MET:CE	2.36	0.56
1:C:158:GLN:HE21	1:C:161:PHE:HE2	1.54	0.56
1:B:84:ASN:O	1:B:85:ASN:C	2.49	0.56
1:A:114:LYS:HE3	5:A:406:HOH:O	2.06	0.56
5:B:389:HOH:O	2:F:76:ALA:HB2	2.06	0.55
1:A:70:ARG:NH1	5:A:422:HOH:O	2.39	0.55
5:B:389:HOH:O	2:F:76:ALA:CB	2.54	0.55
1:D:151:GLU:H	1:D:154:ASN:ND2	2.04	0.55
1:C:165:ASP:OD1	1:C:176:ARG:NH2	2.39	0.55
1:A:181:ARG:HD3	5:B:395:HOH:O	2.07	0.55
1:C:342:VAL:O	1:C:342:VAL:HG13	2.07	0.54
1:C:177:GLU:HB3	1:C:181:ARG:HH21	1.72	0.54
1:D:275:ILE:O	1:D:279:ILE:HG23	2.07	0.54
1:B:26:GLU:OE1	2:E:72:ARG:HB2	2.07	0.54
1:C:58:ALA:CB	5:C:392:HOH:O	2.54	0.54
1:A:35:TRP:CZ2	1:A:39:ILE:HD11	2.43	0.54
1:B:214:ASP:N	2:F:77:SNN:C4	2.71	0.54
1:B:6:GLY:O	1:B:9:VAL:HG13	2.08	0.54
1:C:102:TYR:OH	5:C:388:HOH:O	2.18	0.54
1:C:342:VAL:O	1:C:342:VAL:CG1	2.55	0.53
1:A:181:ARG:HH11	1:A:181:ARG:HG2	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:326:TRP:CZ2	1:D:331:LYS:HE2	2.44	0.53
1:C:151:GLU:H	1:C:154:ASN:ND2	2.07	0.52
1:A:181:ARG:NH2	5:A:402:HOH:O	2.35	0.52
1:D:113:LEU:HD23	1:D:310:ILE:CG1	2.40	0.52
1:C:39:ILE:HD11	1:D:278:LYS:CB	2.39	0.52
1:D:211:VAL:HG21	1:D:223:VAL:HG11	1.90	0.52
1:B:214:ASP:HA	2:F:77:SNM:C4	2.39	0.52
1:D:171:THR:CG2	1:D:189:GLU:CB	2.83	0.52
1:A:111:ASP:CB	5:A:396:HOH:O	2.58	0.52
1:C:163:GLU:O	1:C:166:VAL:HG12	2.10	0.52
1:D:113:LEU:HD23	1:D:310:ILE:HG13	1.91	0.51
1:D:310:ILE:HD12	1:D:310:ILE:O	2.10	0.51
1:C:211:VAL:HG21	1:C:223:VAL:HG11	1.92	0.50
1:C:158:GLN:NE2	1:C:161:PHE:HE2	2.10	0.50
1:A:180:LYS:HB3	1:B:162:SER:OG	2.12	0.50
1:C:194:ILE:HD12	1:C:194:ILE:N	2.26	0.50
1:D:134:LEU:HB3	1:D:139:ILE:HG13	1.94	0.50
1:A:279:ILE:HG13	1:B:39:ILE:CD1	2.43	0.49
5:B:378:HOH:O	2:E:71:MET:N	2.46	0.49
1:C:44:CYS:SG	1:C:58:ALA:HB2	2.51	0.49
1:D:171:THR:HG22	1:D:189:GLU:HB3	1.91	0.49
1:A:279:ILE:HG23	1:B:11:ILE:HG22	1.95	0.48
1:D:145:ILE:CD1	1:D:203:VAL:HG13	2.44	0.48
1:D:145:ILE:HG12	1:D:190:ILE:HB	1.94	0.48
1:C:121:LEU:HD11	1:C:194:ILE:HD13	1.95	0.48
1:A:95:ASN:O	1:A:98:HIS:HB3	2.13	0.48
1:D:132:VAL:CG1	1:D:160:LEU:HD21	2.42	0.48
1:C:117:LYS:HE3	1:C:143:ILE:HD11	1.94	0.48
1:A:143:ILE:HD12	1:A:143:ILE:N	2.29	0.47
5:A:431:HOH:O	1:B:154:ASN:HA	2.13	0.47
1:A:94:ARG:NH2	5:A:431:HOH:O	2.32	0.47
1:B:201:HIS:HB3	1:C:261:GLN:OE1	2.15	0.47
1:C:285:ARG:O	1:D:7:ARG:HG3	2.14	0.47
1:A:177:GLU:O	1:A:181:ARG:HG3	2.14	0.47
1:B:295:ASN:ND2	5:B:390:HOH:O	2.47	0.47
1:D:119:VAL:HG13	1:D:145:ILE:HD12	1.96	0.46
1:D:126:ILE:O	1:D:130:VAL:HG23	2.14	0.46
1:D:274:ASN:HA	1:D:277:HIS:HD2	1.81	0.46
5:C:357:HOH:O	1:D:156:THR:HG22	2.16	0.46
1:A:133:ILE:HD11	1:B:296:ASN:HD22	1.80	0.46
1:D:194:ILE:HD12	1:D:194:ILE:N	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:CYS:HB3	1:A:174:ILE:HD12	1.98	0.46
1:D:176:ARG:NH1	1:D:177:GLU:OE2	2.48	0.46
1:D:44:CYS:SG	1:D:58:ALA:HB2	2.55	0.46
1:C:129:HIS:CE1	1:C:159:VAL:HB	2.51	0.46
1:A:133:ILE:HD11	1:B:296:ASN:ND2	2.31	0.45
1:D:143:ILE:HD12	1:D:143:ILE:N	2.31	0.45
1:C:31:ASN:HD22	1:C:34:LEU:HB2	1.81	0.45
1:C:51:TYR:HH	1:C:66:SER:HG	1.64	0.45
1:D:41:THR:HG23	1:D:65:PHE:CE1	2.52	0.44
1:D:123:CYS:HB3	1:D:174:ILE:HD12	1.98	0.44
1:B:125:GLY:HA3	1:B:295:ASN:HD21	1.81	0.44
1:D:340:SER:HA	1:D:341:PRO:HD2	1.86	0.44
1:B:13:ARG:HD3	1:B:17:GLY:O	2.18	0.44
1:A:36:GLU:O	1:A:40:LYS:HG3	2.18	0.44
5:A:421:HOH:O	1:B:285:ARG:HD3	2.17	0.44
1:D:66:SER:O	1:D:70:ARG:HG3	2.18	0.44
1:D:255:THR:HG21	1:D:319:LEU:HD22	2.00	0.44
1:D:337:MET:HE3	1:D:337:MET:HB3	1.83	0.44
1:C:86:SER:C	1:C:88:GLU:H	2.26	0.44
1:D:112:LYS:C	1:D:310:ILE:HD11	2.43	0.44
1:D:143:ILE:HG13	1:D:188:SER:HB2	2.00	0.44
1:C:49:SER:HB2	1:C:54:ALA:HB2	1.98	0.43
1:C:121:LEU:HD11	1:C:194:ILE:CD1	2.48	0.43
1:C:95:ASN:ND2	1:D:156:THR:HG21	2.34	0.43
1:C:43:TYR:CE1	1:D:281:LEU:HD23	2.53	0.43
1:A:132:VAL:HG11	1:A:160:LEU:HD21	2.01	0.43
1:B:44:CYS:SG	1:B:58:ALA:HB2	2.57	0.43
1:A:94:ARG:HG2	1:B:153:THR:OG1	2.18	0.43
1:C:125:GLY:HA2	1:C:158:GLN:HG2	2.01	0.43
1:D:154:ASN:ND2	1:D:170:LYS:HE2	2.33	0.43
1:D:240:VAL:HG21	2:H:71:MET:HA	2.01	0.43
1:C:29:VAL:HG13	1:C:35:TRP:HB2	2.01	0.43
1:C:348:ASN:O	1:C:349:ARG:CB	2.67	0.43
1:D:121:LEU:HD11	1:D:194:ILE:HD11	2.00	0.43
1:D:224:ASN:O	1:D:228:VAL:HG23	2.19	0.43
1:B:19:LEU:HD11	2:E:72:ARG:HB3	2.01	0.43
1:C:23:GLY:HA2	1:D:243:ILE:HD12	2.00	0.42
1:C:35:TRP:O	1:C:39:ILE:HG23	2.19	0.42
1:C:69:PHE:CE2	1:C:73:LYS:HD2	2.54	0.42
1:C:90:ASN:O	1:C:93:SER:OG	2.35	0.42
1:C:332:ILE:CD1	1:D:332:ILE:HG13	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:310:ILE:HD12	1:D:310:ILE:C	2.43	0.42
1:B:342:VAL:O	1:B:342:VAL:CG2	2.67	0.42
1:A:285:ARG:HD2	5:B:352:HOH:O	2.17	0.42
1:A:285:ARG:CD	1:B:46:ILE:HG23	2.42	0.42
1:B:326:TRP:CH2	2:F:71:MET:HG3	2.54	0.42
1:B:214:ASP:CA	2:F:77:SNN:C4	2.97	0.42
1:B:332:ILE:HD13	1:B:332:ILE:HG21	1.68	0.42
1:D:5:LEU:HA	1:D:78:ILE:HG22	2.00	0.42
1:A:93:SER:O	1:A:94:ARG:C	2.63	0.42
1:A:94:ARG:NH1	5:A:370:HOH:O	2.51	0.42
1:C:14:TYR:H	1:C:18:GLY:HA2	1.84	0.42
1:A:128:ASN:O	1:A:132:VAL:HG22	2.20	0.42
1:C:52:THR:HA	1:C:55:LEU:HB3	2.02	0.41
1:A:123:CYS:HB3	1:A:174:ILE:CD1	2.50	0.41
1:A:160:LEU:O	1:A:177:GLU:HG3	2.20	0.41
1:B:248:PRO:HD3	1:B:337:MET:HE2	2.00	0.41
1:D:151:GLU:O	1:D:154:ASN:HB2	2.20	0.41
5:B:389:HOH:O	2:F:76:ALA:HB3	2.20	0.41
1:C:43:TYR:HE1	1:D:281:LEU:HD23	1.86	0.41
1:C:39:ILE:CD1	1:D:278:LYS:HB3	2.48	0.41
1:C:86:SER:O	1:C:88:GLU:N	2.54	0.41
1:D:274:ASN:HA	1:D:277:HIS:CD2	2.56	0.41
1:D:306:VAL:O	1:D:310:ILE:HG23	2.20	0.41
1:B:35:TRP:O	1:B:39:ILE:HG23	2.21	0.41
1:C:63:LYS:CB	5:C:386:HOH:O	2.68	0.41
1:D:35:TRP:CZ2	1:D:39:ILE:HD11	2.56	0.41
1:D:340:SER:HB3	1:D:343:CYS:HB2	2.01	0.41
1:C:55:LEU:C	1:C:57:THR:H	2.28	0.40
1:B:100:GLN:HG3	1:B:106:PRO:HG3	2.03	0.40
1:B:319:LEU:O	1:B:320:ASN:HB2	2.20	0.40
1:C:181:ARG:NH1	1:D:159:VAL:O	2.55	0.40
1:C:194:ILE:HG12	1:C:200:LEU:HD23	2.04	0.40
1:D:78:ILE:O	1:D:78:ILE:HG13	2.20	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	336/353 (95%)	325 (97%)	11 (3%)	0	100	100
1	B	328/353 (93%)	318 (97%)	10 (3%)	0	100	100
1	C	339/353 (96%)	329 (97%)	10 (3%)	0	100	100
1	D	327/353 (93%)	317 (97%)	10 (3%)	0	100	100
2	E	5/7 (71%)	5 (100%)	0	0	100	100
2	F	5/7 (71%)	5 (100%)	0	0	100	100
All	All	1340/1426 (94%)	1299 (97%)	41 (3%)	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	272/304 (90%)	255 (94%)	17 (6%)	16	14
1	B	269/304 (88%)	252 (94%)	17 (6%)	16	14
1	C	277/304 (91%)	254 (92%)	23 (8%)	10	8
1	D	268/304 (88%)	246 (92%)	22 (8%)	10	8
2	E	4/4 (100%)	3 (75%)	1 (25%)	0	0
2	F	4/4 (100%)	3 (75%)	1 (25%)	0	0
2	G	1/4 (25%)	1 (100%)	0	100	100
2	H	1/4 (25%)	1 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1096/1232 (89%)	1015 (93%)	81 (7%)	13	10

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	9	VAL
1	A	11	ILE
1	A	29	VAL
1	A	56	GLU
1	A	132	VAL
1	A	189	GLU
1	A	220	ILE
1	A	249	LEU
1	A	259	GLU
1	A	260	CYS
1	A	275	ILE
1	A	285	ARG
1	A	317	LEU
1	A	319	LEU
1	A	332	ILE
1	A	342	VAL
1	B	9	VAL
1	B	11	ILE
1	B	39	ILE
1	B	57	THR
1	B	149	GLN
1	B	162	SER
1	B	179	LEU
1	B	188	SER
1	B	192	LEU
1	B	198	THR
1	B	220	ILE
1	B	249	LEU
1	B	275	ILE
1	B	276	ASP
1	B	287	LYS
1	B	342	VAL
1	B	344	SER
1	C	9	VAL
1	C	32	LEU
1	C	39	ILE

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Mol	Chain	Res	Type
1	C	47	THR
1	C	49	SER
1	C	57	THR
1	C	85	ASN
1	C	87	THR
1	C	126	ILE
1	C	132	VAL
1	C	157	ARG
1	C	189	GLU
1	C	198	THR
1	C	214	ASP
1	C	249	LEU
1	C	259	GLU
1	C	273	GLU
1	C	275	ILE
1	C	290	THR
1	C	317	LEU
1	C	319	LEU
1	C	325	ILE
1	C	342	VAL
1	D	1	MET
1	D	7	ARG
1	D	9	VAL
1	D	82	GLU
1	D	126	ILE
1	D	128	ASN
1	D	142	ILE
1	D	179	LEU
1	D	192	LEU
1	D	212	SER
1	D	218	ASN
1	D	240	VAL
1	D	249	LEU
1	D	254	LYS
1	D	257	CYS
1	D	259	GLU
1	D	275	ILE
1	D	279	ILE
1	D	290	THR
1	D	310	ILE
1	D	337	MET
1	D	344	SER

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Mol	Chain	Res	Type
2	E	71	MET
2	F	71	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	95	ASN
1	A	295	ASN
1	A	296	ASN
1	B	295	ASN
1	C	27	GLN
1	C	31	ASN
1	C	59	ASN
1	C	75	ASN
1	C	110	GLN
1	C	129	HIS
1	C	154	ASN
1	C	236	ASN
1	D	95	ASN
1	D	110	GLN
1	D	154	ASN
1	D	277	HIS
1	D	333	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SNN	F	77	2	7,8,8	1.60	2 (28%)	10,11,11	2.38	5 (50%)
2	SNN	E	77	2	7,8,8	1.59	2 (28%)	10,11,11	2.38	5 (50%)

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
2	SNN	F	77	2	-	-	0/1/1/1
2	SNN	E	77	2	-	-	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	77	SNN	C-N1	-3.51	1.33	1.37
2	E	77	SNN	C-N1	-3.48	1.33	1.37
2	F	77	SNN	C5-N1	-2.24	1.33	1.37
2	E	77	SNN	C5-N1	-2.21	1.33	1.37

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	77	SNN	CA-C-N1	4.39	110.75	107.30
2	F	77	SNN	CA-C-N1	4.38	110.74	107.30
2	E	77	SNN	O-C-CA	-3.29	123.82	126.19
2	F	77	SNN	O-C-CA	-3.26	123.84	126.19
2	F	77	SNN	O5-C5-C4	-3.11	122.51	126.48
2	E	77	SNN	O5-C5-C4	-3.10	122.53	126.48
2	E	77	SNN	C4-C5-N1	2.94	111.51	108.02
2	F	77	SNN	C4-C5-N1	2.93	111.50	108.02
2	E	77	SNN	C5-N1-C	-2.30	111.65	113.96
2	F	77	SNN	C5-N1-C	-2.27	111.68	113.96

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	77	SNN	5	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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	SO4	B	351	-	4,4,4	0.28	0	6,6,6	0.46	0
4	SO4	C	351	-	4,4,4	0.28	0	6,6,6	0.21	0

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.

5.7 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	340/353 (96%)	0.76	22 (6%) 25 26	31, 43, 60, 68	0
1	B	334/353 (94%)	0.81	19 (5%) 29 31	33, 44, 57, 71	0
1	C	343/353 (97%)	0.67	11 (3%) 50 53	28, 43, 58, 69	0
1	D	333/353 (94%)	0.76	15 (4%) 38 40	24, 44, 56, 65	0
2	E	6/7 (85%)	2.01	4 (66%) 0 0	62, 63, 65, 67	0
2	F	6/7 (85%)	1.96	3 (50%) 0 0	70, 74, 77, 80	0
2	G	1/7 (14%)	2.77	1 (100%) 0 0	82, 82, 82, 82	0
2	H	1/7 (14%)	1.56	0 100 100	83, 83, 83, 83	0
All	All	1364/1440 (94%)	0.77	75 (5%) 30 32	24, 44, 60, 83	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	347	GLY	4.1
1	D	341	PRO	3.9
1	A	195	ASN	3.4
1	A	87	THR	3.2
1	A	218	ASN	3.1
1	D	226	TYR	3.0
1	D	345	VAL	3.0
2	E	73	THR	3.0
2	F	71	MET	2.9
1	A	348	ASN	2.8
1	A	13	ARG	2.8
2	G	71	MET	2.8
1	D	227	CYS	2.7
1	B	93	SER	2.7
1	A	15	GLY	2.7
1	A	259	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	342	VAL	2.7
1	A	222	TRP	2.7
1	C	68	CYS	2.6
1	A	277	HIS	2.6
2	E	75	ASN	2.6
1	C	85	ASN	2.6
1	C	89	ASN	2.6
2	E	76	ALA	2.6
1	A	86	SER	2.6
1	B	184	GLU	2.5
1	A	213	ALA	2.5
1	B	57	THR	2.5
1	C	28	TYR	2.5
1	B	195	ASN	2.5
1	D	224	ASN	2.5
2	F	73	THR	2.5
1	A	14	TYR	2.4
1	D	260	CYS	2.4
1	D	347	GLY	2.4
1	A	193	ASN	2.4
1	C	1	MET	2.4
1	C	156	THR	2.4
1	D	198	THR	2.4
1	B	56	GLU	2.4
1	B	94	ARG	2.3
1	C	271	GLU	2.3
1	C	3	TYR	2.3
1	B	332	ILE	2.3
1	A	154	ASN	2.3
1	B	344	SER	2.3
1	B	55	LEU	2.3
1	B	307	ILE	2.2
1	A	96	PHE	2.2
1	A	347	GLY	2.2
1	B	58	ALA	2.2
1	B	275	ILE	2.2
1	A	21	GLY	2.2
1	C	66	SER	2.2
1	B	84	ASN	2.2
1	A	29	VAL	2.1
1	B	213	ALA	2.1
1	D	185	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	89	ASN	2.1
1	B	189	GLU	2.1
1	B	198	THR	2.1
1	B	91	ARG	2.1
2	F	76	ALA	2.1
1	B	197	TYR	2.1
1	C	50	SER	2.1
1	D	1	MET	2.0
2	E	71	MET	2.0
1	A	305	ASP	2.0
1	D	346	CYS	2.0
1	A	215	HIS	2.0
1	C	53	ALA	2.0
1	D	222	TRP	2.0
1	A	196	ASP	2.0
1	D	343	CYS	2.0
1	D	197	TYR	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	SNN	F	77	8/8	0.67	0.15	63,65,67,68	0
2	SNN	E	77	8/8	0.68	0.17	63,65,65,67	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($\text{\AA}^2$)	Q<0.9
4	SO4	C	351	5/5	0.77	0.09	85,85,85,85	0
4	SO4	B	351	5/5	0.85	0.09	66,67,68,69	0
3	ZN	D	500	1/1	0.94	0.05	71,71,71,71	0
3	ZN	A	500	1/1	0.99	0.03	50,50,50,50	0
3	ZN	B	500	1/1	0.99	0.03	45,45,45,45	0
3	ZN	C	500	1/1	0.99	0.02	37,37,37,37	0

6.5 Other polymers [i](#)

There are no such residues in this entry.