



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 05:56 AM UTC

PDB ID : 5ODW / pdb_00005odw
Title : Structure of the FpvAI-pyocin S2 complex
Authors : White, P.; Joshi, A.; Kleanthous, C.
Deposited on : 2017-07-06
Resolution : 2.80 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

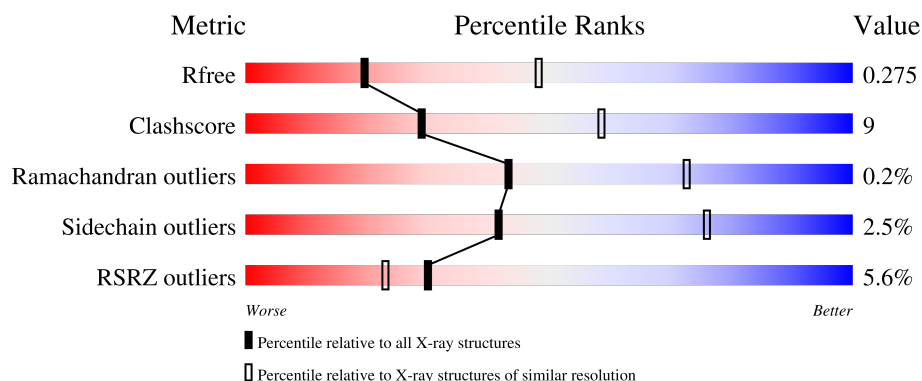
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	815	
1	B	815	
2	C	217	
2	D	217	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 15094 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 Ferripyoverdine receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	771	Total	C	N	O	S	0	0	0
			6105	3840	1044	1209	12			
1	B	740	Total	C	N	O	S	0	0	0
			5874	3696	1008	1158	12			

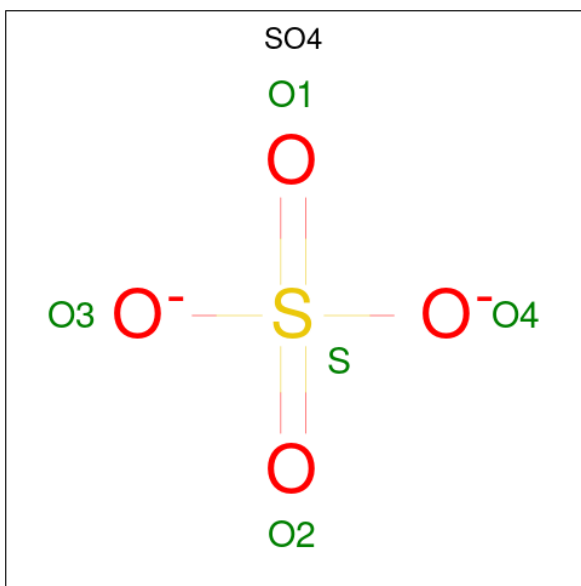
- Molecule 2 is a protein called Pyocin-S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	195	Total	C	N	O	S	0	0	0
			1520	950	264	301	5			
2	D	198	Total	C	N	O	S	0	0	0
			1545	966	267	307	5			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	210	LEU	-	expression tag	UNP Q06584
C	211	GLU	-	expression tag	UNP Q06584
C	212	HIS	-	expression tag	UNP Q06584
C	213	HIS	-	expression tag	UNP Q06584
C	214	HIS	-	expression tag	UNP Q06584
C	215	HIS	-	expression tag	UNP Q06584
C	216	HIS	-	expression tag	UNP Q06584
C	217	HIS	-	expression tag	UNP Q06584
D	210	LEU	-	expression tag	UNP Q06584
D	211	GLU	-	expression tag	UNP Q06584
D	212	HIS	-	expression tag	UNP Q06584
D	213	HIS	-	expression tag	UNP Q06584
D	214	HIS	-	expression tag	UNP Q06584
D	215	HIS	-	expression tag	UNP Q06584
D	216	HIS	-	expression tag	UNP Q06584
D	217	HIS	-	expression tag	UNP Q06584

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).

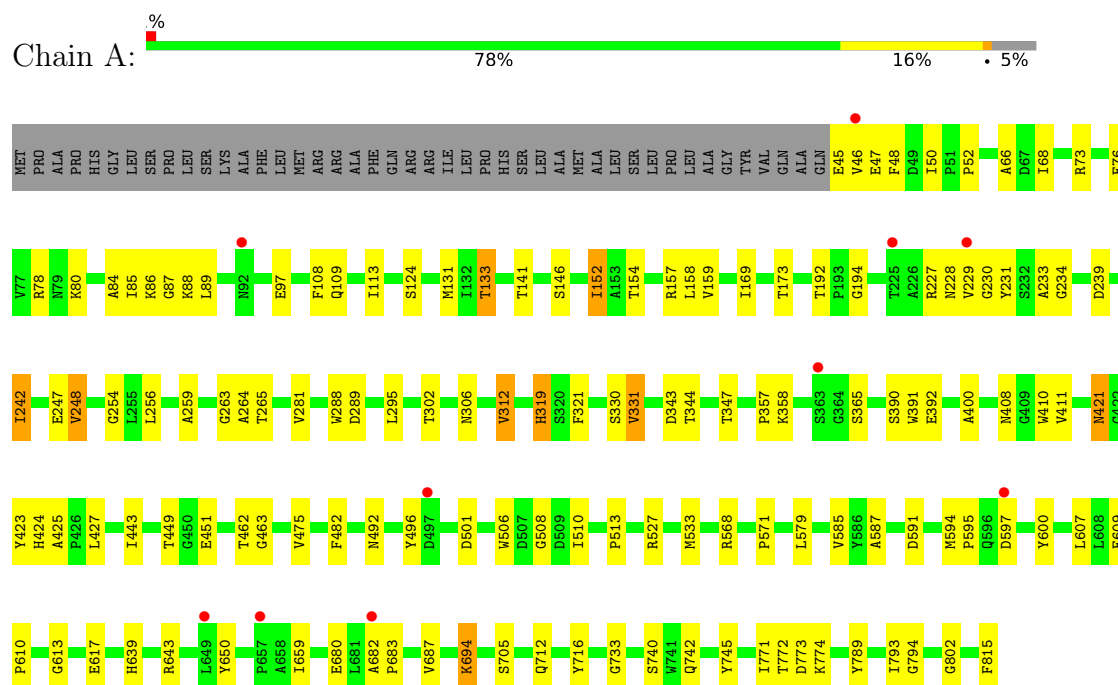


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

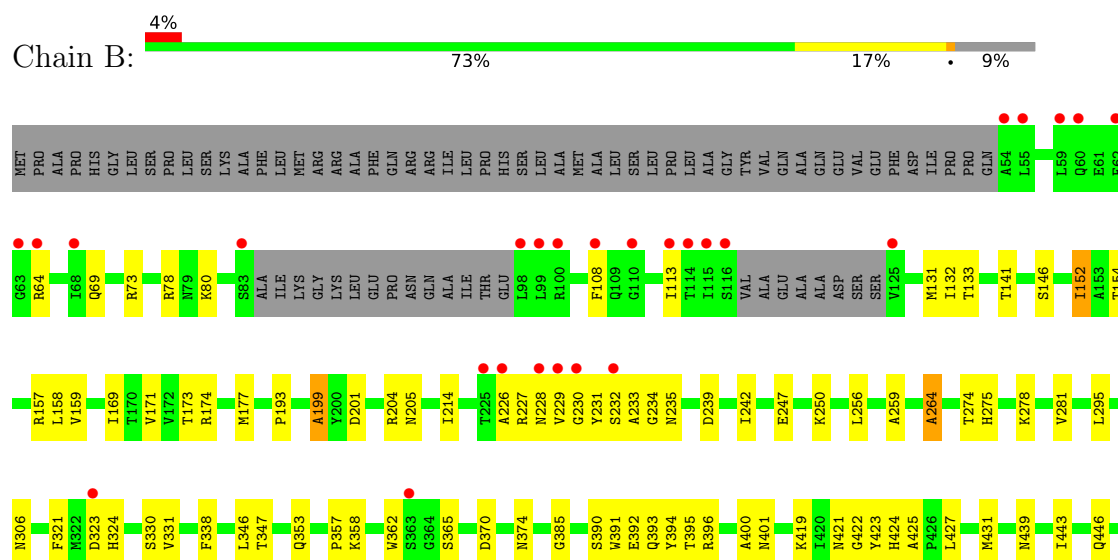
3 Residue-property plots

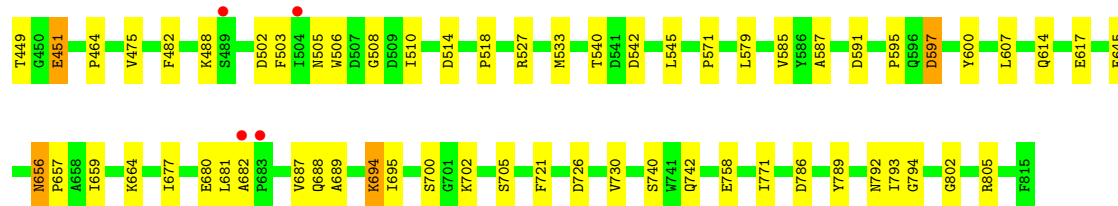
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Ferripyoverdine receptor

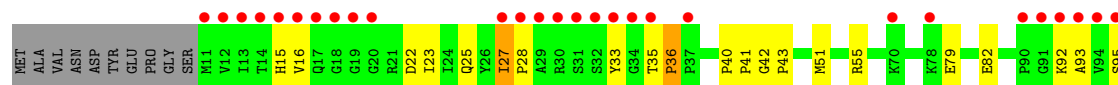


• Molecule 1: Ferripyoverdine receptor

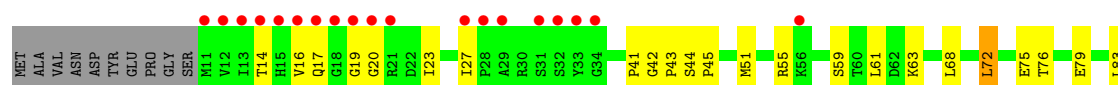




● Molecule 2: Pyocin-S2



● Molecule 2: Pyocin-S2



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	115.52Å 209.39Å 215.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.97 – 2.80 47.97 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.5 (47.97-2.80) 98.5 (47.97-2.80)	Depositor EDS
R_{merge}	0.35	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.61 (at 2.81Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.212 , 0.262 0.228 , 0.275	Depositor DCC
R_{free} test set	3094 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	36.4	Xtriage
Anisotropy	0.603	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 49.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.018 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	15094	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.89% 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: 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	0.80	0/6257	1.19	15/8502 (0.2%)
1	B	0.77	0/6020	1.18	14/8175 (0.2%)
2	C	0.79	0/1545	1.45	15/2079 (0.7%)
2	D	0.77	0/1571	1.45	16/2115 (0.8%)
All	All	0.78	0/15393	1.24	60/20871 (0.3%)

There are no bond length outliers.

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	228	ASN	N-CA-C	-7.71	98.39	109.96
2	D	137	SER	N-CA-C	7.33	119.28	111.28
1	A	146	SER	N-CA-C	7.15	120.20	110.55
1	A	254	GLY	N-CA-C	7.10	121.49	112.83
1	B	321	PHE	N-CA-C	-6.90	104.33	112.89
1	B	656	ASN	CA-C-N	6.88	126.69	119.05
1	B	656	ASN	C-N-CA	6.88	126.69	119.05
1	B	146	SER	N-CA-C	6.85	119.80	110.55
1	A	321	PHE	N-CA-C	-6.84	104.40	112.89
1	A	78	ARG	N-CA-C	6.77	118.66	111.28
1	B	78	ARG	N-CA-C	6.45	118.31	111.28
2	D	94	VAL	N-CA-C	6.35	117.02	111.56
2	C	51	MET	CA-C-N	6.21	128.60	120.28
2	C	51	MET	C-N-CA	6.21	128.60	120.28
1	B	264	ALA	N-CA-C	6.09	117.48	108.60
1	B	199	ALA	N-CA-C	6.01	118.70	108.90
1	A	365	SER	N-CA-C	-6.00	106.57	114.31
2	D	51	MET	CA-C-N	5.92	128.22	120.28
2	D	51	MET	C-N-CA	5.92	128.22	120.28
1	B	514	ASP	N-CA-C	-5.89	98.93	108.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	72	LEU	N-CA-C	5.89	117.70	111.28
2	D	19	GLY	N-CA-C	5.84	119.74	112.73
2	C	96	ALA	CA-C-N	5.81	128.07	120.28
2	C	96	ALA	C-N-CA	5.81	128.07	120.28
1	A	771	ILE	N-CA-C	5.80	115.99	110.42
2	D	75	GLU	N-CA-C	5.79	117.39	111.14
2	D	20	GLY	N-CA-C	5.65	119.51	112.73
1	B	794	GLY	N-CA-C	5.64	123.43	115.30
2	D	101	ASP	CA-C-N	5.58	127.75	120.28
2	D	101	ASP	C-N-CA	5.58	127.75	120.28
2	C	197	ALA	CA-C-N	5.51	127.93	120.65
2	C	197	ALA	C-N-CA	5.51	127.93	120.65
1	B	385	GLY	N-CA-C	5.49	118.24	111.93
1	B	365	SER	N-CA-C	-5.48	108.37	114.62
1	A	794	GLY	N-CA-C	5.40	123.08	115.30
1	A	97	GLU	CA-C-N	5.36	127.46	120.28
1	A	97	GLU	C-N-CA	5.36	127.46	120.28
2	D	55	ARG	CA-C-N	5.33	127.36	120.44
2	D	55	ARG	C-N-CA	5.33	127.36	120.44
2	C	105	ILE	CA-C-N	5.29	127.23	120.56
2	C	105	ILE	C-N-CA	5.29	127.23	120.56
1	A	705	SER	CA-C-N	5.25	127.84	120.28
1	A	705	SER	C-N-CA	5.25	127.84	120.28
2	C	199	ARG	CA-C-N	5.21	127.25	120.28
2	C	199	ARG	C-N-CA	5.21	127.25	120.28
2	D	68	LEU	CA-C-N	5.20	127.50	120.38
2	D	68	LEU	C-N-CA	5.20	127.50	120.38
1	A	87	GLY	N-CA-C	5.15	118.03	111.85
2	C	79	GLU	CA-C-N	5.12	127.01	120.56
2	C	79	GLU	C-N-CA	5.12	127.01	120.56
1	A	228	ASN	N-CA-C	-5.10	102.73	110.28
1	A	319	HIS	N-CA-C	-5.10	102.35	109.69
1	A	687	VAL	N-CA-C	5.09	116.33	108.44
2	D	172	TYR	CA-C-N	5.07	127.03	120.44
2	D	172	TYR	C-N-CA	5.07	127.03	120.44
1	B	705	SER	CA-C-N	5.05	127.56	120.28
1	B	705	SER	C-N-CA	5.05	127.56	120.28
2	C	101	ASP	CA-C-N	5.02	127.01	120.28
2	C	101	ASP	C-N-CA	5.02	127.01	120.28
2	C	164	ALA	N-CA-C	-5.00	105.74	111.14

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	6105	0	5780	95	0
1	B	5874	0	5555	115	0
2	C	1520	0	1525	35	0
2	D	1545	0	1542	31	0
3	A	25	0	0	0	0
3	B	25	0	0	0	0
All	All	15094	0	14402	257	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 (257) 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:A:306:ASN:HD21	1:B:306:ASN:ND2	1.00	1.48
1:A:306:ASN:ND2	1:B:306:ASN:HD21	0.98	1.45
1:B:227:ARG:NH2	1:B:234:GLY:H	1.22	1.33
2:D:95:SER:OG	2:D:98:ASP:OD2	1.53	1.26
1:A:742:GLN:NE2	1:A:793:ILE:O	1.65	1.26
2:D:89:LEU:HD12	2:D:105:ILE:HD11	1.21	1.17
1:A:227:ARG:NH1	1:A:234:GLY:H	1.43	1.16
1:A:227:ARG:HH12	1:A:234:GLY:N	1.46	1.11
1:B:227:ARG:NH2	1:B:234:GLY:N	1.96	1.11
1:B:227:ARG:HH12	1:B:235:ASN:HB2	1.18	1.04
1:A:462:THR:HG22	1:A:475:VAL:HG22	1.40	1.00
2:D:72:LEU:O	2:D:76:THR:HG22	1.61	0.99
1:A:194:GLY:HA2	1:A:712:GLN:HE21	1.26	0.99
1:B:230:GLY:HA3	2:D:43:PRO:CD	1.92	0.99
1:A:76:GLU:O	1:A:80:LYS:NZ	1.98	0.96
1:B:227:ARG:HH21	1:B:234:GLY:H	1.02	0.96
1:B:230:GLY:HA3	2:D:43:PRO:HD3	1.49	0.95
1:A:774:LYS:H	1:A:774:LYS:HD2	1.35	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:ARG:HH12	1:A:234:GLY:H	0.92	0.89
1:A:194:GLY:HA2	1:A:712:GLN:NE2	1.87	0.89
1:B:227:ARG:NH1	1:B:235:ASN:HB2	1.86	0.89
1:B:227:ARG:HH22	1:B:235:ASN:H	1.24	0.85
1:A:229:VAL:HB	2:C:41:PRO:HB2	1.58	0.84
1:B:227:ARG:HH22	1:B:234:GLY:N	1.67	0.83
2:D:89:LEU:HD12	2:D:105:ILE:CD1	2.06	0.83
1:A:694:LYS:HD3	1:A:694:LYS:O	1.80	0.81
1:B:193:PRO:O	1:B:250:LYS:NZ	2.14	0.81
2:C:133:PHE:CE2	2:C:163:LEU:CD2	2.65	0.80
1:B:227:ARG:HH22	1:B:234:GLY:H	1.16	0.79
1:B:742:GLN:OE1	1:B:793:ILE:O	2.00	0.79
1:A:597:ASP:HB2	1:A:600:TYR:HD1	1.48	0.79
1:B:230:GLY:HA3	2:D:43:PRO:HD2	1.66	0.78
2:D:99:ILE:HD11	2:D:190:ALA:HA	1.66	0.77
2:D:89:LEU:CD1	2:D:105:ILE:HD11	2.08	0.77
1:A:227:ARG:NH1	1:A:233:ALA:H	1.84	0.75
1:A:50:ILE:HD12	1:A:85:ILE:HD11	1.69	0.75
1:A:774:LYS:HD2	1:A:774:LYS:N	2.02	0.74
2:D:204:VAL:O	2:D:208:TYR:HD2	1.70	0.74
1:B:227:ARG:HH12	1:B:235:ASN:CB	1.99	0.73
1:B:227:ARG:HH22	1:B:235:ASN:N	1.86	0.73
1:A:680:GLU:HG3	1:A:682:ALA:O	1.89	0.73
2:C:133:PHE:CE2	2:C:163:LEU:HD23	2.23	0.73
1:B:540:THR:HG22	1:B:542:ASP:H	1.53	0.73
1:A:194:GLY:CA	1:A:712:GLN:NE2	2.52	0.72
1:A:600:TYR:O	1:A:607:LEU:HD12	1.90	0.71
2:C:27:ILE:HD12	2:C:27:ILE:N	2.05	0.71
1:B:645:GLU:OE1	1:B:664:LYS:HD3	1.90	0.71
1:B:227:ARG:HE	1:B:232:SER:HA	1.54	0.71
1:B:233:ALA:HB1	1:B:421:ASN:HB3	1.74	0.69
1:B:680:GLU:HG3	1:B:682:ALA:O	1.92	0.68
1:A:230:GLY:HA3	2:C:42:GLY:HA3	1.75	0.68
1:A:597:ASP:HB2	1:A:600:TYR:CD1	2.29	0.68
2:C:132:ASP:OD1	2:C:135:GLN:HB2	1.94	0.67
1:B:199:ALA:HB2	1:B:205:ASN:OD1	1.93	0.67
1:A:66:ALA:HB3	1:A:68:ILE:HG22	1.76	0.66
1:B:227:ARG:NH2	1:B:235:ASN:H	1.94	0.65
1:A:306:ASN:ND2	1:B:306:ASN:ND2	1.81	0.64
2:D:79:GLU:O	2:D:83:LEU:HG	1.97	0.64
1:A:152:ILE:HD13	1:A:169:ILE:HG12	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:ARG:HG3	1:B:131:MET:HE3	1.79	0.64
1:A:73:ARG:HG3	1:A:131:MET:HE3	1.79	0.64
1:B:152:ILE:HD13	1:B:169:ILE:HG12	1.80	0.64
1:B:227:ARG:HH21	1:B:233:ALA:N	1.95	0.63
1:B:597:ASP:HB2	1:B:600:TYR:HD1	1.64	0.63
1:B:681:LEU:HD11	1:B:687:VAL:HG21	1.80	0.62
1:A:52:PRO:HG3	1:A:84:ALA:HB2	1.80	0.62
1:A:694:LYS:HD3	1:A:694:LYS:C	2.23	0.62
1:A:680:GLU:CG	1:A:682:ALA:O	2.48	0.61
1:B:700:SER:OG	1:B:702:LYS:HG2	2.00	0.61
2:C:184:GLN:O	2:C:187:GLU:HG2	2.00	0.61
1:B:347:THR:HB	1:B:401:ASN:HB2	1.82	0.60
1:B:201:ASP:OD1	1:B:204:ARG:HB2	2.00	0.60
1:B:591:ASP:OD1	1:B:614:GLN:HG3	2.02	0.60
2:C:15:HIS:O	2:C:23:ILE:HG13	2.02	0.60
1:B:152:ILE:HG22	1:B:247:GLU:OE1	2.01	0.60
1:B:199:ALA:O	1:B:792:ASN:HB2	2.01	0.60
2:C:15:HIS:HE1	2:C:25:GLN:OE1	1.83	0.59
1:B:502:ASP:OD2	1:B:505:ASN:HB3	2.02	0.59
1:A:227:ARG:NH1	1:A:233:ALA:N	2.51	0.59
1:A:194:GLY:C	1:A:712:GLN:HE22	2.10	0.58
1:B:227:ARG:HH21	1:B:234:GLY:N	1.81	0.58
2:D:95:SER:OG	2:D:98:ASP:CG	2.44	0.58
1:B:132:ILE:HD11	1:B:464:PRO:HG3	1.86	0.58
1:A:410:TRP:CD2	1:A:463:GLY:HA3	2.39	0.57
1:B:231:TYR:CE1	2:D:43:PRO:HG3	2.40	0.57
1:B:656:ASN:OD1	1:B:657:PRO:HD2	2.04	0.56
1:B:239:ASP:HB3	1:B:331:VAL:HG21	1.86	0.56
1:B:680:GLU:CG	1:B:682:ALA:O	2.53	0.56
2:C:95:SER:HB3	2:C:98:ASP:HB2	1.88	0.56
2:D:84:LYS:HG2	2:D:105:ILE:HD13	1.88	0.56
1:A:410:TRP:CE2	1:A:463:GLY:HA3	2.40	0.56
1:A:68:ILE:HD11	1:A:113:ILE:HG23	1.89	0.55
1:B:571:PRO:HD2	1:B:591:ASP:HB3	1.88	0.55
1:B:174:ARG:CZ	1:B:177:MET:HE3	2.37	0.54
1:B:232:SER:OG	1:B:393:GLN:OE1	2.25	0.54
2:C:103:LYS:HA	2:C:186:LEU:HD13	1.89	0.54
2:C:159:HIS:O	2:C:163:LEU:HG	2.07	0.54
2:D:59:SER:O	2:D:63:LYS:HG2	2.07	0.54
1:B:201:ASP:HB3	1:B:362:TRP:O	2.08	0.54
1:A:133:THR:HG21	1:A:159:VAL:HG21	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:ASP:HB3	1:A:331:VAL:HG11	1.90	0.53
1:B:338:PHE:CZ	1:B:346:LEU:HD23	2.44	0.53
1:B:439:ASN:ND2	1:B:502:ASP:OD1	2.40	0.53
2:D:84:LYS:HD3	2:D:102:GLU:HG3	1.89	0.53
1:B:687:VAL:HG12	1:B:688:GLN:N	2.24	0.53
1:A:302:THR:OG1	1:A:306:ASN:OD1	2.10	0.53
2:C:133:PHE:CE2	2:C:163:LEU:HD21	2.44	0.53
1:A:745:TYR:CD1	2:C:33:TYR:HB2	2.44	0.53
1:A:774:LYS:H	1:A:774:LYS:CD	2.13	0.53
1:B:786:ASP:HB2	1:B:805:ARG:HB2	1.91	0.53
1:B:227:ARG:NH2	1:B:233:ALA:H	2.06	0.52
2:D:83:LEU:HD11	2:D:109:LEU:HD13	1.90	0.52
1:B:227:ARG:NH2	1:B:233:ALA:N	2.57	0.52
1:B:323:ASP:OD1	1:B:324:HIS:N	2.42	0.52
1:A:158:LEU:HD21	1:A:475:VAL:HG23	1.92	0.52
1:B:597:ASP:HB2	1:B:600:TYR:CD1	2.45	0.52
1:B:694:LYS:HG2	1:B:695:ILE:N	2.18	0.52
1:A:391:TRP:CZ3	1:A:427:LEU:HD11	2.45	0.51
1:A:613:GLY:HA2	1:A:639:HIS:O	2.10	0.51
1:A:242:ILE:HG22	1:A:312:VAL:HG22	1.92	0.51
2:C:133:PHE:CD2	2:C:163:LEU:HD23	2.45	0.51
2:C:189:LYS:O	2:C:193:LEU:HB2	2.11	0.51
1:A:230:GLY:HA3	2:C:43:PRO:HD2	1.93	0.51
1:A:475:VAL:O	1:A:533:MET:HA	2.10	0.51
1:B:281:VAL:HG22	1:B:295:LEU:HD13	1.94	0.50
1:B:424:HIS:HA	1:B:449:THR:HG22	1.93	0.50
2:D:17:GLN:CD	2:D:17:GLN:H	2.18	0.50
1:A:424:HIS:HA	1:A:449:THR:HG22	1.93	0.50
1:A:745:TYR:CG	2:C:33:TYR:HB2	2.47	0.50
1:B:587:ALA:HA	1:B:617:GLU:O	2.12	0.50
1:A:587:ALA:HA	1:A:617:GLU:O	2.12	0.50
1:B:475:VAL:O	1:B:533:MET:HA	2.13	0.49
1:B:157:ARG:HE	1:B:256:LEU:HD22	1.77	0.49
2:D:188:ASN:N	2:D:188:ASN:HD22	2.10	0.49
1:A:194:GLY:CA	1:A:712:GLN:HE21	2.08	0.48
1:A:48:PHE:O	1:A:86:LYS:HA	2.13	0.48
1:A:158:LEU:CD2	1:A:475:VAL:HG23	2.44	0.48
1:B:687:VAL:CG1	1:B:688:GLN:N	2.76	0.48
2:C:132:ASP:OD1	2:C:135:GLN:OE1	2.31	0.48
1:A:259:ALA:HB1	1:A:595:PRO:HD3	1.96	0.48
1:B:391:TRP:CZ3	1:B:427:LEU:HD11	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:677:ILE:CG2	1:B:689:ALA:HB3	2.44	0.48
2:C:22:ASP:OD2	2:C:165:LYS:HG2	2.13	0.48
2:D:156:LEU:O	2:D:160:MET:HG2	2.14	0.48
1:B:230:GLY:CA	2:D:43:PRO:HD3	2.33	0.47
1:A:392:GLU:O	1:A:423:TYR:HA	2.14	0.47
1:B:677:ILE:HG23	1:B:689:ALA:HB3	1.96	0.47
2:C:15:HIS:CE1	2:C:25:GLN:OE1	2.66	0.47
1:B:721:PHE:O	1:B:726:ASP:HA	2.14	0.47
1:B:227:ARG:NE	1:B:233:ALA:H	2.13	0.47
1:A:492:ASN:HD22	2:C:55:ARG:HH22	1.61	0.47
1:A:194:GLY:C	1:A:712:GLN:NE2	2.72	0.47
1:A:390:SER:O	1:A:425:ALA:HA	2.15	0.47
1:A:571:PRO:HD2	1:A:591:ASP:HB3	1.95	0.47
1:A:659:ILE:HG23	1:A:659:ILE:O	2.13	0.47
1:B:579:LEU:HD11	1:B:585:VAL:HG13	1.96	0.47
1:A:152:ILE:HB	1:A:154:THR:HG22	1.96	0.47
1:A:568:ARG:NH2	1:A:610:PRO:HD2	2.30	0.46
1:A:568:ARG:CZ	1:A:610:PRO:HG2	2.45	0.46
1:A:192:THR:HG21	1:A:248:VAL:HG11	1.96	0.46
1:B:227:ARG:CZ	1:B:233:ALA:H	2.29	0.46
2:C:33:TYR:O	2:C:33:TYR:CG	2.69	0.46
2:D:96:ALA:O	2:D:99:ILE:HG12	2.14	0.46
1:A:501:ASP:OD1	1:A:501:ASP:N	2.49	0.46
1:B:171:VAL:HG22	1:B:247:GLU:HG2	1.98	0.46
2:C:27:ILE:HD12	2:C:27:ILE:H	1.78	0.46
1:A:227:ARG:NH1	1:A:234:GLY:N	2.19	0.46
1:B:392:GLU:O	1:B:423:TYR:HA	2.15	0.46
1:B:506:TRP:CZ2	1:B:508:GLY:HA2	2.50	0.46
1:A:154:THR:HB	1:A:247:GLU:OE1	2.15	0.46
1:A:229:VAL:CB	2:C:41:PRO:HB2	2.38	0.46
1:A:347:THR:O	1:A:400:ALA:HA	2.16	0.46
1:B:742:GLN:CD	1:B:793:ILE:O	2.59	0.46
1:A:281:VAL:HG22	1:A:295:LEU:CD1	2.46	0.45
1:A:772:THR:HG22	1:A:774:LYS:HD2	1.98	0.45
1:A:263:GLY:O	1:A:264:ALA:HB2	2.16	0.45
2:C:35:THR:HA	2:C:36:PRO:HD3	1.82	0.45
1:A:227:ARG:HH12	1:A:233:ALA:C	2.18	0.45
1:B:152:ILE:HB	1:B:154:THR:HG22	1.98	0.45
1:B:230:GLY:HA3	2:D:42:GLY:HA3	1.99	0.45
1:B:789:TYR:CZ	1:B:802:GLY:HA3	2.51	0.45
1:A:157:ARG:HH11	1:A:256:LEU:HD22	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:789:TYR:CZ	1:A:802:GLY:HA3	2.52	0.44
1:B:259:ALA:HB1	1:B:595:PRO:HD3	1.99	0.44
1:B:362:TRP:CH2	1:B:446:GLN:HB2	2.52	0.44
1:B:390:SER:O	1:B:425:ALA:HA	2.17	0.44
1:B:659:ILE:HG23	1:B:659:ILE:O	2.17	0.44
1:B:338:PHE:CE2	1:B:346:LEU:HD23	2.52	0.44
2:D:184:GLN:O	2:D:188:ASN:ND2	2.50	0.44
1:A:46:VAL:HG12	1:A:47:GLU:N	2.33	0.44
1:A:408:ASN:OD1	1:A:410:TRP:HB2	2.18	0.44
2:D:14:THR:HA	2:D:23:ILE:O	2.18	0.44
1:A:579:LEU:HD11	1:A:585:VAL:HG13	1.99	0.44
1:B:230:GLY:CA	2:D:43:PRO:HD2	2.42	0.44
2:C:33:TYR:O	2:C:33:TYR:CD2	2.70	0.44
1:B:357:PRO:O	1:B:358:LYS:HD2	2.17	0.44
1:B:69:GLN:CD	1:B:133:THR:HG23	2.42	0.44
1:B:229:VAL:HB	2:D:41:PRO:HB2	1.99	0.44
1:B:227:ARG:HH12	1:B:235:ASN:H	1.64	0.44
2:C:40:PRO:HA	2:C:41:PRO:HD3	1.90	0.44
2:D:95:SER:CB	2:D:98:ASP:OD2	2.60	0.43
1:A:482:PHE:CE2	1:A:527:ARG:HG2	2.54	0.43
1:B:158:LEU:HD21	1:B:475:VAL:HG23	2.01	0.43
1:B:656:ASN:HA	1:B:657:PRO:HD3	1.74	0.43
1:A:357:PRO:O	1:A:358:LYS:HD2	2.19	0.43
1:A:506:TRP:CZ2	1:A:508:GLY:HA2	2.53	0.43
1:B:64:ARG:O	1:B:275:HIS:CE1	2.71	0.43
1:B:158:LEU:CD2	1:B:475:VAL:HG23	2.49	0.43
1:B:108:PHE:HA	1:B:113:ILE:HG22	2.00	0.43
1:B:347:THR:O	1:B:400:ALA:HA	2.18	0.43
1:B:330:SER:O	1:B:353:GLN:HA	2.19	0.43
1:B:370:ASP:OD1	1:B:374:ASN:N	2.52	0.43
1:B:394:TYR:CZ	1:B:422:GLY:HA3	2.53	0.43
1:B:443:ILE:HG13	1:B:510:ILE:HD13	1.99	0.43
1:B:227:ARG:HH22	1:B:234:GLY:CA	2.27	0.43
1:B:600:TYR:O	1:B:607:LEU:HD12	2.19	0.43
1:A:141:THR:HB	1:A:173:THR:HB	2.01	0.42
1:B:362:TRP:CD2	1:B:431:MET:HE1	2.54	0.42
1:B:681:LEU:CD1	1:B:687:VAL:HG21	2.48	0.42
1:A:443:ILE:HG13	1:A:510:ILE:HD13	2.01	0.42
1:B:214:ILE:HG12	1:B:264:ALA:HB3	1.99	0.42
1:B:656:ASN:O	1:B:659:ILE:O	2.38	0.42
1:B:141:THR:HB	1:B:173:THR:HB	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:GLU:HG2	1:A:88:LYS:HG2	2.01	0.42
2:C:35:THR:O	2:C:35:THR:HG23	2.20	0.42
1:B:69:GLN:CG	1:B:133:THR:HG23	2.50	0.42
1:A:108:PHE:HA	1:A:113:ILE:HG22	2.02	0.41
1:A:650:TYR:OH	1:A:659:ILE:HG23	2.20	0.41
2:D:89:LEU:CD1	2:D:105:ILE:CD1	2.83	0.41
1:A:682:ALA:HB1	1:A:683:PRO:HD2	2.01	0.41
2:C:82:GLU:HA	2:C:82:GLU:OE1	2.20	0.41
1:A:52:PRO:CG	1:A:84:ALA:HB2	2.50	0.41
2:D:44:SER:HA	2:D:45:PRO:HD3	1.93	0.41
1:A:231:TYR:CE2	2:C:43:PRO:HD3	2.56	0.41
1:A:774:LYS:N	1:A:774:LYS:CD	2.73	0.41
1:B:488:LYS:HD3	1:B:518:PRO:HG2	2.02	0.41
2:D:148:SER:HB2	2:D:150:LYS:HG2	2.02	0.41
1:A:233:ALA:HB1	1:A:421:ASN:HB3	2.03	0.41
1:B:69:GLN:NE2	1:B:133:THR:HG21	2.35	0.41
1:B:482:PHE:CE2	1:B:527:ARG:HG2	2.56	0.41
1:A:716:TYR:CD1	1:A:733:GLY:HA3	2.56	0.41
1:A:772:THR:HG22	1:A:773:ASP:N	2.36	0.40
1:A:281:VAL:HG23	1:A:815:PHE:CZ	2.56	0.40
1:B:419:LYS:HD3	1:B:421:ASN:OD1	2.21	0.40
2:C:92:LYS:H	2:C:92:LYS:HG2	1.65	0.40
2:C:93:ALA:HB3	2:C:102:GLU:OE1	2.21	0.40
1:A:288:TRP:O	1:A:319:HIS:HB2	2.21	0.40
1:A:496:TYR:CG	1:A:513:PRO:HB3	2.56	0.40
1:A:594:MET:HE3	1:A:595:PRO:HD2	2.04	0.40
1:B:274:THR:HG21	1:B:278:LYS:HE2	2.03	0.40
1:B:395:THR:HG22	1:B:421:ASN:ND2	2.36	0.40
1:B:503:PHE:CD1	1:B:503:PHE:C	2.98	0.40
1:B:540:THR:HG22	1:B:542:ASP:N	2.30	0.40
1:B:133:THR:HG21	1:B:159:VAL:HG11	2.04	0.40
1:B:394:TYR:OH	1:B:451:GLU:HG3	2.21	0.40
2:C:27:ILE:N	2:C:27:ILE:CD1	2.76	0.40
2:C:148:SER:HB2	2:C:150:LYS:HG2	2.02	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	769/815 (94%)	741 (96%)	28 (4%)	0	100	100
1	B	734/815 (90%)	708 (96%)	25 (3%)	1 (0%)	48	77
2	C	193/217 (89%)	187 (97%)	4 (2%)	2 (1%)	12	38
2	D	196/217 (90%)	190 (97%)	6 (3%)	0	100	100
All	All	1892/2064 (92%)	1826 (96%)	63 (3%)	3 (0%)	43	72

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	28	PRO
1	B	226	ALA
2	C	36	PRO

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	649/684 (95%)	628 (97%)	21 (3%)	34	70
1	B	624/684 (91%)	612 (98%)	12 (2%)	50	81
2	C	163/182 (90%)	159 (98%)	4 (2%)	42	76
2	D	165/182 (91%)	162 (98%)	3 (2%)	51	82
All	All	1601/1732 (92%)	1561 (98%)	40 (2%)	42	76

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	89	LEU
1	A	109	GLN
1	A	124	SER
1	A	133	THR
1	A	152	ILE
1	A	242	ILE
1	A	248	VAL
1	A	265	THR
1	A	289	ASP
1	A	312	VAL
1	A	330	SER
1	A	331	VAL
1	A	343	ASP
1	A	344	THR
1	A	411	VAL
1	A	421	ASN
1	A	451	GLU
1	A	609	GLU
1	A	643	ARG
1	A	694	LYS
1	A	740	SER
1	B	80	LYS
1	B	152	ILE
1	B	242	ILE
1	B	396	ARG
1	B	451	GLU
1	B	545	LEU
1	B	597	ASP
1	B	694	LYS
1	B	730	VAL
1	B	740	SER
1	B	758	GLU
1	B	771	ILE
2	C	16	VAL
2	C	27	ILE
2	C	180	LYS
2	C	184	GLN
2	D	16	VAL
2	D	27	ILE
2	D	61	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	GLN
1	A	109	GLN
1	A	191	HIS
1	A	492	ASN
1	A	528	GLN
1	A	614	GLN
1	A	630	ASN
1	A	642	ASN
1	A	712	GLN
1	A	742	GLN
1	B	191	HIS
1	B	215	ASN
1	B	280	HIS
1	B	306	ASN
1	B	421	ASN
1	B	495	ASN
1	B	528	GLN
1	B	538	ASN
1	B	630	ASN
1	B	712	GLN
1	B	780	ASN
2	C	15	HIS
2	C	65	HIS
2	C	142	GLN
2	D	74	ASN
2	D	175	GLN
2	D	181	GLN
2	D	184	GLN
2	D	188	ASN

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

10 ligands 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	$\# Z > 2$
3	SO4	B	904	-	4,4,4	0.27	0	6,6,6	0.07	0
3	SO4	B	903	-	4,4,4	0.22	0	6,6,6	0.26	0
3	SO4	A	903	-	4,4,4	0.41	0	6,6,6	0.20	0
3	SO4	A	902	-	4,4,4	0.30	0	6,6,6	0.28	0
3	SO4	B	902	-	4,4,4	0.36	0	6,6,6	0.47	0
3	SO4	B	905	-	4,4,4	0.27	0	6,6,6	0.21	0
3	SO4	A	905	-	4,4,4	0.29	0	6,6,6	0.14	0
3	SO4	B	901	-	4,4,4	0.09	0	6,6,6	0.25	0
3	SO4	A	901	-	4,4,4	0.29	0	6,6,6	0.23	0
3	SO4	A	904	-	4,4,4	0.45	0	6,6,6	0.22	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

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

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	771/815 (94%)	0.10	10 (1%) 75 66	8, 29, 51, 76	0
1	B	740/815 (90%)	0.23	31 (4%) 40 32	14, 31, 65, 93	0
2	C	195/217 (89%)	1.03	33 (16%) 4 3	27, 52, 85, 105	0
2	D	198/217 (91%)	1.10	32 (16%) 4 4	28, 55, 89, 113	0
All	All	1904/2064 (92%)	0.35	106 (5%) 30 23	8, 33, 71, 113	0

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	29	ALA	6.1
2	D	18	GLY	5.8
1	B	229	VAL	5.3
2	D	17	GLN	4.9
2	D	19	GLY	4.8
2	C	35	THR	4.7
2	C	14	THR	4.6
2	C	34	GLY	4.6
2	C	18	GLY	4.6
1	B	116	SER	4.3
2	C	31	SER	4.3
2	D	16	VAL	4.2
1	B	230	GLY	4.1
2	C	94	VAL	4.1
2	D	94	VAL	4.0
2	D	32	SER	3.9
2	D	13	ILE	3.8
2	D	20	GLY	3.7
2	C	16	VAL	3.7
2	D	90	PRO	3.6
2	D	34	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
2	D	33	TYR	3.6
2	C	30	ARG	3.5
2	D	21	ARG	3.5
2	C	12	VAL	3.4
1	B	113	ILE	3.4
1	B	125	VAL	3.3
2	C	13	ILE	3.3
2	C	17	GLN	3.2
2	D	12	VAL	3.2
1	B	62	PHE	3.2
1	B	98	LEU	3.2
2	D	14	THR	3.2
2	C	92	LYS	3.1
2	D	95	SER	3.1
2	C	33	TYR	3.0
2	D	11	MET	3.0
2	D	31	SER	3.0
1	B	682	ALA	3.0
1	B	83	SER	2.9
2	C	28	PRO	2.8
1	A	649	LEU	2.8
1	B	504	ILE	2.8
2	D	91	GLY	2.8
2	C	32	SER	2.8
1	B	232	SER	2.8
2	D	88	GLY	2.7
2	D	100	ARG	2.7
1	B	108	PHE	2.7
2	C	11	MET	2.7
2	C	20	GLY	2.7
1	A	46	VAL	2.7
2	D	27	ILE	2.6
1	B	228	ASN	2.6
1	A	229	VAL	2.6
1	B	99	LEU	2.6
2	C	93	ALA	2.6
2	D	96	ALA	2.6
1	B	60	GLN	2.6
1	A	682	ALA	2.6
1	B	100	ARG	2.6
1	B	114	THR	2.5
1	B	64	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
2	D	191	ARG	2.5
1	A	597	ASP	2.5
2	C	19	GLY	2.5
1	B	54	ALA	2.5
1	B	226	ALA	2.5
2	D	56	LYS	2.5
2	D	93	ALA	2.4
1	B	363	SER	2.3
2	C	132	ASP	2.3
2	D	29	ALA	2.3
2	C	91	GLY	2.3
1	B	115	ILE	2.3
2	D	92	LYS	2.3
2	C	95	SER	2.3
1	B	55	LEU	2.2
2	C	27	ILE	2.2
1	B	110	GLY	2.2
2	C	15	HIS	2.2
1	B	683	PRO	2.2
1	B	63	GLY	2.2
2	C	70	LYS	2.2
2	C	90	PRO	2.2
2	D	28	PRO	2.2
2	D	208	TYR	2.2
2	C	118	LYS	2.2
2	D	15	HIS	2.2
1	A	497	ASP	2.1
1	B	59	LEU	2.1
2	C	78	LYS	2.1
2	D	89	LEU	2.1
1	A	363	SER	2.1
1	A	657	PRO	2.1
2	C	205	GLU	2.1
1	A	225	THR	2.0
1	B	225	THR	2.0
2	D	86	GLU	2.0
1	B	489	SER	2.0
2	C	37	PRO	2.0
1	A	92	ASN	2.0
1	B	68	ILE	2.0
2	C	130	ALA	2.0
1	B	323	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
2	C	204	VAL	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
3	SO4	B	905	5/5	0.73	0.21	106,106,107,107	0
3	SO4	A	905	5/5	0.78	0.19	82,84,85,85	0
3	SO4	A	904	5/5	0.86	0.14	67,68,69,70	0
3	SO4	A	901	5/5	0.92	0.10	53,56,58,59	0
3	SO4	B	903	5/5	0.93	0.12	52,53,54,58	0
3	SO4	A	902	5/5	0.93	0.15	53,58,61,61	0
3	SO4	B	904	5/5	0.94	0.09	72,73,74,75	0
3	SO4	B	901	5/5	0.94	0.10	54,55,56,58	0
3	SO4	B	902	5/5	0.95	0.10	54,55,55,55	0
3	SO4	A	903	5/5	0.95	0.08	52,55,56,57	0

6.5 Other polymers [i](#)

There are no such residues in this entry.