



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 10:17 PM UTC

PDB ID : 2WV0 / pdb_00002wv0
Title : Crystal structure of the GntR-HutC family member YvoA from *Bacillus subtilis*
Authors : Resch, M.; Schiltz, E.; Titgemeyer, F.; Muller, Y.A.
Deposited on : 2009-10-12
Resolution : 2.40 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

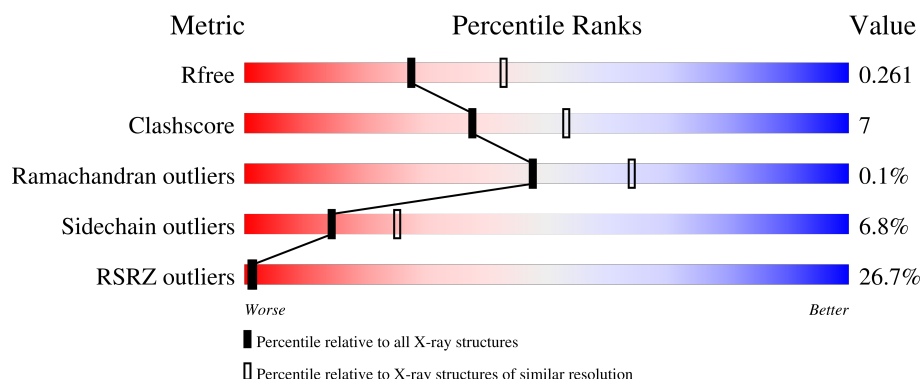
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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 $\leq 5\%$. 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	243	22% 84% 12% .
1	B	243	14% 88% 11% .
1	C	243	7% 90% 8% .
1	D	243	12% 77% 19% .
1	E	243	12% 79% 15% ..

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Mol	Chain	Length	Quality of chain	
1	F	243	12% 79% 16% • •	
1	G	243	16% 81% 15% • •	
1	H	243	72% 67% 20% 5% 8%	
1	I	243	22% 81% 17% •	
1	J	243	72% 85% 11% • •	

2 Entry composition

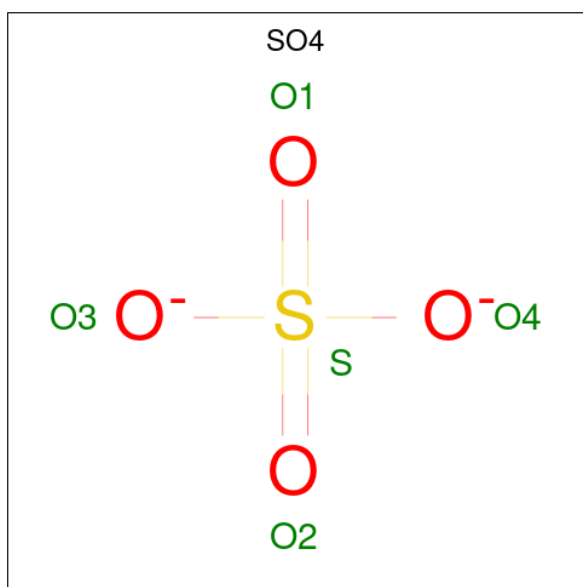
There are 3 unique types of molecules in this entry. The entry contains 18689 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 HTH-TYPE TRANSCRIPTIONAL REPRESSOR YVOA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	243	Total	C	N	O	S	0	3	0
			1911	1207	330	364	10			
1	B	242	Total	C	N	O	S	0	3	0
			1872	1185	321	355	11			
1	C	242	Total	C	N	O	S	0	0	0
			1871	1180	323	358	10			
1	D	242	Total	C	N	O	S	0	5	0
			1913	1211	330	361	11			
1	E	234	Total	C	N	O	S	0	0	0
			1777	1119	306	343	9			
1	F	237	Total	C	N	O	S	0	2	0
			1853	1171	316	355	11			
1	G	237	Total	C	N	O	S	0	0	0
			1779	1123	302	345	9			
1	H	224	Total	C	N	O	S	0	0	0
			1485	922	267	291	5			
1	I	242	Total	C	N	O	S	0	0	0
			1842	1164	314	354	10			
1	J	235	Total	C	N	O	S	0	0	0
			1542	960	278	296	8			

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	I	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	I	1	Total	O	S	0	0
			5	4	1		

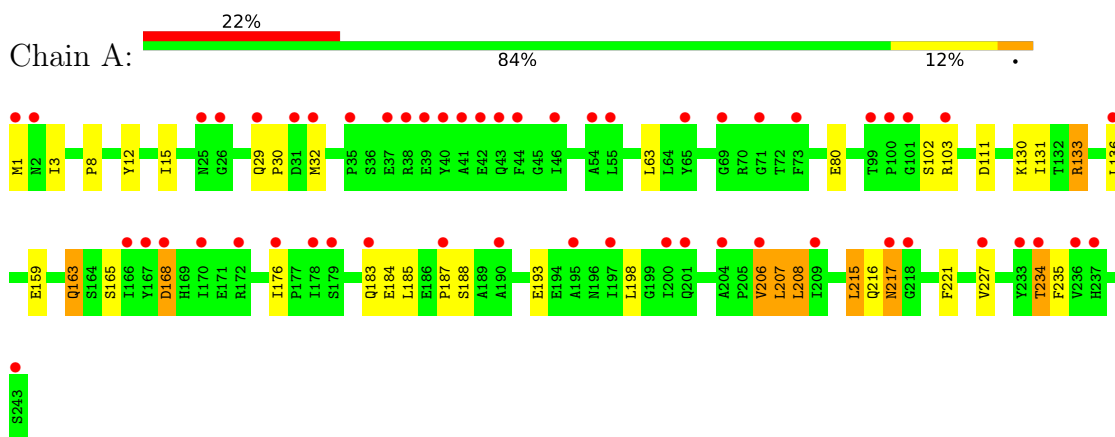
- Molecule 3 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	132	Total	O		0	0
			132	132			
3	B	109	Total	O		0	0
			109	109			
3	C	103	Total	O		0	0
			103	103			
3	D	113	Total	O		0	0
			113	113			
3	E	50	Total	O		0	0
			50	50			
3	F	93	Total	O		0	0
			93	93			
3	G	38	Total	O		0	0
			38	38			
3	H	24	Total	O		0	0
			24	24			
3	I	80	Total	O		0	0
			80	80			
3	J	27	Total	O		0	0
			27	27			

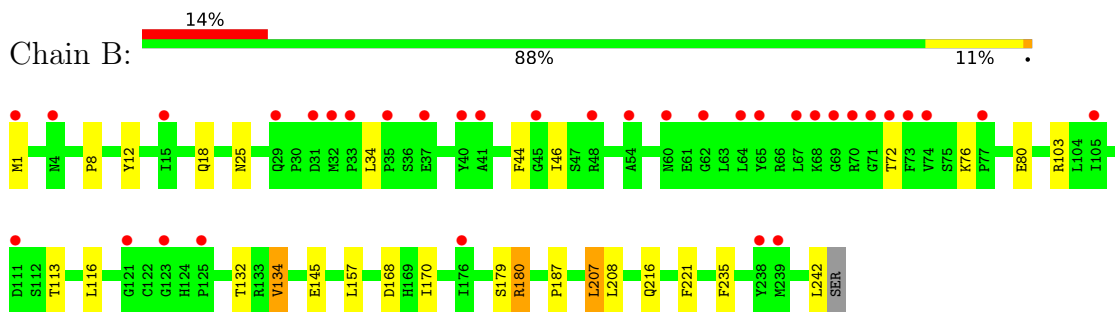
3 Residue-property plots

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.

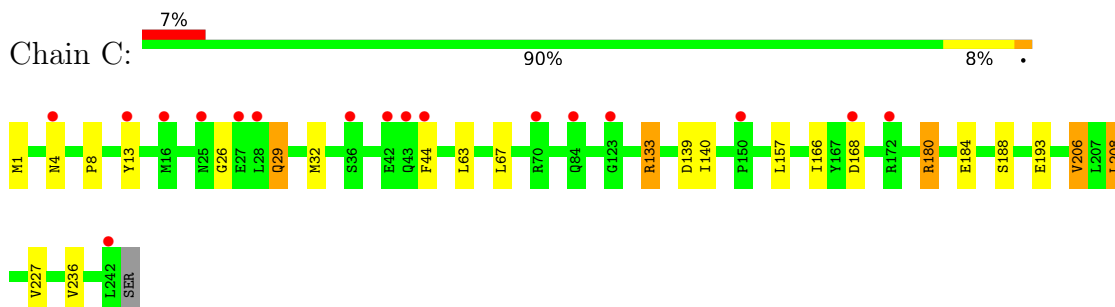
• Molecule 1: HTH-TYPE TRANSCRIPTIONAL REPRESSOR YVOA



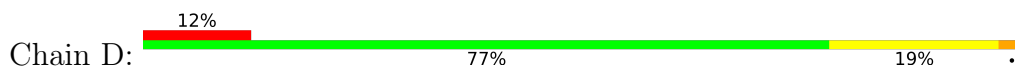
• Molecule 1: HTH-TYPE TRANSCRIPTIONAL REPRESSOR YVOA

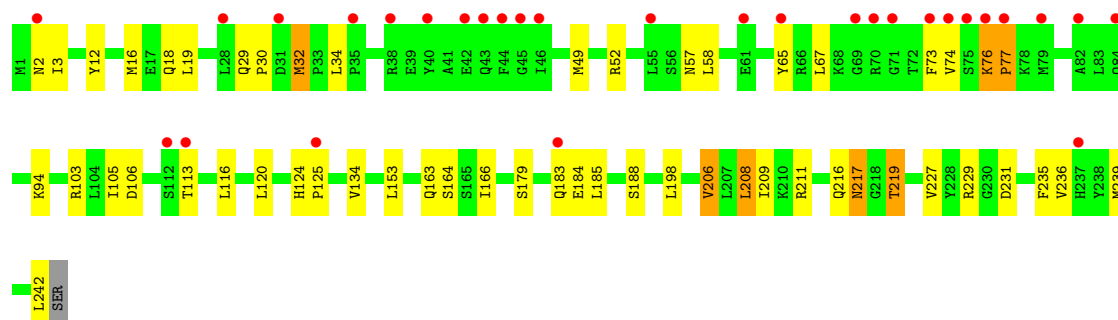


• Molecule 1: HTH-TYPE TRANSCRIPTIONAL REPRESSOR YVOA

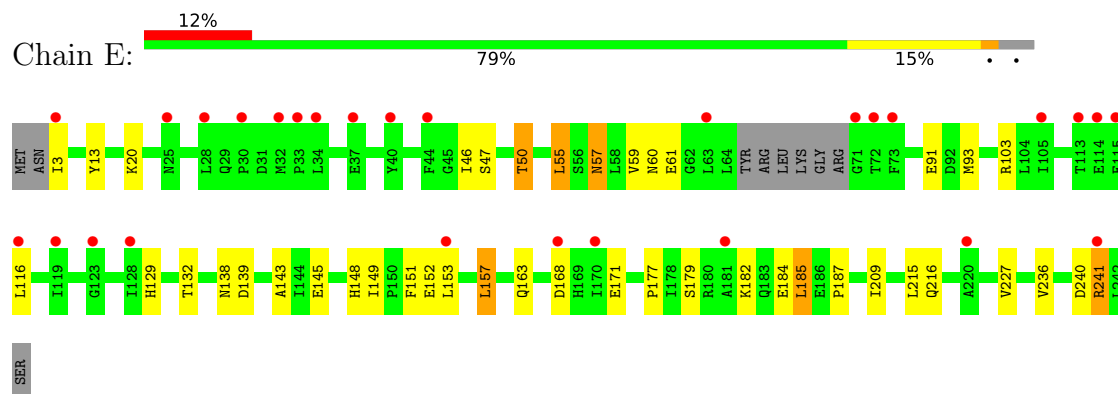


• Molecule 1: HTH-TYPE TRANSCRIPTIONAL REPRESSOR YVOA

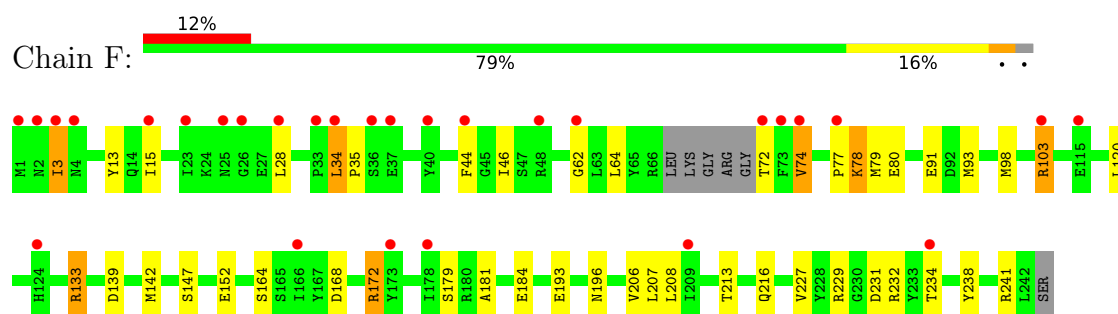




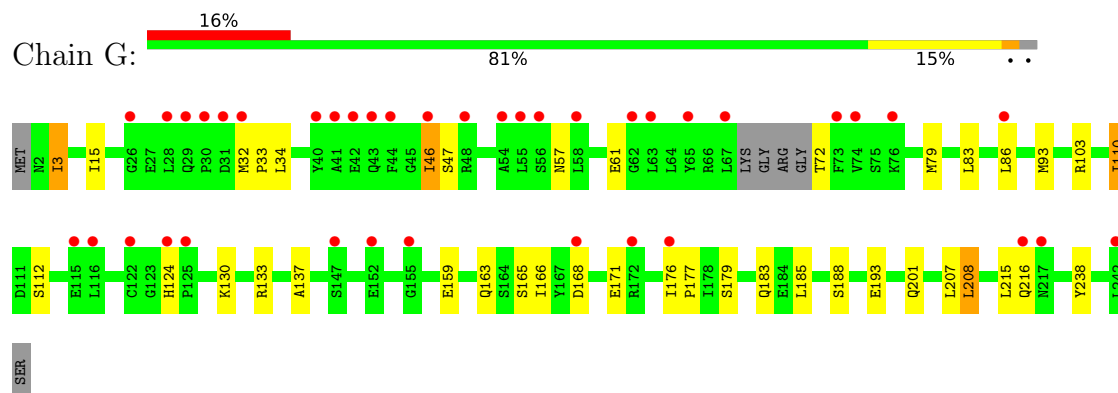
• Molecule 1: HTH-TYPE TRANSCRIPTIONAL REPRESSOR YVOA



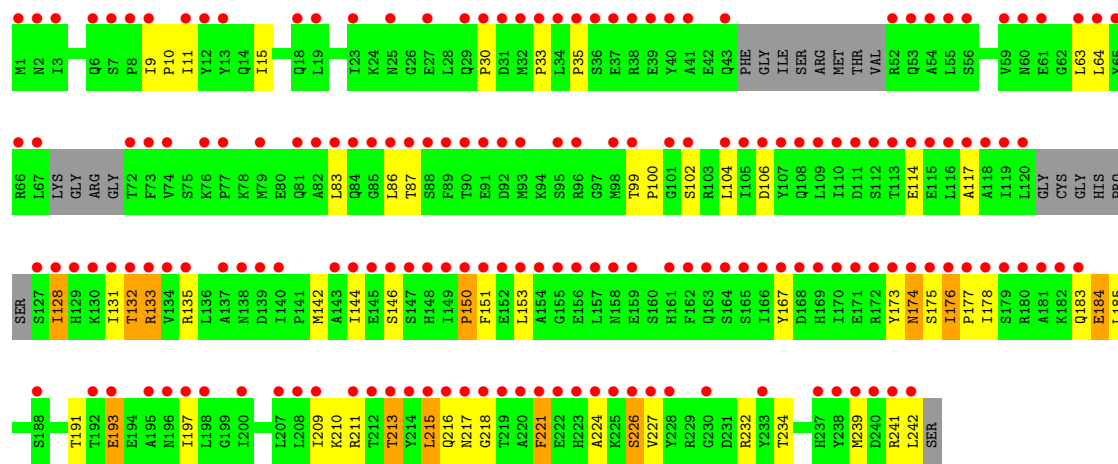
• Molecule 1: HTH-TYPE TRANSCRIPTIONAL REPRESSOR YVOA



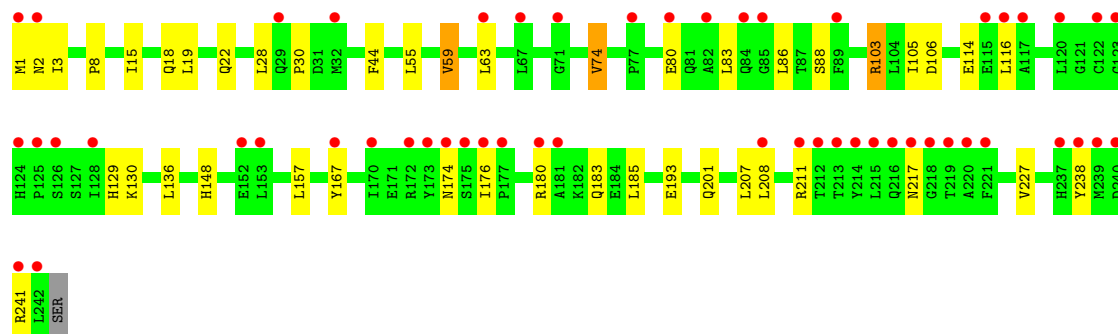
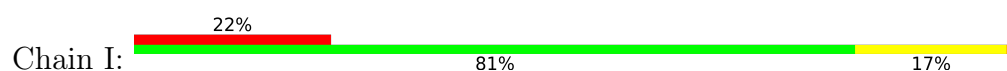
• Molecule 1: HTH-TYPE TRANSCRIPTIONAL REPRESSOR YVOA



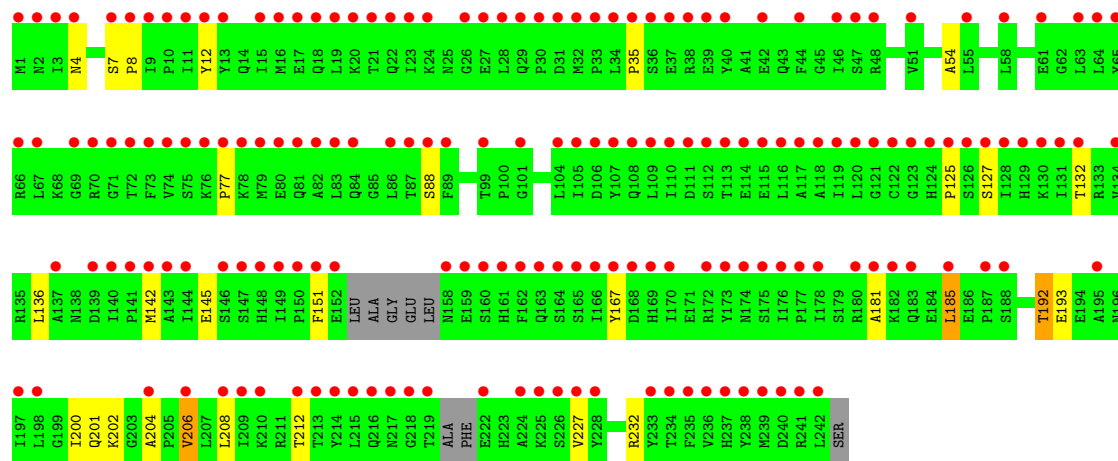
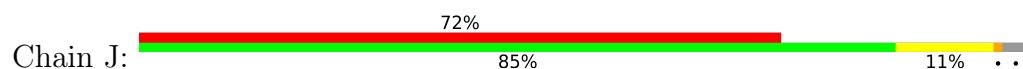
• Molecule 1: HTH-TYPE TRANSCRIPTIONAL REPRESSOR YVOA



• Molecule 1: HTH-TYPE TRANSCRIPTIONAL REPRESSOR YVOA



• Molecule 1: HTH-TYPE TRANSCRIPTIONAL REPRESSOR YVOA



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	208.41Å 137.08Å 120.19Å 90.00° 94.97° 90.00°	Depositor
Resolution (Å)	114.00 – 2.40 114.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.3 (114.00-2.40) 99.3 (114.00-2.40)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.80 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.199 , 0.255 0.258 , 0.261	Depositor DCC
R_{free} test set	6247 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å ²)	47.1	Xtriage
Anisotropy	0.121	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 54.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	18689	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.94% 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	0.63	0/1957	0.89	2/2650 (0.1%)
1	B	0.57	0/1918	0.86	2/2601 (0.1%)
1	C	0.59	0/1908	0.87	1/2586 (0.0%)
1	D	0.64	0/1966	0.93	0/2661
1	E	0.51	0/1812	0.85	0/2460
1	F	0.57	0/1895	0.85	0/2566
1	G	0.50	0/1813	0.82	0/2463
1	H	1.81	31/1504 (2.1%)	1.14	13/2057 (0.6%)
1	I	0.81	3/1879 (0.2%)	0.88	1/2549 (0.0%)
1	J	0.61	1/1567 (0.1%)	0.95	3/2144 (0.1%)
All	All	0.78	35/18219 (0.2%)	0.90	22/24737 (0.1%)

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	215	LEU	C-O	23.76	1.54	1.23
1	H	128	ILE	C-N	20.37	1.60	1.33
1	H	87	THR	C-N	19.98	1.60	1.33
1	H	133	ARG	CZ-NH1	19.75	1.60	1.32
1	H	215	LEU	C-N	15.91	1.55	1.33
1	I	217	ASN	CG-OD1	15.38	1.52	1.23
1	H	128	ILE	C-O	14.12	1.40	1.24
1	H	216	GLN	C-N	12.84	1.52	1.33
1	I	241	ARG	C-O	11.59	1.38	1.24
1	H	150	PRO	C-N	10.83	1.48	1.33
1	H	226	SER	CB-OG	10.00	1.62	1.42
1	H	102	SER	CB-OG	9.77	1.61	1.42
1	I	180	ARG	CZ-NH1	9.57	1.46	1.32
1	H	221	PHE	CG-CD2	8.24	1.56	1.38
1	H	217	ASN	N-CA	8.22	1.56	1.46
1	H	173	TYR	C-O	7.85	1.33	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	178	ILE	C-O	7.82	1.32	1.24
1	H	217	ASN	C-O	7.49	1.33	1.24
1	H	132	THR	C-N	7.48	1.43	1.33
1	H	174	ASN	C-O	7.47	1.33	1.24
1	H	100	PRO	N-CD	7.38	1.58	1.47
1	H	167	TYR	CG-CD2	6.79	1.53	1.39
1	H	104	LEU	C-O	6.78	1.32	1.24
1	J	7	SER	CB-OG	6.60	1.55	1.42
1	H	133	ARG	CD-NE	6.53	1.55	1.46
1	H	151	PHE	C-O	6.50	1.32	1.24
1	H	150	PRO	C-O	6.45	1.32	1.24
1	H	221	PHE	CE2-CZ	6.18	1.57	1.38
1	H	99	THR	C-N	5.94	1.40	1.33
1	H	132	THR	C-O	5.87	1.31	1.24
1	H	218	GLY	N-CA	5.56	1.53	1.45
1	H	128	ILE	CA-C	5.47	1.59	1.52
1	H	175	SER	CA-CB	5.31	1.61	1.53
1	H	213	THR	CB-OG1	5.10	1.51	1.43
1	H	173	TYR	C-N	5.08	1.40	1.33

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	77	PRO	N-CA-CB	10.30	110.13	103.23
1	H	128	ILE	O-C-N	9.16	134.02	122.57
1	H	33	PRO	N-CA-CB	7.87	110.20	103.35
1	H	35	PRO	N-CA-CB	7.76	110.56	103.34
1	J	35	PRO	N-CA-CB	7.35	110.30	103.39
1	H	30	PRO	N-CA-CB	7.29	110.11	103.33
1	J	125	PRO	N-CA-CB	6.86	110.14	102.60
1	H	215	LEU	O-C-N	6.60	130.75	122.43
1	C	180	ARG	N-CA-C	6.50	118.09	108.60
1	H	174	ASN	OD1-CG-ND2	5.93	128.53	122.60
1	H	87	THR	O-C-N	5.82	130.60	123.21
1	H	99	THR	O-C-N	5.79	126.23	121.31
1	H	174	ASN	O-C-N	5.66	129.74	122.39
1	A	216	GLN	CA-C-N	5.60	128.05	120.38
1	A	216	GLN	C-N-CA	5.60	128.05	120.38
1	H	221	PHE	CG-CD2-CE2	-5.45	111.43	120.70
1	H	173	TYR	O-C-N	5.44	129.82	122.59
1	H	221	PHE	CB-CG-CD2	-5.34	111.61	120.70
1	B	76	LYS	CA-C-N	5.16	124.92	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	76	LYS	C-N-CA	5.16	124.92	119.76
1	H	216	GLN	O-C-N	5.13	129.06	122.39
1	I	217	ASN	OD1-CG-ND2	5.01	127.61	122.60

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	1911	0	1895	40	0
1	B	1872	0	1829	20	0
1	C	1871	0	1831	16	0
1	D	1913	0	1904	40	0
1	E	1777	0	1699	23	0
1	F	1853	0	1818	33	0
1	G	1779	0	1690	28	0
1	H	1485	0	1220	39	0
1	I	1842	0	1780	25	0
1	J	1542	0	1222	15	0
2	A	10	0	0	0	0
2	B	10	0	0	0	0
2	C	10	0	0	0	0
2	D	10	0	0	0	0
2	E	5	0	0	0	0
2	F	10	0	0	0	0
2	G	10	0	0	0	0
2	I	10	0	0	0	0
3	A	132	0	0	3	0
3	B	109	0	0	0	0
3	C	103	0	0	2	0
3	D	113	0	0	1	0
3	E	50	0	0	0	0
3	F	93	0	0	2	0
3	G	38	0	0	3	0
3	H	24	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	I	80	0	0	5	0
3	J	27	0	0	0	0
All	All	18689	0	16888	244	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 7.

All (244) 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:G:93:MET:CE	1:G:137:ALA:HB2	1.63	1.27
1:F:103:ARG:HG2	1:F:103:ARG:HH11	1.03	1.17
1:G:93:MET:HE3	1:G:137:ALA:CB	1.73	1.15
1:H:176:ILE:HG22	1:H:177:PRO:HD2	1.15	1.14
1:G:93:MET:HE3	1:G:137:ALA:HB2	1.09	1.08
1:D:16:MET:HE1	1:D:57:ASN:HD22	1.13	1.05
1:H:176:ILE:CG2	1:H:177:PRO:HD2	1.86	1.05
1:H:176:ILE:HG22	1:H:177:PRO:CD	1.94	0.96
1:D:30:PRO:HB3	1:D:76:LYS:HD3	1.45	0.95
1:F:103:ARG:HH11	1:F:103:ARG:CG	1.81	0.92
1:H:133:ARG:NH1	1:H:135:ARG:HH22	1.68	0.92
1:F:103:ARG:HG2	1:F:103:ARG:NH1	1.77	0.88
1:H:150:PRO:HB2	1:H:153:LEU:HD13	1.56	0.87
1:C:139:ASP:OD1	1:F:103:ARG:NH2	2.08	0.86
1:D:12:TYR:HD1	1:D:16:MET:HE3	1.42	0.85
1:G:93:MET:CE	1:G:137:ALA:CB	2.42	0.83
1:A:103[B]:ARG:HH11	1:I:103:ARG:HH21	1.24	0.83
1:C:13:TYR:OH	1:C:139:ASP:OD2	1.98	0.81
1:H:86:LEU:CD1	1:H:211:ARG:NH2	2.45	0.79
1:A:103[B]:ARG:HE	1:I:103:ARG:HE	1.31	0.79
1:C:180:ARG:HB2	1:D:239:MET:O	1.81	0.79
1:I:183:GLN:OE1	1:I:211:ARG:HD3	1.83	0.78
1:D:16:MET:HE1	1:D:57:ASN:ND2	1.95	0.78
1:A:80:GLU:HG2	1:B:242:LEU:HD23	1.65	0.77
1:D:12:TYR:CD1	1:D:16:MET:HE3	2.20	0.76
1:A:80:GLU:HG2	1:B:242:LEU:CD2	2.17	0.75
1:D:76:LYS:NZ	1:D:77:PRO:HD3	2.01	0.75
1:D:185:LEU:HD22	1:D:209:ILE:HG12	1.68	0.74
1:A:103[B]:ARG:NH1	1:I:103:ARG:HH21	1.86	0.73
1:B:113:THR:HG22	1:B:116:LEU:HB2	1.73	0.71
1:F:34:LEU:HD11	1:F:72:THR:OG1	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:13:TYR:OH	1:E:139:ASP:OD2	2.10	0.70
1:G:3:ILE:HD11	1:G:15:ILE:HG13	1.73	0.70
1:I:83:LEU:HD23	1:I:238:TYR:HE2	1.57	0.70
1:C:184:GLU:HG2	1:D:236:VAL:HG22	1.72	0.70
1:A:103[A]:ARG:HD2	3:I:2054:HOH:O	1.92	0.70
1:A:29[A]:GLN:HG2	1:A:32:MET:HG3	1.74	0.70
1:A:103[B]:ARG:HH11	1:I:103:ARG:NH2	1.92	0.67
1:F:77:PRO:HB2	1:F:79:MET:HE3	1.78	0.65
1:H:174:ASN:HB3	1:H:176:ILE:HD11	1.79	0.65
1:A:176[A]:ILE:HG23	1:A:215:LEU:HG	1.79	0.65
1:D:16:MET:HE2	1:D:57:ASN:HB2	1.79	0.64
1:C:26:GLY:O	1:C:29:GLN:NE2	2.31	0.64
1:H:144:ILE:HG12	1:H:197:ILE:HD11	1.80	0.64
1:E:93:MET:HE3	1:E:93:MET:HA	1.79	0.63
1:B:12:TYR:OH	1:D:106:ASP:OD1	2.10	0.63
1:G:201:GLN:HG3	3:G:2032:HOH:O	1.98	0.62
1:G:93:MET:HE2	1:G:137:ALA:HB2	1.75	0.62
1:D:217:ASN:HB3	1:D:219:THR:HG23	1.82	0.62
1:A:183:GLN:HE21	1:A:185:LEU:HD11	1.65	0.62
1:I:201:GLN:HG3	3:I:2069:HOH:O	1.99	0.61
1:D:76:LYS:HZ2	1:D:77:PRO:HD3	1.64	0.61
1:G:93:MET:HE3	1:G:137:ALA:HB1	1.77	0.61
1:D:16:MET:CE	1:D:57:ASN:HB2	2.30	0.61
1:A:103[A]:ARG:NH2	3:A:2054:HOH:O	2.33	0.61
1:F:179:SER:OG	1:F:216:GLN:HA	2.01	0.61
1:A:207:LEU:HG	1:B:187:PRO:HD3	1.82	0.60
1:F:64:LEU:HD23	1:F:74:VAL:HA	1.84	0.60
1:B:1:MET:HE3	1:B:18:GLN:HB2	1.82	0.60
1:A:176[A]:ILE:CG2	1:A:215:LEU:HG	2.31	0.60
1:C:236:VAL:HG22	1:D:184:GLU:HG2	1.84	0.59
1:H:11:ILE:O	1:H:15:ILE:HG12	2.02	0.59
1:D:183:GLN:NE2	1:D:235:PHE:CE2	2.71	0.59
1:H:174:ASN:CB	1:H:176:ILE:CD1	2.80	0.59
1:H:183:GLN:HE21	1:H:185:LEU:HD21	1.68	0.59
1:G:79:MET:HB3	1:G:83:LEU:HD13	1.84	0.59
1:A:159:GLU:O	1:A:163:GLN:HG2	2.03	0.58
1:A:227:VAL:HG23	1:I:8:PRO:HG3	1.85	0.58
1:H:176:ILE:HD12	1:H:176:ILE:H	1.69	0.58
1:H:174:ASN:CB	1:H:176:ILE:HD11	2.33	0.58
1:D:179:SER:HB2	1:D:216:GLN:HA	1.86	0.58
1:H:146:SER:O	1:H:224:ALA:HA	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:83:LEU:HD23	1:G:238:TYR:HE2	1.69	0.57
1:F:93:MET:HE3	1:F:93:MET:HA	1.86	0.57
1:A:206:VAL:CG1	1:A:227:VAL:HG13	2.34	0.57
1:J:192:THR:HB	1:J:202:LYS:HD2	1.87	0.57
1:H:176:ILE:HD12	1:H:176:ILE:N	2.20	0.56
1:I:185:LEU:HD23	1:I:207:LEU:HD13	1.86	0.56
1:J:206:VAL:CG1	1:J:227:VAL:HG13	2.35	0.56
1:E:47:SER:HB3	1:E:50:THR:HG22	1.87	0.56
1:E:116:LEU:HD21	1:E:148:HIS:CD2	2.41	0.56
1:D:30:PRO:HA	1:D:74:VAL:HB	1.87	0.56
1:G:34:LEU:HD13	1:G:72:THR:HG22	1.88	0.55
1:C:140:ILE:HD11	1:F:196:ASN:HB3	1.89	0.55
1:G:159:GLU:HG3	1:G:163:GLN:NE2	2.21	0.55
1:B:179:SER:HB2	1:B:216:GLN:HA	1.89	0.55
1:A:234:THR:HG22	3:A:2121:HOH:O	2.07	0.54
1:A:103[B]:ARG:NE	1:I:103:ARG:HE	2.01	0.54
1:H:144:ILE:CG1	1:H:197:ILE:HD11	2.38	0.54
1:A:206:VAL:HG13	1:A:227:VAL:HG13	1.89	0.53
1:D:16:MET:CE	1:D:57:ASN:HD22	2.04	0.53
1:E:20:LYS:HE3	1:E:138:ASN:OD1	2.09	0.53
1:A:103[B]:ARG:HE	1:I:103:ARG:NE	2.03	0.53
1:A:29[B]:GLN:HG3	1:A:30:PRO:HD2	1.91	0.53
1:G:165:SER:HB3	1:G:168:ASP:HB2	1.90	0.53
1:H:174:ASN:C	1:H:176:ILE:CD1	2.82	0.53
1:D:76:LYS:HZ3	1:D:77:PRO:HD3	1.72	0.52
1:A:8:PRO:HG2	1:I:227:VAL:HG23	1.91	0.52
1:C:180:ARG:NH1	3:C:2066:HOH:O	2.42	0.52
1:A:12:TYR:OH	1:I:106:ASP:OD1	2.27	0.52
1:E:103:ARG:HD2	1:G:103:ARG:HB2	1.91	0.52
1:H:174:ASN:HB2	1:H:176:ILE:CD1	2.40	0.52
1:J:200:ILE:HD12	1:J:204:ALA:HB3	1.92	0.52
1:F:44:PHE:HB2	1:F:46:ILE:HG12	1.92	0.52
1:H:209:ILE:HB	1:H:226:SER:HB2	1.92	0.51
1:F:152:GLU:HG2	3:F:2045:HOH:O	2.10	0.51
1:J:181:ALA:HA	1:J:212:THR:O	2.11	0.51
1:D:183:GLN:HE22	1:D:235:PHE:HE2	1.59	0.51
1:A:183:GLN:NE2	1:A:235:PHE:CE2	2.80	0.50
1:J:206:VAL:HG13	1:J:227:VAL:HG13	1.92	0.50
1:D:76:LYS:HZ2	1:D:77:PRO:CD	2.23	0.50
1:H:176:ILE:CG2	1:H:177:PRO:CD	2.71	0.50
1:H:185:LEU:HD22	1:H:209:ILE:HG12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:184:GLU:HG2	1:H:210:LYS:HB3	1.93	0.50
1:I:55:LEU:O	1:I:59:VAL:HG13	2.12	0.50
1:I:1:MET:HE1	1:I:15:ILE:HG23	1.95	0.49
1:A:1:MET:HE1	1:A:15:ILE:HG23	1.94	0.49
1:I:129:HIS:O	1:I:148:HIS:HA	2.12	0.49
1:A:133:ARG:HD3	3:A:2071:HOH:O	2.13	0.49
1:A:188:SER:HB2	1:A:208:LEU:HD22	1.95	0.49
1:D:65:TYR:CZ	1:D:73:PHE:HB2	2.47	0.48
1:B:180:ARG:HH21	1:B:180:ARG:HB2	1.78	0.48
1:E:91:GLU:CD	1:F:241:ARG:HH22	2.21	0.48
1:I:2:ASN:C	1:I:18:GLN:HE22	2.20	0.48
1:J:132:THR:HA	1:J:145:GLU:O	2.13	0.48
1:H:174:ASN:O	1:H:176:ILE:HD11	2.13	0.48
1:B:103:ARG:HD2	1:D:103:ARG:HD3	1.95	0.48
1:F:168:ASP:HB3	1:F:172:ARG:NH2	2.28	0.48
1:A:131:ILE:HG22	1:A:133:ARG:HD2	1.94	0.48
1:B:44:PHE:HB2	1:B:46:ILE:HG12	1.95	0.48
1:H:239:MET:HE3	1:I:86:LEU:HD13	1.96	0.48
1:D:105:ILE:HD11	1:D:134:VAL:HG22	1.96	0.48
1:E:171:GLU:HG2	1:E:177:PRO:HA	1.97	0.47
1:E:185:LEU:HD12	1:E:209:ILE:HG12	1.97	0.47
1:F:13:TYR:OH	1:F:139:ASP:OD2	2.18	0.47
1:F:78:LYS:C	1:F:79:MET:HE2	2.38	0.47
1:F:98:MET:HE1	1:F:232:ARG:HH21	1.79	0.47
1:B:103:ARG:HB3	1:B:134:VAL:HG13	1.97	0.47
1:G:176:ILE:HG13	1:G:177:PRO:HD2	1.97	0.47
1:H:106:ASP:CB	1:J:12:TYR:OH	2.62	0.47
1:D:49:MET:HE1	1:D:52:ARG:NH2	2.30	0.47
1:F:34:LEU:HB2	1:F:35:PRO:HD2	1.98	0.46
1:H:114:GLU:HA	1:H:117:ALA:HB3	1.98	0.46
1:A:215:LEU:HD13	1:A:221:PHE:CD1	2.50	0.46
1:G:179:SER:HB2	1:G:216:GLN:HA	1.98	0.46
1:H:174:ASN:C	1:H:176:ILE:HD11	2.41	0.46
1:A:187:PRO:HD3	1:B:207:LEU:HG	1.98	0.46
1:A:217:ASN:HD22	1:A:217:ASN:HA	1.53	0.46
1:C:1:MET:HE2	1:C:44:PHE:HZ	1.81	0.46
1:D:29:GLN:HB2	1:D:32:MET:HG3	1.98	0.46
1:D:188:SER:HB2	1:D:208:LEU:HD22	1.98	0.45
1:E:129:HIS:HB2	1:E:149:ILE:HB	1.99	0.45
1:H:174:ASN:C	1:H:176:ILE:HD12	2.42	0.45
1:A:102:SER:O	1:A:103[A]:ARG:NE	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:GLN:HE22	1:A:235:PHE:HE2	1.63	0.45
1:B:34:LEU:HD13	1:B:72:THR:HG23	1.98	0.45
1:E:187:PRO:HD3	1:F:207:LEU:HG	1.98	0.45
1:F:133:ARG:NH1	1:F:164:SER:O	2.49	0.45
1:G:32:MET:HG2	1:G:33:PRO:HD2	1.98	0.45
1:G:171:GLU:HG2	1:G:177:PRO:HA	1.97	0.45
1:C:29:GLN:HB3	1:C:32:MET:HG3	1.98	0.45
1:E:132:THR:HA	1:E:145:GLU:O	2.17	0.45
1:H:86:LEU:CD1	1:H:211:ARG:HH21	2.27	0.45
1:E:179:SER:HB2	1:E:216:GLN:HA	1.99	0.44
1:H:191:THR:HG21	1:J:4:ASN:ND2	2.33	0.44
1:C:133:ARG:CZ	1:C:166:ILE:HD12	2.47	0.44
1:E:55:LEU:O	1:E:59:VAL:HG23	2.18	0.44
1:H:86:LEU:HD11	1:H:211:ARG:NH2	2.27	0.44
1:H:153:LEU:HD23	1:H:221:PHE:HA	1.99	0.44
1:J:12:TYR:HB2	1:J:54:ALA:HB2	1.99	0.44
1:J:185:LEU:HA	1:J:208:LEU:O	2.18	0.44
1:F:3:ILE:HD11	1:F:15:ILE:HG13	1.98	0.44
1:G:103:ARG:NH1	3:G:2012:HOH:O	2.49	0.44
1:D:105:ILE:HD11	1:D:134:VAL:CG2	2.46	0.44
1:I:80:GLU:CD	1:I:80:GLU:H	2.26	0.44
1:B:80:GLU:CD	1:B:80:GLU:H	2.26	0.44
1:F:229:ARG:HB3	1:F:231:ASP:OD1	2.17	0.44
1:H:142:MET:HE1	1:H:232:ARG:HB3	1.99	0.44
1:F:103:ARG:CG	1:F:103:ARG:NH1	2.52	0.44
1:I:174:ASN:HB3	1:I:176:ILE:HG22	2.00	0.44
1:B:170:ILE:HD13	1:B:221:PHE:CD2	2.53	0.44
1:I:88:SER:HB3	1:I:167:TYR:CD1	2.52	0.43
1:B:132:THR:HA	1:B:145:GLU:O	2.18	0.43
1:D:49:MET:HE1	1:D:52:ARG:CZ	2.48	0.43
1:E:185:LEU:CD1	1:E:209:ILE:HG12	2.48	0.43
1:I:30:PRO:HA	1:I:74:VAL:HG22	1.99	0.43
1:C:206:VAL:CG1	1:C:227:VAL:HG13	2.49	0.43
1:E:182:LYS:HD3	1:F:238:TYR:CZ	2.54	0.43
1:G:176:ILE:HG23	1:G:215:LEU:HD22	1.99	0.43
1:G:183:GLN:HE21	1:G:185:LEU:HD11	1.84	0.43
1:I:1:MET:N	3:I:2001:HOH:O	2.52	0.43
1:F:181:ALA:HB2	1:F:213:THR:HG23	1.99	0.43
1:H:227:VAL:HG23	1:J:8:PRO:HG2	2.01	0.43
1:J:88:SER:HB2	1:J:167:TYR:CD2	2.54	0.43
1:E:129:HIS:CE1	1:E:157:LEU:HD22	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:127:SER:O	1:J:151:PHE:HB2	2.19	0.42
1:J:206:VAL:HG11	1:J:227:VAL:HG13	2.00	0.42
1:A:80:GLU:CG	1:B:242:LEU:HD23	2.43	0.42
1:C:133:ARG:NH1	1:C:166:ILE:HD12	2.34	0.42
1:C:188:SER:HB2	1:C:208:LEU:HD22	2.00	0.42
1:H:86:LEU:HD12	1:H:211:ARG:NH2	2.28	0.42
1:E:143:ALA:HA	1:E:227:VAL:O	2.19	0.42
1:I:18:GLN:O	1:I:22:GLN:HG3	2.20	0.42
1:C:8:PRO:HG3	1:F:227:VAL:HG23	2.02	0.42
1:I:1:MET:SD	1:I:44:PHE:HZ	2.43	0.42
1:D:183:GLN:HE21	1:D:185:LEU:HD21	1.85	0.42
1:B:34:LEU:HB2	1:B:72:THR:HG23	2.00	0.42
1:E:241:ARG:NH1	1:F:91:GLU:OE1	2.52	0.42
1:G:185:LEU:HD23	1:G:207:LEU:HD13	2.02	0.42
1:F:62:GLY:HA2	3:F:2016:HOH:O	2.19	0.41
1:F:34:LEU:HB2	1:F:35:PRO:CD	2.50	0.41
1:C:133:ARG:CD	3:C:2054:HOH:O	2.68	0.41
1:E:236:VAL:HG22	1:F:184:GLU:HG2	2.02	0.41
1:G:188:SER:HB2	1:G:208:LEU:HD22	2.01	0.41
1:H:211:ARG:HG2	1:H:213:THR:HG22	2.03	0.41
1:A:206:VAL:HG11	1:A:227:VAL:HG13	2.01	0.41
1:H:174:ASN:HB3	1:H:176:ILE:CD1	2.45	0.41
1:F:142:MET:HE2	1:F:232:ARG:NH1	2.36	0.41
1:A:184:GLU:HA	1:B:235:PHE:O	2.21	0.41
1:A:215:LEU:HB3	1:A:217:ASN:HB2	2.03	0.41
1:G:57:ASN:O	1:G:61:GLU:HB2	2.20	0.41
1:D:29:GLN:HA	1:D:30:PRO:HD3	1.97	0.41
1:D:229:ARG:HB3	1:D:231:ASP:OD1	2.20	0.41
1:E:184:GLU:HG3	1:F:234:THR:CG2	2.51	0.41
1:G:110:ILE:CD1	1:G:130:LYS:HD2	2.51	0.41
1:H:193:GLU:CD	1:H:193:GLU:H	2.29	0.41
1:D:2:ASN:O	1:D:18:GLN:NE2	2.41	0.41
1:D:124:HIS:HA	1:D:125:PRO:HA	1.92	0.41
1:D:206:VAL:HG13	1:D:227:VAL:HG13	2.02	0.41
1:E:129:HIS:NE2	1:E:151:PHE:HD2	2.18	0.41
1:G:46:ILE:HG23	1:G:47:SER:N	2.35	0.41
1:G:133:ARG:HD3	3:G:2019:HOH:O	2.20	0.41
1:A:103[A]:ARG:CD	3:I:2054:HOH:O	2.60	0.41
1:E:57:ASN:O	1:E:61:GLU:HB2	2.21	0.41
1:A:103[B]:ARG:HD3	3:I:2039:HOH:O	2.20	0.40
1:D:113:THR:HG1	1:D:116:LEU:HB2	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:142:MET:HE1	1:J:232:ARG:HG2	2.04	0.40
1:B:8:PRO:HG3	1:D:227:VAL:HG23	2.04	0.40
1:G:112:SER:HB3	1:G:124:HIS:ND1	2.37	0.40
1:D:76:LYS:HA	1:D:77:PRO:HD3	1.83	0.40
1:D:77:PRO:HG3	3:D:2035:HOH:O	2.22	0.40
1:F:98:MET:HE1	1:F:232:ARG:NH2	2.36	0.40
1:H:9:ILE:HA	1:H:10:PRO:HD3	1.96	0.40
1:A:165:SER:HB3	1:A:168:ASP:HB2	2.04	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	244/243 (100%)	240 (98%)	4 (2%)	0	100	100
1	B	243/243 (100%)	239 (98%)	4 (2%)	0	100	100
1	C	240/243 (99%)	238 (99%)	2 (1%)	0	100	100
1	D	245/243 (101%)	237 (97%)	7 (3%)	1 (0%)	30	43
1	E	230/243 (95%)	223 (97%)	7 (3%)	0	100	100
1	F	235/243 (97%)	230 (98%)	5 (2%)	0	100	100
1	G	233/243 (96%)	230 (99%)	3 (1%)	0	100	100
1	H	216/243 (89%)	202 (94%)	13 (6%)	1 (0%)	24	37
1	I	240/243 (99%)	236 (98%)	4 (2%)	0	100	100
1	J	229/243 (94%)	214 (93%)	15 (7%)	0	100	100
All	All	2355/2430 (97%)	2289 (97%)	64 (3%)	2 (0%)	48	64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	128	ILE
1	D	77	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	207/213 (97%)	191 (92%)	16 (8%)	12	20
1	B	198/213 (93%)	191 (96%)	7 (4%)	32	53
1	C	200/213 (94%)	190 (95%)	10 (5%)	22	38
1	D	208/213 (98%)	188 (90%)	20 (10%)	8	12
1	E	186/213 (87%)	171 (92%)	15 (8%)	11	18
1	F	200/213 (94%)	186 (93%)	14 (7%)	14	24
1	G	183/213 (86%)	176 (96%)	7 (4%)	29	49
1	H	114/213 (54%)	102 (90%)	12 (10%)	6	10
1	I	193/213 (91%)	178 (92%)	15 (8%)	11	20
1	J	111/213 (52%)	105 (95%)	6 (5%)	20	35
All	All	1800/2130 (84%)	1678 (93%)	122 (7%)	14	25

All (122) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ILE
1	A	63	LEU
1	A	111	ASP
1	A	130	LYS
1	A	133	ARG
1	A	136	LEU
1	A	163	GLN
1	A	168	ASP
1	A	193	GLU
1	A	198	LEU
1	A	206	VAL
1	A	207	LEU

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Mol	Chain	Res	Type
1	A	208	LEU
1	A	215	LEU
1	A	217	ASN
1	A	234	THR
1	B	25	ASN
1	B	134	VAL
1	B	157	LEU
1	B	168	ASP
1	B	180	ARG
1	B	207	LEU
1	B	208	LEU
1	C	4	ASN
1	C	29	GLN
1	C	63	LEU
1	C	67	LEU
1	C	133	ARG
1	C	157	LEU
1	C	168	ASP
1	C	193	GLU
1	C	206	VAL
1	C	208	LEU
1	D	3	ILE
1	D	19	LEU
1	D	32	MET
1	D	34	LEU
1	D	58	LEU
1	D	67	LEU
1	D	76	LYS
1	D	94	LYS
1	D	120	LEU
1	D	153	LEU
1	D	163	GLN
1	D	164	SER
1	D	166	ILE
1	D	198	LEU
1	D	206	VAL
1	D	208	LEU
1	D	211	ARG
1	D	217	ASN
1	D	219	THR
1	D	242	LEU
1	E	3	ILE

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Mol	Chain	Res	Type
1	E	46	ILE
1	E	50	THR
1	E	55	LEU
1	E	57	ASN
1	E	60	ASN
1	E	152	GLU
1	E	153	LEU
1	E	157	LEU
1	E	163	GLN
1	E	168	ASP
1	E	185	LEU
1	E	215	LEU
1	E	240	ASP
1	E	241	ARG
1	F	3	ILE
1	F	28	LEU
1	F	34	LEU
1	F	74	VAL
1	F	78	LYS
1	F	80	GLU
1	F	103	ARG
1	F	120	LEU
1	F	133	ARG
1	F	147	SER
1	F	172	ARG
1	F	193	GLU
1	F	206	VAL
1	F	208	LEU
1	G	3	ILE
1	G	46	ILE
1	G	86	LEU
1	G	110	ILE
1	G	166	ILE
1	G	193	GLU
1	G	208	LEU
1	H	63	LEU
1	H	64	LEU
1	H	83	LEU
1	H	131	ILE
1	H	132	THR
1	H	176	ILE
1	H	184	GLU

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Mol	Chain	Res	Type
1	H	193	GLU
1	H	215	LEU
1	H	234	THR
1	H	241	ARG
1	H	242	LEU
1	I	3	ILE
1	I	19	LEU
1	I	28	LEU
1	I	59	VAL
1	I	63	LEU
1	I	74	VAL
1	I	103	ARG
1	I	105	ILE
1	I	114	GLU
1	I	116	LEU
1	I	130	LYS
1	I	136	LEU
1	I	157	LEU
1	I	193	GLU
1	I	208	LEU
1	J	136	LEU
1	J	185	LEU
1	J	192	THR
1	J	193	GLU
1	J	201	GLN
1	J	206	VAL

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	6	GLN
1	A	22	GLN
1	A	217	ASN
1	B	22	GLN
1	B	25	ASN
1	B	148	HIS
1	B	223	HIS
1	C	84	GLN
1	D	57	ASN
1	D	148	HIS
1	D	217	ASN
1	E	25	ASN

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Mol	Chain	Res	Type
1	E	60	ASN
1	E	108	GLN
1	E	148	HIS
1	E	163	GLN
1	E	174	ASN
1	F	53	GLN
1	F	60	ASN
1	F	148	HIS
1	G	163	GLN
1	G	196	ASN
1	H	148	HIS
1	H	161	HIS
1	H	183	GLN
1	H	196	ASN
1	I	57	ASN
1	J	4	ASN
1	J	14	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

15 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
2	SO4	A	1244	-	4,4,4	0.28	0	6,6,6	0.48	0
2	SO4	D	1243	-	4,4,4	0.26	0	6,6,6	0.16	0
2	SO4	D	1244	-	4,4,4	0.26	0	6,6,6	0.45	0
2	SO4	G	1243	-	4,4,4	0.26	0	6,6,6	0.27	0
2	SO4	G	1244	-	4,4,4	0.32	0	6,6,6	0.23	0
2	SO4	A	1245	-	4,4,4	0.24	0	6,6,6	0.17	0
2	SO4	B	1244	-	4,4,4	0.20	0	6,6,6	0.23	0
2	SO4	C	1243	-	4,4,4	0.26	0	6,6,6	0.44	0
2	SO4	E	1243	-	4,4,4	0.19	0	6,6,6	0.31	0
2	SO4	I	1243	-	4,4,4	0.22	0	6,6,6	0.28	0
2	SO4	I	1244	-	4,4,4	0.20	0	6,6,6	0.51	0
2	SO4	F	1243	-	4,4,4	0.29	0	6,6,6	0.37	0
2	SO4	F	1244	-	4,4,4	0.20	0	6,6,6	0.42	0
2	SO4	C	1244	-	4,4,4	0.32	0	6,6,6	0.37	0
2	SO4	B	1243	-	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	H	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	H	87:THR	C	88:SER	N	1.60

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	243/243 (100%)	1.48	54 (22%) 2 2	35, 60, 79, 87	3 (1%)
1	B	242/243 (99%)	1.14	35 (14%) 6 4	28, 61, 76, 80	3 (1%)
1	C	242/243 (99%)	0.89	17 (7%) 22 19	45, 58, 71, 82	0
1	D	242/243 (99%)	1.10	30 (12%) 8 6	32, 56, 72, 76	5 (2%)
1	E	234/243 (96%)	1.18	28 (11%) 9 6	54, 67, 87, 95	0
1	F	237/243 (97%)	1.18	29 (12%) 8 6	40, 63, 79, 85	2 (0%)
1	G	237/243 (97%)	1.35	39 (16%) 4 3	57, 69, 83, 89	0
1	H	224/243 (92%)	2.94	174 (77%) 0 0	62, 74, 86, 93	0
1	I	242/243 (99%)	1.41	53 (21%) 2 2	49, 63, 79, 93	0
1	J	235/243 (96%)	2.64	175 (74%) 0 0	62, 74, 87, 91	0
All	All	2378/2430 (97%)	1.52	634 (26%) 1 1	28, 65, 83, 95	13 (0%)

All (634) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	147	SER	7.1
1	H	222	GLU	6.4
1	H	129	HIS	6.4
1	H	162	PHE	6.3
1	H	167	TYR	5.9
1	J	160	SER	5.5
1	J	111	ASP	5.5
1	D	45	GLY	5.5
1	H	40	TYR	5.5
1	H	149	ILE	5.5
1	H	131	ILE	5.5
1	H	213	THR	5.3
1	H	127	SER	5.3

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Mol	Chain	Res	Type	RSRZ
1	J	122	CYS	5.2
1	H	221	PHE	5.2
1	H	177	PRO	5.2
1	J	112	SER	5.0
1	J	236	VAL	5.0
1	H	79	MET	5.0
1	H	108	GLN	4.9
1	I	123	GLY	4.9
1	H	154	ALA	4.9
1	J	214	TYR	4.9
1	H	242	LEU	4.9
1	H	107	TYR	4.8
1	H	41	ALA	4.8
1	H	65	TYR	4.7
1	H	168	ASP	4.7
1	H	106	ASP	4.7
1	H	119	ILE	4.6
1	G	29	GLN	4.6
1	H	120	LEU	4.6
1	H	214	TYR	4.6
1	I	242	LEU	4.5
1	H	172	ARG	4.5
1	I	173	TYR	4.5
1	J	161	HIS	4.5
1	H	176	ILE	4.4
1	H	67	LEU	4.4
1	H	37	GLU	4.4
1	J	1	MET	4.4
1	H	7	SER	4.4
1	G	31	ASP	4.4
1	H	180	ARG	4.3
1	H	64	LEU	4.3
1	H	165	SER	4.3
1	H	148	HIS	4.3
1	J	162	PHE	4.3
1	H	39	GLU	4.3
1	I	219	THR	4.2
1	B	67	LEU	4.2
1	F	34	LEU	4.2
1	H	220	ALA	4.2
1	B	1	MET	4.2
1	J	125	PRO	4.2

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Mol	Chain	Res	Type	RSRZ
1	J	11	ILE	4.2
1	H	56	SER	4.2
1	H	31	ASP	4.2
1	I	217	ASN	4.2
1	H	178	ILE	4.1
1	J	176	ILE	4.1
1	I	216	GLN	4.1
1	H	1	MET	4.1
1	J	27	GLU	4.1
1	J	178	ILE	4.1
1	I	152	GLU	4.0
1	J	116	LEU	4.0
1	H	217	ASN	4.0
1	J	152	GLU	4.0
1	G	43	GLN	4.0
1	H	61	GLU	4.0
1	H	105	ILE	4.0
1	H	112	SER	4.0
1	J	126	SER	4.0
1	H	116	LEU	4.0
1	H	113	THR	4.0
1	H	89	PHE	3.9
1	J	166	ILE	3.9
1	H	173	TYR	3.9
1	J	114	GLU	3.9
1	J	174	ASN	3.9
1	J	16	MET	3.9
1	A	243	SER	3.9
1	B	73	PHE	3.9
1	I	239	MET	3.9
1	I	174	ASN	3.9
1	H	73	PHE	3.8
1	J	158	ASN	3.8
1	A	168	ASP	3.8
1	J	29	GLN	3.8
1	H	228	TYR	3.8
1	J	70	ARG	3.8
1	A	71	GLY	3.8
1	H	66	ARG	3.8
1	J	167	TYR	3.8
1	H	81	GLN	3.8
1	J	219	THR	3.8

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Mol	Chain	Res	Type	RSRZ
1	J	2	ASN	3.8
1	J	124	HIS	3.7
1	F	44	PHE	3.7
1	I	2	ASN	3.7
1	J	40	TYR	3.7
1	F	1	MET	3.7
1	H	88	SER	3.7
1	J	222	GLU	3.7
1	H	83	LEU	3.7
1	J	31	ASP	3.7
1	J	147	SER	3.7
1	J	48	ARG	3.7
1	H	156	GLU	3.6
1	D	79[A]	MET	3.6
1	H	128	ILE	3.6
1	H	12	TYR	3.6
1	H	169	HIS	3.6
1	H	29	GLN	3.6
1	J	64	LEU	3.6
1	I	172	ARG	3.6
1	J	106	ASP	3.6
1	F	36	SER	3.6
1	H	130	LYS	3.6
1	J	28	LEU	3.6
1	J	113	THR	3.6
1	H	179	SER	3.6
1	J	36	SER	3.6
1	B	48	ARG	3.6
1	H	181	ALA	3.6
1	I	117	ALA	3.6
1	J	30	PRO	3.6
1	J	51	VAL	3.5
1	J	163	GLN	3.5
1	J	175	SER	3.5
1	I	218	GLY	3.5
1	J	15	ILE	3.5
1	J	13	TYR	3.5
1	J	108	GLN	3.5
1	H	19	LEU	3.5
1	J	120	LEU	3.5
1	J	242	LEU	3.5
1	J	9	ILE	3.5

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Mol	Chain	Res	Type	RSRZ
1	J	46	ILE	3.5
1	F	2	ASN	3.5
1	H	60	ASN	3.5
1	J	42	GLU	3.5
1	J	76	LYS	3.5
1	H	212	THR	3.5
1	F	33	PRO	3.5
1	H	36	SER	3.5
1	J	33	PRO	3.5
1	J	150	PRO	3.5
1	H	152	GLU	3.4
1	J	63	LEU	3.4
1	H	33	PRO	3.4
1	D	82	ALA	3.4
1	I	176	ILE	3.4
1	H	159	GLU	3.4
1	H	87	THR	3.4
1	H	219	THR	3.4
1	J	132	THR	3.4
1	H	144	ILE	3.4
1	J	144	ILE	3.4
1	J	217	ASN	3.4
1	H	43	GLN	3.4
1	H	183	GLN	3.4
1	H	132	THR	3.4
1	I	177	PRO	3.4
1	H	101	GLY	3.4
1	J	117	ALA	3.4
1	I	175	SER	3.4
1	A	217	ASN	3.3
1	H	174	ASN	3.3
1	H	59	VAL	3.3
1	J	17	GLU	3.3
1	H	9	ILE	3.3
1	A	31	ASP	3.3
1	G	65	TYR	3.3
1	J	74	VAL	3.3
1	B	69	GLY	3.3
1	H	166	ILE	3.3
1	J	151	PHE	3.3
1	J	183	GLN	3.3
1	A	2	ASN	3.3

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Mol	Chain	Res	Type	RSRZ
1	I	238	TYR	3.3
1	J	233	TYR	3.3
1	H	96	ARG	3.3
1	H	153	LEU	3.3
1	J	72	THR	3.3
1	J	75	SER	3.2
1	H	151	PHE	3.2
1	C	70	ARG	3.2
1	H	34	LEU	3.2
1	H	84	GLN	3.2
1	H	161	HIS	3.2
1	I	29	GLN	3.2
1	E	44	PHE	3.2
1	H	35	PRO	3.2
1	H	27	GLU	3.2
1	J	215	LEU	3.2
1	H	233	TYR	3.2
1	H	18	GLN	3.2
1	A	25	ASN	3.2
1	H	2	ASN	3.2
1	J	80	GLU	3.2
1	J	123	GLY	3.2
1	I	122	CYS	3.2
1	A	41	ALA	3.1
1	I	180	ARG	3.1
1	G	67	LEU	3.1
1	I	215	LEU	3.1
1	D	69	GLY	3.1
1	G	74	VAL	3.1
1	J	71	GLY	3.1
1	J	128	ILE	3.1
1	G	172	ARG	3.1
1	H	143	ALA	3.1
1	J	216	GLN	3.1
1	J	32	MET	3.1
1	J	185	LEU	3.1
1	B	40	TYR	3.1
1	H	72	THR	3.1
1	H	238	TYR	3.1
1	J	238	TYR	3.1
1	H	53	GLN	3.1
1	H	150	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
1	J	35	PRO	3.1
1	H	92	ASP	3.1
1	J	44	PHE	3.1
1	D	71	GLY	3.1
1	J	173	TYR	3.1
1	G	122	CYS	3.1
1	I	208	LEU	3.1
1	B	105	ILE	3.1
1	E	115	GLU	3.0
1	J	73	PHE	3.0
1	J	121	GLY	3.0
1	J	82	ALA	3.0
1	F	37	GLU	3.0
1	H	104	LEU	3.0
1	J	21	THR	3.0
1	H	109	LEU	3.0
1	H	52	ARG	3.0
1	I	221	PHE	3.0
1	J	235	PHE	3.0
1	H	197	ILE	3.0
1	J	81	GLN	3.0
1	H	137	ALA	3.0
1	J	104	LEU	3.0
1	J	226	SER	3.0
1	A	43	GLN	3.0
1	E	123	GLY	3.0
1	C	42	GLU	2.9
1	H	54	ALA	2.9
1	J	55	LEU	2.9
1	J	58	LEU	2.9
1	G	152	GLU	2.9
1	J	131	ILE	2.9
1	J	159	GLU	2.9
1	J	38	ARG	2.9
1	J	224	ALA	2.9
1	F	173	TYR	2.9
1	I	214	TYR	2.9
1	H	102	SER	2.9
1	I	84	GLN	2.9
1	I	32	MET	2.9
1	J	23	ILE	2.9
1	H	134	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	J	129	HIS	2.9
1	H	211	ARG	2.9
1	A	40	TYR	2.9
1	J	79	MET	2.9
1	J	239	MET	2.9
1	H	146	SER	2.9
1	J	4	ASN	2.9
1	J	110	ILE	2.9
1	H	30	PRO	2.9
1	B	239[A]	MET	2.9
1	H	163	GLN	2.9
1	J	115	GLU	2.9
1	J	218	GLY	2.9
1	F	3	ILE	2.8
1	J	24	LYS	2.8
1	J	209	ILE	2.8
1	H	224	ALA	2.8
1	J	118	ALA	2.8
1	H	198	LEU	2.8
1	B	37	GLU	2.8
1	E	73	PHE	2.8
1	H	135	ARG	2.8
1	J	210	LYS	2.8
1	D	112	SER	2.8
1	E	170	ILE	2.8
1	J	146	SER	2.8
1	H	111	ASP	2.8
1	H	216	GLN	2.8
1	G	73	PHE	2.8
1	H	38	ARG	2.8
1	J	172	ARG	2.8
1	G	124	HIS	2.8
1	J	12	TYR	2.8
1	H	170	ILE	2.8
1	J	77	PRO	2.8
1	J	213	THR	2.8
1	I	116	LEU	2.8
1	J	168	ASP	2.8
1	B	65	TYR	2.8
1	I	170	ILE	2.8
1	J	127	SER	2.8
1	G	30	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	34	LEU	2.8
1	F	72	THR	2.8
1	B	70	ARG	2.8
1	D	76	LYS	2.8
1	J	22	GLN	2.8
1	F	40	TYR	2.7
1	J	67	LEU	2.7
1	C	16	MET	2.7
1	B	29	GLN	2.7
1	J	37	GLU	2.7
1	A	237	HIS	2.7
1	A	44	PHE	2.7
1	J	3	ILE	2.7
1	B	60	ASN	2.7
1	E	33	PRO	2.7
1	A	167	TYR	2.7
1	B	64	LEU	2.7
1	C	242	LEU	2.7
1	J	86	LEU	2.7
1	G	54	ALA	2.7
1	D	43	GLN	2.7
1	G	62	GLY	2.7
1	H	200	ILE	2.7
1	H	8	PRO	2.7
1	D	2	ASN	2.7
1	A	236	VAL	2.7
1	D	70	ARG	2.7
1	I	80	GLU	2.7
1	J	237	HIS	2.7
1	H	85	GLY	2.7
1	J	10	PRO	2.7
1	A	172	ARG	2.7
1	B	32	MET	2.7
1	D	75	SER	2.7
1	H	63	LEU	2.7
1	H	175	SER	2.7
1	I	120	LEU	2.7
1	J	83	LEU	2.7
1	J	109	LEU	2.7
1	A	37	GLU	2.7
1	J	234	THR	2.7
1	J	18	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
1	J	240	ASP	2.6
1	H	155	GLY	2.6
1	A	209	ILE	2.6
1	E	241	ARG	2.6
1	J	66	ARG	2.6
1	G	63	LEU	2.6
1	D	65	TYR	2.6
1	H	99	THR	2.6
1	B	33	PRO	2.6
1	J	119	ILE	2.6
1	I	241	ARG	2.6
1	C	28	LEU	2.6
1	H	74	VAL	2.6
1	H	91	GLU	2.6
1	H	82	ALA	2.6
1	H	117	ALA	2.6
1	J	212	THR	2.6
1	C	13	TYR	2.6
1	H	237	HIS	2.6
1	J	225	LYS	2.6
1	I	71	GLY	2.6
1	I	77	PRO	2.6
1	E	116	LEU	2.6
1	I	124	HIS	2.6
1	I	213	THR	2.6
1	A	233	TYR	2.6
1	A	176[A]	ILE	2.6
1	D	61	GLU	2.6
1	J	208	LEU	2.6
1	F	4[A]	ASN	2.6
1	G	217	ASN	2.6
1	I	212	THR	2.6
1	J	137	ALA	2.6
1	J	78	LYS	2.6
1	J	130	LYS	2.6
1	G	26	GLY	2.5
1	H	32	MET	2.5
1	H	98	MET	2.5
1	J	177	PRO	2.5
1	D	44	PHE	2.5
1	F	28	LEU	2.5
1	G	28	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	H	192	THR	2.5
1	I	126	SER	2.5
1	J	47	SER	2.5
1	A	65	TYR	2.5
1	D	77	PRO	2.5
1	H	77	PRO	2.5
1	F	166	ILE	2.5
1	I	115	GLU	2.5
1	A	73	PHE	2.5
1	H	157	LEU	2.5
1	H	138	ASN	2.5
1	E	220	ALA	2.5
1	F	234	THR	2.5
1	J	164	SER	2.5
1	A	103[A]	ARG	2.5
1	A	1	MET	2.5
1	F	26	GLY	2.5
1	G	55	LEU	2.5
1	I	63	LEU	2.5
1	J	69	GLY	2.5
1	J	65	TYR	2.5
1	J	107	TYR	2.5
1	A	166	ILE	2.5
1	G	176	ILE	2.5
1	H	11	ILE	2.5
1	J	105	ILE	2.5
1	I	67	LEU	2.5
1	H	164	SER	2.5
1	G	76	LYS	2.4
1	A	136	LEU	2.4
1	G	58	LEU	2.4
1	J	34	LEU	2.4
1	D	84	GLN	2.4
1	D	74	VAL	2.4
1	B	54	ALA	2.4
1	H	118	ALA	2.4
1	J	181	ALA	2.4
1	J	195	ALA	2.4
1	D	42	GLU	2.4
1	H	114	GLU	2.4
1	F	62	GLY	2.4
1	H	140	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	J	170	ILE	2.4
1	J	198	LEU	2.4
1	F	73	PHE	2.4
1	G	48	ARG	2.4
1	A	32	MET	2.4
1	H	158	ASN	2.4
1	A	190	ALA	2.4
1	A	100	PRO	2.4
1	J	88	SER	2.4
1	J	140	ILE	2.4
1	E	63	LEU	2.4
1	D	237[A]	HIS	2.4
1	H	225	LYS	2.4
1	J	39	GLU	2.4
1	A	69	GLY	2.4
1	H	230	GLY	2.4
1	G	46	ILE	2.4
1	I	211	ARG	2.4
1	J	19	LEU	2.4
1	E	40	TYR	2.4
1	I	89	PHE	2.4
1	A	227	VAL	2.4
1	I	125	PRO	2.3
1	E	3	ILE	2.3
1	E	128	ILE	2.3
1	G	168	ASP	2.3
1	H	13	TYR	2.3
1	J	227	VAL	2.3
1	C	4	ASN	2.3
1	A	39	GLU	2.3
1	A	204	ALA	2.3
1	A	234	THR	2.3
1	B	72	THR	2.3
1	B	71	GLY	2.3
1	C	172	ARG	2.3
1	H	241	ARG	2.3
1	A	170	ILE	2.3
1	C	43	GLN	2.3
1	E	105	ILE	2.3
1	I	237	HIS	2.3
1	J	228	TYR	2.3
1	C	27	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	37	GLU	2.3
1	F	115	GLU	2.3
1	G	42	GLU	2.3
1	H	193	GLU	2.3
1	J	61	GLU	2.3
1	H	90	THR	2.3
1	G	155	GLY	2.3
1	H	95	SER	2.3
1	J	7	SER	2.3
1	J	101	GLY	2.3
1	H	86	LEU	2.3
1	H	208	LEU	2.3
1	I	128	ILE	2.3
1	J	149	ILE	2.3
1	G	44	PHE	2.3
1	A	42	GLU	2.3
1	G	40	TYR	2.3
1	I	167	TYR	2.3
1	J	241	ARG	2.3
1	A	200	ILE	2.3
1	I	153	LEU	2.3
1	J	142	MET	2.3
1	C	168	ASP	2.3
1	G	115	GLU	2.3
1	H	171	GLU	2.3
1	J	206	VAL	2.3
1	J	180	ARG	2.3
1	I	181	ALA	2.2
1	A	26	GLY	2.2
1	A	201	GLN	2.2
1	B	62	GLY	2.2
1	H	218	GLY	2.2
1	J	169	HIS	2.2
1	H	226	SER	2.2
1	H	145	GLU	2.2
1	J	89	PHE	2.2
1	J	8	PRO	2.2
1	F	25	ASN	2.2
1	J	204	ALA	2.2
1	A	29[A]	GLN	2.2
1	H	223	HIS	2.2
1	B	68	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	71	GLY	2.2
1	D	28	LEU	2.2
1	G	147	SER	2.2
1	J	165	SER	2.2
1	D	31	ASP	2.2
1	A	38	ARG	2.2
1	E	25	ASN	2.2
1	H	76	LYS	2.2
1	E	32	MET	2.2
1	D	46	ILE	2.2
1	F	48	ARG	2.2
1	A	206	VAL	2.2
1	H	182	LYS	2.2
1	H	25	ASN	2.2
1	H	6	GLN	2.2
1	A	101	GLY	2.2
1	B	238	TYR	2.2
1	E	153	LEU	2.2
1	G	116	LEU	2.2
1	G	242	LEU	2.2
1	H	207	LEU	2.2
1	F	178	ILE	2.2
1	H	3	ILE	2.2
1	G	56	SER	2.2
1	H	139	ASP	2.2
1	H	240	ASP	2.2
1	I	240	ASP	2.2
1	H	133	ARG	2.2
1	B	125	PRO	2.2
1	H	227	VAL	2.1
1	C	84	GLN	2.1
1	G	216	GLN	2.1
1	H	196	ASN	2.1
1	C	123	GLY	2.1
1	H	55	LEU	2.1
1	H	215	LEU	2.1
1	J	99	THR	2.1
1	A	46	ILE	2.1
1	F	23	ILE	2.1
1	A	187	PRO	2.1
1	F	77	PRO	2.1
1	J	20	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	J	182	LYS	2.1
1	F	74	VAL	2.1
1	J	134	VAL	2.1
1	J	148	HIS	2.1
1	D	183	GLN	2.1
1	A	54	ALA	2.1
1	B	45	GLY	2.1
1	B	123	GLY	2.1
1	G	86	LEU	2.1
1	B	15	ILE	2.1
1	B	176	ILE	2.1
1	E	119	ILE	2.1
1	F	15	ILE	2.1
1	D	38	ARG	2.1
1	D	40	TYR	2.1
1	F	103	ARG	2.1
1	H	188	SER	2.1
1	C	150	PRO	2.1
1	G	32	MET	2.1
1	D	55	LEU	2.1
1	E	28	LEU	2.1
1	A	99	THR	2.1
1	J	26	GLY	2.1
1	A	197	ILE	2.1
1	B	111	ASP	2.1
1	B	77	PRO	2.1
1	D	125	PRO	2.1
1	F	124	HIS	2.1
1	H	93	MET	2.1
1	H	239	MET	2.1
1	A	183	GLN	2.1
1	B	74	VAL	2.1
1	E	181	ALA	2.1
1	H	195	ALA	2.1
1	A	55	LEU	2.1
1	B	4[A]	ASN	2.1
1	C	25	ASN	2.1
1	A	218	GLY	2.1
1	B	121	GLY	2.1
1	D	113	THR	2.1
1	E	113	THR	2.1
1	H	115	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	209	ILE	2.1
1	H	23	ILE	2.1
1	H	110	ILE	2.1
1	H	209	ILE	2.1
1	B	31	ASP	2.1
1	A	179	SER	2.1
1	E	30	PRO	2.1
1	J	84	GLN	2.0
1	G	41	ALA	2.0
1	J	143	ALA	2.0
1	E	114	GLU	2.0
1	A	178	ILE	2.0
1	E	72	THR	2.0
1	J	87	THR	2.0
1	J	197	ILE	2.0
1	A	35	PRO	2.0
1	B	35	PRO	2.0
1	J	187	PRO	2.0
1	C	44	PHE	2.0
1	D	73	PHE	2.0
1	A	195	ALA	2.0
1	B	41	ALA	2.0
1	I	82	ALA	2.0
1	I	220	ALA	2.0
1	I	85	GLY	2.0
1	D	35	PRO	2.0
1	E	168	ASP	2.0
1	G	125	PRO	2.0
1	I	1	MET	2.0
1	J	139	ASP	2.0
1	J	141	PRO	2.0
1	C	36	SER	2.0
1	J	188	SER	2.0

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

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

6.3 Carbohydrates ⓘ

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
2	SO4	F	1243	5/5	0.89	0.15	61,63,64,64	0
2	SO4	G	1243	5/5	0.92	0.10	77,77,78,78	0
2	SO4	I	1244	5/5	0.93	0.11	55,57,60,60	0
2	SO4	B	1243	5/5	0.95	0.11	67,68,68,69	0
2	SO4	C	1243	5/5	0.95	0.10	50,53,55,56	0
2	SO4	E	1243	5/5	0.95	0.09	59,59,60,60	0
2	SO4	I	1243	5/5	0.96	0.12	47,48,50,51	0
2	SO4	G	1244	5/5	0.96	0.10	54,55,56,57	0
2	SO4	B	1244	5/5	0.97	0.07	47,48,48,49	0
2	SO4	A	1245	5/5	0.97	0.09	55,55,56,58	0
2	SO4	F	1244	5/5	0.98	0.06	43,44,45,46	0
2	SO4	D	1243	5/5	0.98	0.08	54,54,56,56	0
2	SO4	D	1244	5/5	0.98	0.06	36,37,38,39	0
2	SO4	A	1244	5/5	0.98	0.07	38,39,40,41	0
2	SO4	C	1244	5/5	0.98	0.06	40,41,42,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.