



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 01:34 PM UTC

PDB ID : 1DW9 / pdb_00001dw9
Title : Structure of cyanase reveals that a novel dimeric and decameric arrangement of subunits is required for formation of the enzyme active site
Authors : Walsh, M.A.; Otwinowski, Z.; Perrakis, A.; Anderson, P.M.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on : 1999-12-03
Resolution : 1.65 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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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

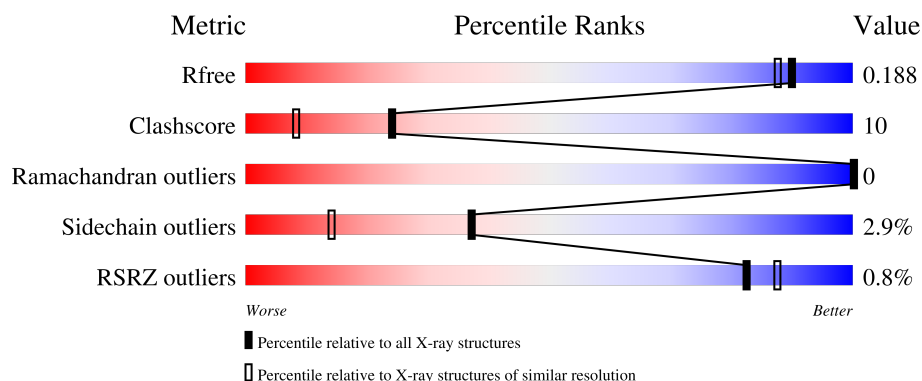
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.65 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	2563 (1.66-1.66)
Clashscore	190562	2662 (1.66-1.66)
Ramachandran outliers	187476	2621 (1.66-1.66)
Sidechain outliers	187428	2621 (1.66-1.66)
RSRZ outliers	180081	2564 (1.66-1.66)

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	156	 83% 14% .
1	B	156	 81% 15% .
1	C	156	 77% 18% . .
1	D	156	 76% 20% .
1	E	156	 71% 26% . .

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Mol	Chain	Length	Quality of chain
1	F	156	
1	G	156	
1	H	156	
1	I	156	
1	J	156	

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
3	SO4	A	1159[A]	-	X	X	-
3	SO4	E	1159	-	-	X	-
3	SO4	H	1159	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 14178 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 CYANATE LYASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	156	Total	C	N	O	S	Se	0	10	0
			1234	796	201	232	1	4			
1	B	156	Total	C	N	O	S	Se	0	8	0
			1226	793	200	228	1	4			
1	C	156	Total	C	N	O	S	Se	0	8	0
			1223	790	200	228	1	4			
1	D	156	Total	C	N	O	S	Se	0	5	0
			1212	782	199	226	1	4			
1	E	156	Total	C	N	O	S	Se	0	7	0
			1221	785	199	232	1	4			
1	F	156	Total	C	N	O	S	Se	0	5	0
			1214	782	199	228	1	4			
1	G	156	Total	C	N	O	S	Se	0	6	0
			1214	781	200	228	1	4			
1	H	156	Total	C	N	O	S	Se	0	5	0
			1215	781	199	230	1	4			
1	I	156	Total	C	N	O	S	Se	0	4	0
			1210	780	199	226	1	4			
1	J	156	Total	C	N	O	S	Se	0	5	0
			1214	782	199	228	1	4			

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cl	0	0
			1	1		
2	B	1	Total	Cl	0	0
			1	1		
2	C	1	Total	Cl	0	0
			1	1		
2	D	1	Total	Cl	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	E	1	Total	Cl	0	0
			1	1		
2	F	1	Total	Cl	0	0
			1	1		
2	G	1	Total	Cl	0	0
			1	1		
2	H	1	Total	Cl	0	0
			1	1		
2	I	1	Total	Cl	0	0
			1	1		
2	J	1	Total	Cl	0	0
			1	1		

- 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	1
			10	8	2		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		
3	I	1	Total	O	S	0	0
			5	4	1		
3	I	1	Total	O	S	0	0
			5	4	1		
3	J	1	Total	O	S	0	0
			5	4	1		
3	J	1	Total	O	S	0	0
			5	4	1		
3	J	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	187	Total	O	0	0
			187	187		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	5	Total O 5 5	0	0
4	A	5	Total O 5 5	0	0
4	B	209	Total O 209 209	0	0
4	B	1	Total O 1 1	0	0
4	C	194	Total O 194 194	0	0
4	C	3	Total O 3 3	0	0
4	D	186	Total O 186 186	0	0
4	D	1	Total O 1 1	0	0
4	E	177	Total O 177 177	0	0
4	E	1	Total O 1 1	0	0
4	E	2	Total O 2 2	0	0
4	F	156	Total O 156 156	0	0
4	F	4	Total O 4 4	0	0
4	F	1	Total O 1 1	0	0
4	G	179	Total O 179 179	0	0
4	G	1	Total O 1 1	0	0
4	G	1	Total O 1 1	0	0
4	G	1	Total O 1 1	0	0
4	H	178	Total O 178 178	0	0
4	H	1	Total O 1 1	0	0
4	I	179	Total O 179 179	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	I	2	Total 2	O 2	0	0
4	J	188	Total 188	O 188	0	0
4	J	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: CYANATE LYASE

Chain A: 



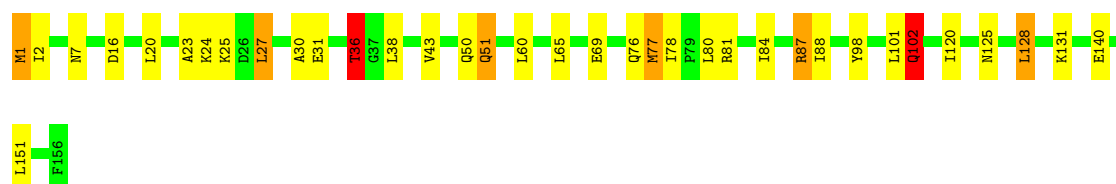
- Molecule 1: CYANATE LYASE

Chain B: 



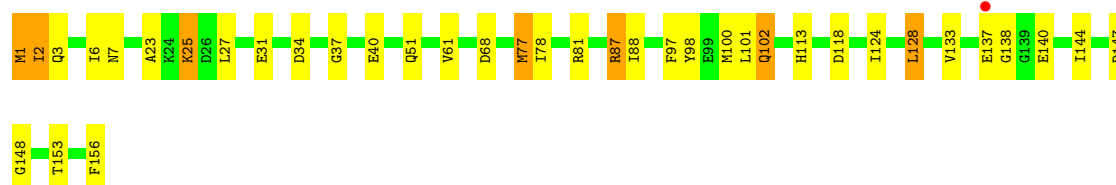
- Molecule 1: CYANATE LYASE

Chain C: 



- Molecule 1: CYANATE LYASE

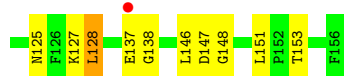
Chain D: 



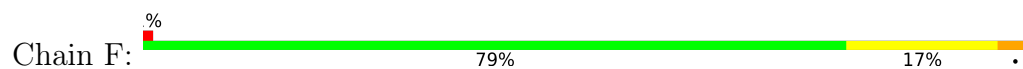
- Molecule 1: CYANATE LYASE

Chain E: 

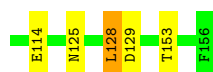
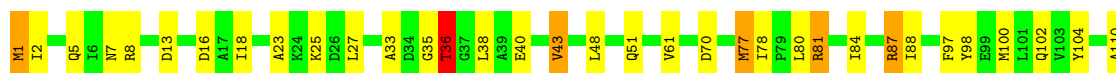




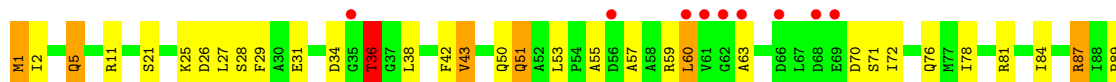
• Molecule 1: CYANATE LYASE



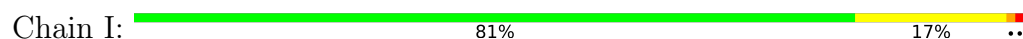
• Molecule 1: CYANATE LYASE



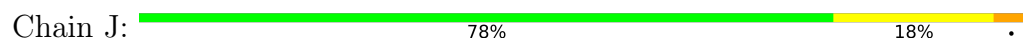
• Molecule 1: CYANATE LYASE



• Molecule 1: CYANATE LYASE



• Molecule 1: CYANATE LYASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	76.34Å 81.03Å 82.30Å 70.30° 72.20° 66.40°	Depositor
Resolution (Å)	20.00 – 1.65 20.00 – 1.65	Depositor EDS
% Data completeness (in resolution range)	94.2 (20.00-1.65) 93.9 (20.00-1.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.22 (at 1.66Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.150 , 0.189 0.152 , 0.188	Depositor DCC
R_{free} test set	9436 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	13.3	Xtriage
Anisotropy	0.334	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 51.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	14178	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.20% 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, CL

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	1.14	3/1301 (0.2%)	1.80	17/1754 (1.0%)
1	B	1.18	3/1276 (0.2%)	1.80	20/1721 (1.2%)
1	C	1.13	3/1277 (0.2%)	1.76	20/1723 (1.2%)
1	D	1.18	7/1250 (0.6%)	1.78	24/1687 (1.4%)
1	E	1.14	2/1269 (0.2%)	1.82	33/1712 (1.9%)
1	F	1.16	1/1252 (0.1%)	1.78	24/1689 (1.4%)
1	G	1.15	4/1260 (0.3%)	1.84	28/1699 (1.6%)
1	H	1.21	3/1253 (0.2%)	2.00	50/1690 (3.0%)
1	I	1.10	2/1243 (0.2%)	1.63	14/1676 (0.8%)
1	J	1.22	3/1252 (0.2%)	1.84	26/1689 (1.5%)
All	All	1.16	31/12633 (0.2%)	1.81	256/17040 (1.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	1	0
1	J	0	2
All	All	1	4

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	1	MSE	SE-CE	-18.72	1.39	1.95
1	C	1	MSE	SE-CE	-9.91	1.65	1.95
1	D	138	GLY	CA-C	8.73	1.58	1.52
1	B	1	MSE	SE-CE	-8.57	1.69	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	1	MSE	SE-CE	-8.23	1.70	1.95
1	B	1	MSE	CG-SE	-7.89	1.71	1.95
1	A	1	MSE	SE-CE	-7.82	1.72	1.95
1	H	1	MSE	SE-CE	-7.67	1.72	1.95
1	C	1	MSE	CG-SE	-7.66	1.72	1.95
1	A	77	MSE	SE-CE	-7.41	1.73	1.95
1	A	1	MSE	CG-SE	-7.39	1.73	1.95
1	G	1	MSE	CG-SE	-7.14	1.74	1.95
1	G	77	MSE	SE-CE	-6.88	1.74	1.95
1	I	1	MSE	CG-SE	-6.75	1.75	1.95
1	E	77	MSE	SE-CE	-6.24	1.76	1.95
1	I	1	MSE	SE-CE	-6.00	1.77	1.95
1	H	1	MSE	CG-SE	-5.63	1.78	1.95
1	D	113	HIS	ND1-CE1	5.63	1.38	1.32
1	E	100	MSE	SE-CE	-5.50	1.78	1.95
1	J	77	MSE	SE-CE	-5.48	1.79	1.95
1	D	100	MSE	SE-CE	-5.45	1.79	1.95
1	D	1	MSE	SE-CE	-5.42	1.79	1.95
1	D	1	MSE	CG-SE	-5.26	1.79	1.95
1	F	77	MSE	SE-CE	-5.22	1.79	1.95
1	G	100	MSE	SE-CE	-5.21	1.79	1.95
1	D	77	MSE	SE-CE	-5.21	1.79	1.95
1	H	100	MSE	SE-CE	-5.15	1.80	1.95
1	J	1	MSE	CG-SE	-5.13	1.80	1.95
1	B	77	MSE	SE-CE	-5.05	1.80	1.95
1	D	148	GLY	CA-C	5.01	1.56	1.52
1	C	77	MSE	SE-CE	-5.01	1.80	1.95

All (256) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1	MSE	CG-SE-CE	18.50	139.62	98.92
1	B	1	MSE	CG-SE-CE	15.08	132.09	98.92
1	G	1	MSE	CG-SE-CE	14.21	130.18	98.92
1	H	102	GLN	OE1-CD-NE2	-12.77	109.83	122.60
1	B	156	PHE	CA-CB-CG	12.06	125.86	113.80
1	A	1	MSE	CG-SE-CE	11.86	125.02	98.92
1	E	137	GLU	CB-CG-CD	11.73	132.54	112.60
1	J	1	MSE	CG-SE-CE	11.67	124.60	98.92
1	J	36	THR	N-CA-CB	-10.83	93.54	110.44
1	G	36	THR	N-CA-CB	-10.60	93.13	110.40
1	J	36	THR	OG1-CB-CG2	10.41	130.11	109.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	36	THR	N-CA-CB	-10.39	94.23	110.44
1	E	36	THR	N-CA-CB	-9.76	95.22	110.44
1	C	36	THR	OG1-CB-CG2	9.61	128.52	109.30
1	E	36	THR	OG1-CB-CG2	9.52	128.34	109.30
1	H	36	THR	CA-C-O	9.34	129.42	119.14
1	H	36	THR	O-C-N	-8.90	110.56	122.49
1	H	53	LEU	CA-C-O	-8.78	112.81	120.19
1	H	21	SER	CA-C-O	8.76	130.01	120.82
1	F	23	ALA	O-C-N	8.73	132.11	122.15
1	H	36	THR	N-CA-CB	-8.66	97.79	110.53
1	A	113	HIS	CA-C-O	-8.57	111.34	120.42
1	H	60	LEU	N-CA-C	8.52	120.56	111.28
1	A	61	VAL	CA-C-N	8.34	129.41	119.99
1	A	61	VAL	C-N-CA	8.34	129.41	119.99
1	G	36	THR	OG1-CB-CG2	8.34	125.97	109.30
1	D	156	PHE	CA-CB-CG	8.27	122.07	113.80
1	C	125	ASN	OD1-CG-ND2	8.13	130.73	122.60
1	B	69	GLU	CB-CG-CD	8.12	126.40	112.60
1	B	7	ASN	CA-CB-CG	8.09	120.69	112.60
1	F	69	GLU	CA-C-O	-8.05	112.02	120.55
1	H	36	THR	CA-C-N	7.89	136.07	120.77
1	H	36	THR	C-N-CA	7.89	136.07	120.77
1	E	138	GLY	O-C-N	7.84	132.89	122.70
1	B	124	ILE	O-C-N	7.82	128.94	121.98
1	E	62	GLY	O-C-N	7.75	129.63	122.19
1	F	23	ALA	CA-C-O	-7.62	112.34	120.42
1	A	20	LEU	CA-C-O	-7.61	112.48	120.55
1	H	11	ARG	NE-CZ-NH1	7.43	128.93	121.50
1	A	102	GLN	OE1-CD-NE2	-7.39	115.21	122.60
1	H	76	GLN	OE1-CD-NE2	7.35	129.95	122.60
1	F	7	ASN	CA-CB-CG	7.28	119.88	112.60
1	B	124	ILE	CA-C-O	-7.20	113.82	120.73
1	D	31	GLU	CA-CB-CG	7.18	128.46	114.10
1	J	40	GLU	CA-C-O	-7.11	113.01	120.55
1	E	23	ALA	O-C-N	7.04	130.17	122.15
1	G	23	ALA	O-C-N	7.03	130.17	122.15
1	A	97	PHE	CA-CB-CG	-7.01	106.79	113.80
1	G	8	ARG	NE-CZ-NH2	-7.00	112.90	119.20
1	H	97	PHE	CA-CB-CG	-7.00	106.80	113.80
1	J	55	ALA	CA-C-O	-7.00	113.13	120.55
1	C	140	GLU	O-C-N	6.99	131.62	123.17
1	E	147	ASP	CA-C-N	-6.96	116.25	121.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	147	ASP	C-N-CA	-6.96	116.25	121.61
1	J	7	ASN	CA-CB-CG	6.93	119.53	112.60
1	F	102	GLN	OE1-CD-NE2	-6.91	115.69	122.60
1	H	71	SER	O-C-N	-6.90	113.26	122.23
1	G	18	ILE	CA-C-O	6.88	128.14	120.85
1	D	102	GLN	OE1-CD-NE2	-6.83	115.77	122.60
1	J	51	GLN	OE1-CD-NE2	-6.77	115.83	122.60
1	B	70	ASP	CA-C-O	-6.76	113.25	120.42
1	H	135	ASP	CA-C-O	-6.73	114.14	119.66
1	C	50	GLN	OE1-CD-NE2	6.69	129.29	122.60
1	E	7	ASN	OD1-CG-ND2	-6.67	115.92	122.60
1	I	1	MSE	CG-SE-CE	6.67	113.61	98.92
1	F	147	ASP	CA-C-N	-6.67	116.48	121.61
1	F	147	ASP	C-N-CA	-6.67	116.48	121.61
1	H	127	LYS	CA-CB-CG	6.67	127.44	114.10
1	E	87	ARG	CD-NE-CZ	-6.64	115.11	124.40
1	J	32	ILE	CA-C-O	-6.63	114.05	120.95
1	J	57	ALA	O-C-N	-6.58	114.66	122.15
1	B	125	ASN	OD1-CG-ND2	6.56	129.16	122.60
1	D	128[A]	LEU	N-CA-CB	-6.56	99.43	111.37
1	D	128[B]	LEU	N-CA-CB	-6.56	99.43	111.37
1	G	23	ALA	CA-C-O	-6.51	113.52	120.42
1	H	34	ASP	CA-CB-CG	-6.48	106.12	112.60
1	J	55	ALA	O-C-N	6.44	128.95	122.12
1	B	87	ARG	CD-NE-CZ	-6.41	115.43	124.40
1	G	125	ASN	OD1-CG-ND2	6.40	129.00	122.60
1	C	7	ASN	CA-CB-CG	6.34	118.94	112.60
1	G	81	ARG	NE-CZ-NH1	6.33	127.83	121.50
1	G	61	VAL	CA-C-N	6.32	127.00	119.98
1	G	61	VAL	C-N-CA	6.32	127.00	119.98
1	C	16	ASP	O-C-N	6.32	128.82	122.12
1	F	19	LEU	CA-C-N	-6.29	111.35	120.29
1	F	19	LEU	C-N-CA	-6.29	111.35	120.29
1	G	35	GLY	CA-C-O	6.26	125.93	119.10
1	A	87	ARG	CD-NE-CZ	-6.26	115.64	124.40
1	C	30	ALA	O-C-N	6.24	128.49	122.07
1	D	124	ILE	CA-C-O	-6.23	115.26	120.80
1	E	102	GLN	OE1-CD-NE2	-6.19	116.41	122.60
1	H	25	LYS	CA-C-O	6.19	126.55	119.18
1	I	140	GLU	O-C-N	6.13	130.38	123.27
1	H	87	ARG	CD-NE-CZ	-6.13	115.82	124.40
1	A	20	LEU	O-C-N	6.12	128.61	122.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	26	ASP	CA-C-O	6.11	128.80	121.65
1	F	4	SER	O-C-N	-6.11	115.78	123.17
1	B	61	VAL	CA-C-N	6.10	126.76	119.98
1	B	61	VAL	C-N-CA	6.10	126.76	119.98
1	G	97	PHE	CA-CB-CG	-6.10	107.70	113.80
1	H	5	GLN	CB-CA-C	-6.08	99.76	109.80
1	I	60[A]	LEU	N-CA-CB	6.05	118.74	109.91
1	I	60[B]	LEU	N-CA-CB	6.05	118.74	109.91
1	E	153	THR	O-C-N	6.02	130.22	123.05
1	D	140	GLU	O-C-N	6.02	130.25	123.27
1	G	8	ARG	CD-NE-CZ	-6.02	115.97	124.40
1	B	23	ALA	O-C-N	6.01	129.01	122.15
1	E	153	THR	CA-C-O	-6.01	114.28	120.54
1	D	23	ALA	O-C-N	5.98	128.97	122.15
1	D	153	THR	O-C-N	5.98	130.04	123.22
1	I	124	ILE	O-C-N	5.97	126.58	121.98
1	D	25	LYS	CA-C-O	5.95	126.26	119.18
1	J	87	ARG	CA-CB-CG	-5.94	102.22	114.10
1	H	89	PRO	O-C-N	5.94	130.36	123.06
1	E	5	GLN	CA-C-N	-5.93	115.55	122.14
1	E	5	GLN	C-N-CA	-5.93	115.55	122.14
1	E	7	ASN	CA-CB-CG	5.92	118.52	112.60
1	D	7	ASN	CA-CB-CG	5.90	118.50	112.60
1	F	97	PHE	CA-CB-CG	-5.90	107.90	113.80
1	G	129	ASP	O-C-N	5.90	129.98	123.25
1	H	51	GLN	O-C-N	5.88	129.95	123.25
1	A	23	ALA	O-C-N	5.87	128.84	122.15
1	A	96	ARG	NE-CZ-NH2	-5.87	113.92	119.20
1	D	34	ASP	CA-C-N	-5.87	114.29	122.86
1	D	34	ASP	C-N-CA	-5.87	114.29	122.86
1	H	55	ALA	CA-C-O	-5.83	114.37	120.55
1	J	135	ASP	CA-C-O	-5.81	114.89	119.66
1	C	87	ARG	CD-NE-CZ	-5.80	116.28	124.40
1	D	87	ARG	CA-CB-CG	-5.80	102.50	114.10
1	B	70	ASP	O-C-N	5.78	128.74	122.15
1	H	36	THR	N-CA-C	-5.77	106.40	113.50
1	A	5	GLN	OE1-CD-NE2	-5.76	116.84	122.60
1	H	57	ALA	CA-C-N	5.76	127.93	120.44
1	H	57	ALA	C-N-CA	5.76	127.93	120.44
1	J	68	ASP	CA-CB-CG	5.76	118.36	112.60
1	H	1	MSE	CG-SE-CE	5.74	111.56	98.92
1	G	16	ASP	CA-C-O	-5.74	114.47	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	25[A]	LYS	CA-C-O	5.73	126.21	119.28
1	G	25[B]	LYS	CA-C-O	5.73	126.21	119.28
1	H	135	ASP	O-C-N	5.72	129.83	121.54
1	G	77	MSE	CG-SE-CE	-5.69	86.40	98.92
1	H	43	VAL	N-CA-C	5.69	115.89	110.42
1	G	5	GLN	OE1-CD-NE2	-5.68	116.92	122.60
1	H	59	ARG	CD-NE-CZ	5.67	132.34	124.40
1	H	5	GLN	CA-C-N	-5.66	115.79	122.36
1	H	5	GLN	C-N-CA	-5.66	115.79	122.36
1	D	138	GLY	O-C-N	5.66	129.91	122.55
1	E	127	LYS	CA-CB-CG	5.64	125.39	114.10
1	F	42	PHE	CA-C-O	5.64	126.58	120.55
1	G	18	ILE	O-C-N	-5.64	116.03	121.83
1	G	43	VAL	O-C-N	5.63	127.33	121.87
1	H	110	ALA	O-C-N	5.63	128.57	122.15
1	E	55	ALA	N-CA-C	5.62	118.13	111.33
1	E	87	ARG	CA-CB-CG	-5.61	102.88	114.10
1	D	68	ASP	CA-CB-CG	5.59	118.19	112.60
1	J	102	GLN	O-C-N	-5.58	116.21	122.12
1	I	5	GLN	OE1-CD-NE2	-5.57	117.03	122.60
1	F	4	SER	CA-C-O	5.56	127.68	121.40
1	B	96	ARG	NE-CZ-NH2	5.55	124.20	119.20
1	C	69	GLU	CA-C-O	-5.54	114.67	120.55
1	I	97	PHE	O-C-N	-5.54	115.45	122.27
1	E	23	ALA	CA-C-O	-5.54	114.55	120.42
1	G	7	ASN	OD1-CG-ND2	-5.53	117.07	122.60
1	J	97	PHE	CA-CB-CG	-5.53	108.27	113.80
1	J	19	LEU	CA-C-O	-5.51	114.71	120.55
1	B	87	ARG	CA-CB-CG	-5.50	103.09	114.10
1	H	70	ASP	CA-C-O	-5.50	113.88	120.10
1	G	87	ARG	CD-NE-CZ	-5.50	116.70	124.40
1	I	97	PHE	CA-CB-CG	-5.50	108.30	113.80
1	J	113	HIS	CA-C-O	-5.49	114.73	120.55
1	D	2	ILE	CA-C-O	5.47	127.38	121.36
1	G	40	GLU	CA-C-O	-5.47	114.72	120.63
1	J	19	LEU	O-C-N	5.47	127.92	122.12
1	D	6	ILE	CA-C-O	-5.47	115.19	119.46
1	F	87	ARG	CD-NE-CZ	-5.46	116.75	124.40
1	B	65	LEU	CA-C-O	5.45	126.02	119.59
1	H	87	ARG	CA-CB-CG	-5.45	103.20	114.10
1	E	30	ALA	CA-C-O	-5.45	114.77	120.55
1	F	8	ARG	CD-NE-CZ	-5.44	116.78	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	102	GLN	OE1-CD-NE2	-5.44	117.16	122.60
1	D	40	GLU	CA-C-O	-5.42	113.98	120.10
1	H	21	SER	O-C-N	-5.41	116.49	122.07
1	D	87	ARG	CD-NE-CZ	-5.41	116.83	124.40
1	E	40[A]	GLU	CA-C-O	-5.40	114.83	120.55
1	E	40[B]	GLU	CA-C-O	-5.40	114.83	120.55
1	E	68	ASP	CA-CB-CG	5.40	118.00	112.60
1	D	147	ASP	CA-C-N	-5.39	118.46	122.18
1	D	147	ASP	C-N-CA	-5.39	118.46	122.18
1	A	102	GLN	O-C-N	-5.39	115.91	122.22
1	H	72	ILE	CA-C-O	-5.39	115.34	120.95
1	J	23	ALA	O-C-N	5.38	128.29	122.15
1	G	13	ASP	CA-CB-CG	5.38	117.98	112.60
1	E	62	GLY	CA-C-O	-5.37	115.22	120.75
1	A	138	GLY	CA-C-O	-5.35	115.02	121.98
1	D	61	VAL	CA-C-N	5.35	125.92	119.98
1	D	61	VAL	C-N-CA	5.35	125.92	119.98
1	C	76	GLN	OE1-CD-NE2	5.35	127.95	122.60
1	H	102	GLN	O-C-N	-5.34	115.98	122.22
1	F	8	ARG	NE-CZ-NH2	-5.33	114.40	119.20
1	F	8	ARG	NE-CZ-NH1	5.33	126.83	121.50
1	E	137	GLU	CA-C-O	5.33	126.10	119.12
1	E	16	ASP	CA-CB-CG	5.30	117.91	112.60
1	I	68	ASP	CA-CB-CG	5.30	117.90	112.60
1	H	59	ARG	CA-CB-CG	-5.30	103.50	114.10
1	G	153	THR	O-C-N	5.29	129.21	123.13
1	F	133	VAL	O-C-N	-5.27	117.06	123.02
1	H	36	THR	CB-CA-C	5.26	118.87	109.29
1	J	14	LEU	CA-C-O	5.26	126.35	120.82
1	H	102	GLN	CG-CD-NE2	5.26	124.29	116.40
1	E	125	ASN	OD1-CG-ND2	5.24	127.84	122.60
1	C	36	THR	CA-CB-OG1	5.24	117.46	109.60
1	E	148	GLY	CA-C-O	5.24	126.13	121.57
1	I	101[A]	LEU	O-C-N	-5.24	116.18	122.15
1	I	101[B]	LEU	O-C-N	-5.24	116.18	122.15
1	H	36	THR	OG1-CB-CG2	5.24	119.78	109.30
1	B	19	LEU	CA-C-O	-5.23	114.88	120.42
1	B	110	ALA	O-C-N	5.22	127.44	122.07
1	J	5	GLN	CA-C-N	-5.22	116.35	122.14
1	J	5	GLN	C-N-CA	-5.22	116.35	122.14
1	C	51	GLN	OE1-CD-NE2	-5.21	117.39	122.60
1	H	11	ARG	NH1-CZ-NH2	-5.21	112.53	119.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	50	GLN	OE1-CD-NE2	5.21	127.81	122.60
1	G	77	MSE	O-C-N	5.19	128.83	122.96
1	C	102	GLN	OE1-CD-NE2	-5.18	117.42	122.60
1	F	19	LEU	O-C-N	5.18	128.06	122.15
1	H	71	SER	CA-C-N	5.18	127.56	120.46
1	H	71	SER	C-N-CA	5.18	127.56	120.46
1	J	148	GLY	O-C-N	5.18	127.91	123.25
1	F	51	GLN	O-C-N	5.18	129.05	123.10
1	H	114	GLU	CA-C-O	-5.18	114.93	120.42
1	E	61	VAL	CA-C-N	5.16	125.70	119.98
1	E	61	VAL	C-N-CA	5.16	125.70	119.98
1	C	23	ALA	O-C-N	5.15	128.03	122.15
1	F	51	GLN	CA-C-O	-5.14	115.95	121.45
1	C	16	ASP	CA-C-O	-5.14	115.10	120.55
1	H	42	PHE	CA-CB-CG	-5.12	108.68	113.80
1	H	138	GLY	O-C-N	5.12	129.35	122.70
1	F	40[A]	GLU	O-C-N	5.11	127.54	122.12
1	F	40[B]	GLU	O-C-N	5.11	127.54	122.12
1	F	65	LEU	CA-C-O	5.11	125.33	119.35
1	C	140	GLU	CA-C-O	-5.10	115.63	121.40
1	I	87	ARG	CD-NE-CZ	-5.10	117.27	124.40
1	H	29	PHE	O-C-N	-5.09	116.72	122.12
1	I	73	LEU	O-C-N	5.07	127.93	122.15
1	E	113	HIS	CB-CG-CD2	-5.07	124.61	131.20
1	I	70	ASP	CA-C-O	-5.07	115.18	120.55
1	B	19	LEU	CA-C-N	-5.03	113.15	120.29
1	B	19	LEU	C-N-CA	-5.03	113.15	120.29
1	A	29	PHE	CA-CB-CG	-5.03	108.77	113.80
1	A	129	ASP	CA-CB-CG	5.01	117.61	112.60
1	C	87	ARG	CA-CB-CG	-5.01	104.07	114.10
1	C	65	LEU	CA-C-O	5.01	125.21	119.35
1	J	55	ALA	CA-C-N	-5.01	113.57	120.28
1	J	55	ALA	C-N-CA	-5.01	113.57	120.28
1	E	16	ASP	O-C-N	5.01	127.43	122.12
1	A	113	HIS	N-CA-C	-5.01	105.90	111.36

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	C	36	THR	CB

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	68	ASP	Mainchain
1	B	7	ASN	Mainchain
1	J	132	LYS	Mainchain
1	J	7	ASN	Mainchain

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1234	0	1301	19	0
1	B	1226	0	1294	22	0
1	C	1223	0	1288	40	0
1	D	1212	0	1276	28	0
1	E	1221	0	1275	35	0
1	F	1214	0	1273	21	0
1	G	1214	0	1268	37	0
1	H	1215	0	1268	43	0
1	I	1210	0	1271	23	0
1	J	1214	0	1273	17	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
3	A	15	0	0	6	0
3	B	10	0	0	1	0
3	C	5	0	0	0	0
3	D	15	0	0	2	0
3	E	15	0	0	2	0
3	F	10	0	0	1	0
3	G	10	0	0	0	0
3	H	15	0	0	2	0
3	I	10	0	0	0	0
3	J	15	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	197	0	0	1	0
4	B	210	0	0	4	0
4	C	197	0	0	4	0
4	D	187	0	0	5	0
4	E	180	0	0	2	0
4	F	161	0	0	1	0
4	G	182	0	0	1	0
4	H	179	0	0	4	0
4	I	181	0	0	5	0
4	J	191	0	0	2	0
All	All	14178	0	12787	251	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 10.

All (251) 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:128[B]:LEU:CD1	1:G:128[B]:LEU:HD22	1.29	1.59
1:H:128[B]:LEU:CG	1:H:128[B]:LEU:CD1	2.00	1.39
1:G:128[B]:LEU:CD1	1:G:128[B]:LEU:CD2	1.99	1.38
1:G:128[B]:LEU:CD1	1:G:128[B]:LEU:CG	2.03	1.36
1:H:128[B]:LEU:CB	1:H:128[B]:LEU:CD2	2.06	1.33
1:H:128[B]:LEU:CB	1:H:128[B]:LEU:CG	2.15	1.22
3:A:1159[A]:SO4:S	3:A:1159[A]:SO4:O3	1.99	1.19
1:H:1:MSE:HE3	1:H:2:ILE:HG22	1.16	1.13
1:D:2:ILE:HD11	1:D:78[A]:ILE:HD11	1.31	1.12
1:C:2:ILE:HD11	1:C:78[A]:ILE:HD11	1.32	1.11
1:I:1:MSE:HE2	1:I:2:ILE:HG22	1.26	1.11
1:G:128[B]:LEU:HD22	1:G:128[B]:LEU:HD11	1.16	1.08
1:B:2:ILE:HD11	1:B:78[A]:ILE:HD11	1.35	1.08
1:G:2:ILE:HD11	1:G:78[A]:ILE:HD11	1.34	1.07
1:E:2:ILE:HD11	1:E:78[A]:ILE:HD11	1.36	1.07
1:J:2:ILE:HD11	1:J:78[A]:ILE:HD11	1.35	1.06
1:F:2:ILE:HD11	1:F:78[A]:ILE:HD11	1.37	1.05
3:A:1159[A]:SO4:O3	3:A:1159[A]:SO4:O4	1.74	1.04
1:I:2:ILE:HD11	1:I:78:ILE:HD11	1.37	1.03
1:H:2:ILE:HD11	1:H:78[A]:ILE:HD11	1.39	1.02
1:A:2:ILE:HD11	1:A:78[B]:ILE:HD11	1.44	0.99
1:G:1:MSE:HE2	1:G:2:ILE:HG22	1.44	0.98
1:B:1:MSE:HE2	1:B:2:ILE:HG22	1.48	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:25:LYS:HE2	4:J:2045:HOH:O	1.67	0.95
1:H:128[B]:LEU:CB	1:H:128[B]:LEU:HD22	1.95	0.95
1:H:128[B]:LEU:CB	1:H:128[B]:LEU:HD23	1.94	0.94
1:E:27[B]:LEU:HD23	1:E:31[B]:GLU:CD	1.93	0.92
1:C:128[B]:LEU:HD21	1:H:108:LEU:HD21	1.49	0.92
1:A:1:MSE:HE2	1:A:2:ILE:HG22	1.52	0.92
1:A:128[B]:LEU:CD2	1:A:128[B]:LEU:HG	1.99	0.92
1:H:1:MSE:CE	1:H:2:ILE:HG22	1.97	0.91
1:H:128[B]:LEU:CD2	1:H:128[B]:LEU:HB3	2.01	0.91
1:C:27[A]:LEU:HD12	1:C:31:GLU:CD	1.96	0.91
1:B:1:MSE:CE	1:B:2:ILE:HG22	2.04	0.88
1:E:27[B]:LEU:HD22	1:E:31[B]:GLU:HG3	1.56	0.86
3:A:1159[A]:SO4:O4	3:A:1159[A]:SO4:O2	1.95	0.85
1:A:1:MSE:CE	1:A:2:ILE:HG22	2.09	0.82
1:E:114:GLU:HG3	1:F:1:MSE:HE1	1.62	0.81
1:B:114:GLU:HG3	1:D:1:MSE:HE1	1.63	0.80
1:J:1:MSE:HE3	1:J:2:ILE:HG22	1.62	0.80
3:A:1159[A]:SO4:S	3:A:1159[A]:SO4:O4	0.39	0.79
1:G:1:MSE:HE3	4:G:2003:HOH:O	1.84	0.78
1:G:1:MSE:CE	1:G:2:ILE:HG22	2.13	0.78
1:H:128[B]:LEU:CD1	1:H:128[B]:LEU:CD2	2.63	0.77
1:C:1:MSE:HE3	1:I:114:GLU:HG3	1.68	0.76
1:G:128[B]:LEU:CD1	1:G:128[B]:LEU:CB	2.64	0.75
1:A:128[B]:LEU:CD2	1:A:128[B]:LEU:CG	2.65	0.74
1:G:2:ILE:CD1	1:G:78[A]:ILE:HD11	2.15	0.74
1:B:1:MSE:HE3	4:B:2004:HOH:O	1.86	0.74
1:D:133[A]:VAL:HG11	4:D:2078:HOH:O	1.89	0.72
1:E:27[B]:LEU:CD2	1:E:31[B]:GLU:HG3	2.19	0.72
1:D:1:MSE:SE	4:F:2019:HOH:O	2.56	0.72
3:A:1159[A]:SO4:O3	3:A:1159[A]:SO4:O1	2.08	0.72
1:D:2:ILE:HD11	1:D:78[A]:ILE:CD1	2.16	0.71
1:B:2:ILE:HD11	1:B:78[A]:ILE:CD1	2.17	0.71
1:I:25:LYS:CB	1:I:27[B]:LEU:HD13	2.20	0.71
1:J:1:MSE:CE	1:J:2:ILE:HG22	2.21	0.69
1:D:25:LYS:HB3	1:D:27[A]:LEU:HD13	1.75	0.69
1:F:1:MSE:HE3	1:F:2:ILE:HG22	1.75	0.69
1:E:27[B]:LEU:HD23	1:E:31[B]:GLU:OE1	1.94	0.67
1:J:151:LEU:HD23	4:J:2177:HOH:O	1.96	0.66
1:E:36:THR:CG2	1:E:38:LEU:H	2.10	0.65
1:I:77:MSE:SE	4:I:2052:HOH:O	2.65	0.65
3:A:1159[A]:SO4:S	3:A:1159[A]:SO4:O1	1.05	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:128[B]:LEU:HD22	1:H:128[B]:LEU:HB3	1.71	0.64
1:C:128[B]:LEU:CD1	1:C:128[B]:LEU:CD2	2.77	0.63
1:I:60[B]:LEU:HD13	4:I:2090:HOH:O	1.99	0.63
1:C:36:THR:CG2	1:C:38:LEU:H	2.12	0.62
1:D:1:MSE:HE3	1:D:2:ILE:HG22	1.81	0.62
1:F:2:ILE:HD11	1:F:78[A]:ILE:CD1	2.23	0.62
4:D:2030:HOH:O	1:J:1:MSE:SE	2.67	0.61
1:H:60:LEU:HD22	4:H:2060:HOH:O	1.99	0.61
1:J:2:ILE:HD11	1:J:78[A]:ILE:CD1	2.24	0.61
1:C:20:LEU:HG	1:C:24:LYS:HE3	1.82	0.61
1:E:27[B]:LEU:CD2	1:E:31[B]:GLU:CG	2.80	0.60
1:C:1:MSE:CE	1:I:114:GLU:HG3	2.30	0.60
1:E:36:THR:HG23	1:E:38:LEU:H	1.67	0.59
1:I:25:LYS:HB2	1:I:27[B]:LEU:HD13	1.84	0.59
1:C:36:THR:HG23	1:C:38:LEU:H	1.67	0.58
1:H:2:ILE:CD1	1:H:78[A]:ILE:HD11	2.23	0.58
1:I:25:LYS:HB3	1:I:27[B]:LEU:CD1	2.32	0.58
1:F:1:MSE:HE3	1:F:2:ILE:CG2	2.34	0.58
1:B:78[A]:ILE:HD13	1:D:118:ASP:HB2	1.86	0.58
1:C:84:ILE:HD11	1:H:101[B]:LEU:HG	1.85	0.58
1:I:2:ILE:CD1	1:I:78:ILE:HD11	2.25	0.58
1:J:36:THR:CG2	1:J:38:LEU:H	2.17	0.57
1:F:51:GLN:NE2	1:F:81:ARG:HH21	2.02	0.57
1:G:36:THR:HG23	1:G:38:LEU:HB2	1.87	0.57
1:B:78[A]:ILE:HD13	1:D:118:ASP:CB	2.34	0.57
1:C:131:LYS:HD2	4:C:2078:HOH:O	2.04	0.57
1:E:51:GLN:NE2	1:E:81:ARG:HH21	2.04	0.56
1:H:63:ALA:HB3	4:H:2093:HOH:O	2.04	0.56
1:H:128[B]:LEU:CB	1:H:128[B]:LEU:CD1	2.83	0.56
1:I:25:LYS:HB3	1:I:27[B]:LEU:HD13	1.86	0.56
1:E:27[B]:LEU:CD2	1:E:31[B]:GLU:CD	2.74	0.55
1:D:51:GLN:NE2	1:D:81:ARG:HH21	2.05	0.55
1:G:36:THR:CG2	1:G:38:LEU:H	2.20	0.55
1:B:24:LYS:HE2	1:E:70:ASP:OD1	2.06	0.55
1:D:1:MSE:HE3	1:D:2:ILE:CG2	2.37	0.55
1:G:36:THR:HG21	1:G:43:VAL:HG21	1.89	0.55
1:H:128[B]:LEU:HD23	1:H:128[B]:LEU:HB3	1.72	0.55
1:E:87:ARG:NH1	1:F:87:ARG:NH1	2.55	0.55
1:H:128[B]:LEU:CD1	1:H:128[B]:LEU:HD22	2.37	0.54
1:H:28:SER:OG	1:H:31[A]:GLU:HG3	2.07	0.54
1:H:1:MSE:HE3	1:H:2:ILE:CG2	2.11	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:36:THR:HG23	1:J:38:LEU:H	1.73	0.54
1:C:1:MSE:HE1	4:I:2138:HOH:O	2.08	0.54
1:B:114:GLU:HG3	1:D:1:MSE:CE	2.35	0.54
1:G:114:GLU:HG3	1:H:1:MSE:CE	2.38	0.54
1:C:1:MSE:HE3	1:I:114:GLU:CG	2.37	0.53
1:C:128[B]:LEU:HD21	1:H:108:LEU:CD2	2.33	0.53
1:B:1:MSE:HE3	1:B:2:ILE:HG22	1.88	0.53
1:B:20:LEU:HG	1:B:24:LYS:HE3	1.91	0.53
1:B:131[A]:LYS:HD2	4:B:2185:HOH:O	2.09	0.53
1:C:24:LYS:HE2	1:G:70:ASP:OD1	2.10	0.52
1:G:33:ALA:O	1:G:36:THR:HB	2.10	0.52
1:F:1:MSE:CE	1:F:2:ILE:HG22	2.39	0.52
1:C:2:ILE:CD1	1:C:78[A]:ILE:HD11	2.21	0.52
1:E:114:GLU:HG3	1:F:1:MSE:CE	2.38	0.52
1:C:128[B]:LEU:CD2	1:C:128[B]:LEU:HD13	2.40	0.51
1:E:33:ALA:O	1:E:36:THR:HB	2.10	0.51
1:I:2:ILE:HD11	1:I:78:ILE:CD1	2.27	0.51
1:B:69:GLU:HG3	4:B:2131:HOH:O	2.09	0.51
1:I:20:LEU:HG	1:I:24:LYS:HE3	1.92	0.51
1:E:27[B]:LEU:HD23	1:E:31[B]:GLU:CG	2.41	0.51
1:E:128[A]:LEU:HD21	1:G:104:TYR:CD1	2.44	0.51
1:A:2:ILE:HD11	1:A:78[B]:ILE:CD1	2.31	0.51
1:J:87:ARG:NH1	3:J:1159:SO4:O2	2.43	0.51
1:G:51:GLN:NE2	1:G:81:ARG:HH21	2.08	0.51
1:C:51:GLN:NE2	1:C:81:ARG:HH21	2.09	0.51
1:E:88:ILE:HD12	1:E:98:TYR:CZ	2.46	0.51
1:G:128[B]:LEU:CD1	1:G:128[B]:LEU:HB3	2.41	0.51
1:C:60[A]:LEU:HD12	4:C:2101:HOH:O	2.11	0.50
1:H:36:THR:CG2	1:H:38:LEU:H	2.25	0.50
1:B:77:MSE:HG2	4:B:2137:HOH:O	2.11	0.50
1:E:128[B]:LEU:HD12	1:E:146:LEU:HD23	1.94	0.50
1:D:25:LYS:HE2	4:D:2046:HOH:O	2.11	0.50
1:B:1:MSE:HE2	1:B:2:ILE:CG2	2.33	0.50
1:D:1:MSE:CE	1:D:2:ILE:HG22	2.41	0.50
1:E:2:ILE:HD11	1:E:78[A]:ILE:CD1	2.26	0.50
1:H:51:GLN:NE2	1:H:81:ARG:HH21	2.09	0.50
1:D:25:LYS:CB	1:D:27[A]:LEU:HD13	2.40	0.49
1:I:84:ILE:HD11	1:J:101[B]:LEU:HG	1.94	0.49
1:F:35:GLY:N	3:F:1159:SO4:O4	2.35	0.49
1:D:27[A]:LEU:HD12	4:D:2055:HOH:O	2.10	0.49
1:C:88[A]:ILE:HD12	1:C:98:TYR:CZ	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:2138:HOH:O	1:F:151:LEU:HD13	2.13	0.48
1:E:104:TYR:HB3	1:G:128[B]:LEU:HD11	1.94	0.48
1:I:152:PRO:HG2	1:I:154:LYS:HE2	1.95	0.48
1:F:128[B]:LEU:HG	1:F:129:ASP:N	2.29	0.48
1:G:36:THR:HG22	1:G:38:LEU:H	1.79	0.48
1:C:87:ARG:NH1	3:H:1159:SO4:O2	2.46	0.48
1:A:104:TYR:CD1	1:D:128[A]:LEU:HD21	2.49	0.48
1:B:51:GLN:NE2	1:B:81:ARG:HH21	2.12	0.47
1:C:128[B]:LEU:CD2	1:C:128[B]:LEU:CG	2.92	0.47
1:I:1:MSE:CE	1:I:2:ILE:H	2.27	0.47
1:H:5:GLN:HG3	4:H:2026:HOH:O	2.15	0.47
1:I:64:LYS:HE2	4:I:2064:HOH:O	2.14	0.47
1:A:133[A]:VAL:CG2	1:A:141:ARG:HB2	2.44	0.47
1:E:27[B]:LEU:CD2	1:E:31[B]:GLU:OE1	2.61	0.47
1:A:70:ASP:OD1	1:I:24:LYS:HE2	2.15	0.47
1:E:36:THR:HG22	1:E:38:LEU:H	1.80	0.47
1:A:51:GLN:NE2	1:A:81:ARG:HH21	2.13	0.47
1:A:104:TYR:CG	1:D:128[A]:LEU:HD21	2.50	0.47
1:D:97:PHE:CE1	1:D:144:ILE:HD13	2.49	0.47
1:I:51:GLN:NE2	1:I:81:ARG:HH21	2.12	0.47
1:C:128[B]:LEU:HD21	1:H:108:LEU:HD11	1.95	0.47
1:A:77:MSE:HG2	4:A:2112:HOH:O	2.14	0.46
1:E:87:ARG:HD2	3:E:1159:SO4:O3	2.16	0.46
1:J:51:GLN:NE2	1:J:81:ARG:HH21	2.13	0.46
3:E:1159:SO4:O4	1:G:87:ARG:NH1	2.47	0.46
1:G:114:GLU:HG3	1:H:1:MSE:HE1	1.98	0.46
1:B:78[A]:ILE:CD1	1:D:118:ASP:HB2	2.46	0.45
1:D:97:PHE:HE1	1:D:144:ILE:HD13	1.82	0.45
1:H:128[B]:LEU:HD22	1:H:128[B]:LEU:HD13	1.98	0.45
1:A:80:LEU:HD13	1:A:80:LEU:C	2.41	0.45
1:C:101[B]:LEU:HG	1:H:84:ILE:HD11	1.96	0.45
1:E:36:THR:HG21	1:E:43:VAL:HG21	1.98	0.45
1:C:120:ILE:HD11	1:C:151:LEU:HD12	1.98	0.45
1:J:36:THR:HG21	1:J:43:VAL:HG21	1.97	0.45
1:E:25:LYS:HB3	1:E:27[A]:LEU:HD13	1.98	0.45
1:A:84:ILE:HD11	1:D:101[B]:LEU:HG	1.99	0.45
1:G:87:ARG:NH1	1:H:87:ARG:NH1	2.65	0.45
1:F:88:ILE:HD12	1:F:98:TYR:CZ	2.52	0.45
1:D:87:ARG:NH1	3:D:1159:SO4:O4	2.49	0.45
1:H:87:ARG:NH1	3:H:1159:SO4:O3	2.50	0.45
1:C:36:THR:HG21	1:C:43:VAL:HG21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:77:MSE:HB3	1:F:77:MSE:HE2	1.80	0.44
1:J:77:MSE:HB3	1:J:77:MSE:HE2	1.71	0.44
1:H:36:THR:HG21	1:H:43:VAL:HG21	2.00	0.44
1:C:25:LYS:HB2	1:C:27[A]:LEU:HD22	1.98	0.44
1:I:80:LEU:HD13	1:I:80:LEU:C	2.43	0.44
1:C:25:LYS:CB	1:C:27[A]:LEU:HD22	2.47	0.44
1:E:151:LEU:HD23	4:E:2170:HOH:O	2.18	0.43
1:I:60[B]:LEU:HD11	4:I:2042:HOH:O	2.17	0.43
1:G:80:LEU:C	1:G:80:LEU:HD13	2.43	0.43
1:A:87:ARG:NH1	1:J:87:ARG:NH1	2.66	0.43
1:F:127:LYS:HE3	1:F:127:LYS:HB2	1.91	0.43
1:A:133[A]:VAL:HG23	1:A:141:ARG:HB2	2.01	0.43
1:A:1:MSE:HE3	1:A:2:ILE:HG22	1.94	0.43
1:C:88[B]:ILE:HD11	1:H:87:ARG:HD3	2.01	0.43
1:E:29:PHE:CE2	1:G:110:ALA:HB1	2.54	0.43
1:G:88:ILE:HD12	1:G:98:TYR:CZ	2.54	0.43
1:D:77:MSE:HG2	4:D:2108:HOH:O	2.18	0.43
1:F:128[B]:LEU:HD12	1:F:146:LEU:HD23	2.01	0.43
1:D:37:GLY:N	3:D:1160:SO4:O3	2.41	0.42
1:F:6:ILE:HD13	1:G:48:LEU:HD22	2.02	0.42
1:J:3:GLN:HB3	1:J:77:MSE:HE3	2.00	0.42
1:C:102:GLN:HE22	1:H:84:ILE:H	1.66	0.42
1:D:3:GLN:HB3	1:D:77:MSE:HE3	2.01	0.42
1:G:78[A]:ILE:HD12	1:H:113:HIS:HB3	2.01	0.42
1:H:151:LEU:HD11	4:H:2137:HOH:O	2.20	0.42
1:A:77:MSE:HE2	1:A:77:MSE:HB3	1.56	0.42
1:G:77:MSE:HB3	1:G:77:MSE:HE2	1.45	0.42
1:C:151:LEU:HD11	4:C:2160:HOH:O	2.20	0.42
1:C:77:MSE:HE2	1:C:77:MSE:HB3	1.69	0.42
1:E:77:MSE:HE2	1:E:77:MSE:HB3	1.58	0.42
1:B:108:LEU:HD21	1:F:128[B]:LEU:HD11	2.02	0.42
1:E:78[A]:ILE:HD12	1:F:113:HIS:HB3	2.02	0.42
1:F:25:LYS:HB2	1:F:27:LEU:HD22	2.01	0.41
1:D:77:MSE:HE2	1:D:77:MSE:HB3	1.71	0.41
1:E:101[B]:LEU:HG	1:G:84:ILE:HD11	2.02	0.41
1:C:36:THR:HG22	1:C:38:LEU:H	1.83	0.41
1:C:77:MSE:HG2	4:C:2123:HOH:O	2.21	0.41
1:E:28:SER:H	1:E:31[B]:GLU:HG2	1.84	0.41
1:E:104:TYR:HB3	1:G:128[B]:LEU:CD1	2.51	0.41
1:J:88:ILE:HD12	1:J:98:TYR:CZ	2.56	0.41
3:B:1159:SO4:O4	1:F:87:ARG:NH1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:128[B]:LEU:CD2	1:G:128[B]:LEU:HD11	2.06	0.41
1:H:36:THR:HG22	1:H:38:LEU:H	1.85	0.41
1:G:36:THR:HG23	1:G:38:LEU:H	1.85	0.40
1:C:78[A]:ILE:HD12	1:I:113:HIS:HB3	2.04	0.40
1:D:88:ILE:HD12	1:D:98:TYR:CZ	2.57	0.40
1:B:3:GLN:HB3	1:B:77:MSE:HE3	2.03	0.40
1:E:104:TYR:CB	1:G:128[B]:LEU:CD1	2.98	0.40
1:B:88:ILE:HD12	1:B:98:TYR:CZ	2.56	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	165/156 (106%)	162 (98%)	3 (2%)	0	100	100
1	B	162/156 (104%)	159 (98%)	3 (2%)	0	100	100
1	C	162/156 (104%)	159 (98%)	3 (2%)	0	100	100
1	D	159/156 (102%)	156 (98%)	3 (2%)	0	100	100
1	E	161/156 (103%)	158 (98%)	3 (2%)	0	100	100
1	F	159/156 (102%)	156 (98%)	3 (2%)	0	100	100
1	G	160/156 (103%)	157 (98%)	3 (2%)	0	100	100
1	H	159/156 (102%)	156 (98%)	3 (2%)	0	100	100
1	I	158/156 (101%)	155 (98%)	3 (2%)	0	100	100
1	J	159/156 (102%)	156 (98%)	3 (2%)	0	100	100
All	All	1604/1560 (103%)	1574 (98%)	30 (2%)	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	138/123 (112%)	136 (99%)	2 (1%)	59	39
1	B	135/123 (110%)	129 (96%)	6 (4%)	25	6
1	C	135/123 (110%)	128 (95%)	7 (5%)	21	4
1	D	132/123 (107%)	130 (98%)	2 (2%)	57	37
1	E	134/123 (109%)	127 (95%)	7 (5%)	21	4
1	F	132/123 (107%)	128 (97%)	4 (3%)	36	13
1	G	133/123 (108%)	129 (97%)	4 (3%)	36	13
1	H	132/123 (107%)	127 (96%)	5 (4%)	29	7
1	I	131/123 (106%)	126 (96%)	5 (4%)	29	7
1	J	132/123 (107%)	126 (96%)	6 (4%)	24	5
All	All	1334/1230 (108%)	1286 (96%)	48 (4%)	37	9

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	80	LEU
1	A	102	GLN
1	B	78[A]	ILE
1	B	78[B]	ILE
1	B	80	LEU
1	B	102	GLN
1	B	128[A]	LEU
1	B	128[B]	LEU
1	C	27[A]	LEU
1	C	27[B]	LEU
1	C	36	THR
1	C	80	LEU
1	C	102	GLN
1	C	128[A]	LEU
1	C	128[B]	LEU
1	D	102	GLN

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Mol	Chain	Res	Type
1	D	137	GLU
1	E	27[A]	LEU
1	E	27[B]	LEU
1	E	36	THR
1	E	80	LEU
1	E	102	GLN
1	E	128[A]	LEU
1	E	128[B]	LEU
1	F	27	LEU
1	F	102	GLN
1	F	128[A]	LEU
1	F	128[B]	LEU
1	G	36	THR
1	G	102	GLN
1	G	128[A]	LEU
1	G	128[B]	LEU
1	H	27	LEU
1	H	36	THR
1	H	102	GLN
1	H	128[A]	LEU
1	H	128[B]	LEU
1	I	1	MSE
1	I	80	LEU
1	I	102	GLN
1	I	128[A]	LEU
1	I	128[B]	LEU
1	J	36	THR
1	J	80	LEU
1	J	102	GLN
1	J	127	LYS
1	J	128[A]	LEU
1	J	128[B]	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	51	GLN
1	A	102	GLN
1	B	51	GLN
1	B	102	GLN
1	C	51	GLN

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Mol	Chain	Res	Type
1	C	102	GLN
1	D	51	GLN
1	D	102	GLN
1	E	51	GLN
1	E	102	GLN
1	F	51	GLN
1	F	102	GLN
1	G	51	GLN
1	G	102	GLN
1	H	51	GLN
1	H	102	GLN
1	I	51	GLN
1	I	102	GLN
1	J	51	GLN
1	J	102	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](#)

Of 34 ligands modelled in this entry, 10 are monoatomic - leaving 24 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
3	SO4	I	1158	-	4,4,4	0.64	0	6,6,6	0.63	0
3	SO4	I	1159	-	4,4,4	0.64	0	6,6,6	0.50	0
3	SO4	A	1159[B]	-	4,4,4	0.63	0	6,6,6	0.79	0
3	SO4	F	1158	-	4,4,4	0.72	0	6,6,6	0.40	0
3	SO4	D	1158	-	4,4,4	0.68	0	6,6,6	0.47	0
3	SO4	C	1158	-	4,4,4	0.63	0	6,6,6	0.44	0
3	SO4	D	1159	-	4,4,4	0.55	0	6,6,6	1.19	1 (16%)
3	SO4	B	1158	-	4,4,4	0.68	0	6,6,6	0.44	0
3	SO4	E	1158	-	4,4,4	0.66	0	6,6,6	0.37	0
3	SO4	H	1158	-	4,4,4	0.74	0	6,6,6	0.39	0
3	SO4	J	1159	-	4,4,4	0.63	0	6,6,6	0.81	0
3	SO4	G	1158	-	4,4,4	0.72	0	6,6,6	0.47	0
3	SO4	B	1159	-	4,4,4	0.52	0	6,6,6	1.11	0
3	SO4	J	1160	-	4,4,4	0.62	0	6,6,6	0.56	0
3	SO4	H	1160	-	4,4,4	0.65	0	6,6,6	0.30	0
3	SO4	A	1159[A]	-	4,4,4	8.15	4 (100%)	6,6,6	7.92	4 (66%)
3	SO4	D	1160	-	4,4,4	0.68	0	6,6,6	0.40	0
3	SO4	E	1160	-	4,4,4	0.64	0	6,6,6	0.37	0
3	SO4	A	1158	-	4,4,4	0.63	0	6,6,6	0.73	0
3	SO4	E	1159	-	4,4,4	0.82	0	6,6,6	1.04	0
3	SO4	H	1159	-	4,4,4	0.64	0	6,6,6	0.89	0
3	SO4	J	1158	-	4,4,4	0.70	0	6,6,6	0.93	0
3	SO4	G	1159	-	4,4,4	0.61	0	6,6,6	0.35	0
3	SO4	F	1159	-	4,4,4	0.64	0	6,6,6	0.56	0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1159[A]	SO4	O4-S	-13.21	0.39	1.48
3	A	1159[A]	SO4	O1-S	-6.66	1.05	1.44
3	A	1159[A]	SO4	O3-S	6.29	1.99	1.48
3	A	1159[A]	SO4	O2-S	2.70	1.60	1.44

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1159[A]	SO4	O4-S-O1	-12.65	43.45	109.56
3	A	1159[A]	SO4	O4-S-O3	-11.37	45.86	108.54
3	A	1159[A]	SO4	O4-S-O2	7.20	147.21	109.56
3	A	1159[A]	SO4	O3-S-O1	-5.72	79.64	109.56
3	D	1159	SO4	O3-S-O2	2.06	120.33	109.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1159	SO4	1	0
3	J	1159	SO4	1	0
3	B	1159	SO4	1	0
3	A	1159[A]	SO4	6	0
3	D	1160	SO4	1	0
3	E	1159	SO4	2	0
3	H	1159	SO4	2	0
3	F	1159	SO4	1	0

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	152/156 (97%)	-0.53	0 100 100	7, 14, 24, 42	10 (6%)
1	B	152/156 (97%)	-0.55	0 100 100	8, 13, 24, 45	8 (5%)
1	C	152/156 (97%)	-0.56	0 100 100	7, 13, 25, 41	8 (5%)
1	D	152/156 (97%)	-0.54	1 (0%) 84 89	8, 14, 25, 37	5 (3%)
1	E	152/156 (97%)	-0.53	1 (0%) 84 89	8, 14, 23, 31	7 (4%)
1	F	152/156 (97%)	-0.40	1 (0%) 84 89	8, 15, 26, 35	5 (3%)
1	G	152/156 (97%)	-0.48	0 100 100	8, 15, 25, 43	5 (3%)
1	H	152/156 (97%)	-0.16	9 (5%) 28 32	8, 16, 33, 41	5 (3%)
1	I	152/156 (97%)	-0.46	0 100 100	8, 15, 28, 41	4 (2%)
1	J	152/156 (97%)	-0.52	0 100 100	8, 14, 23, 44	5 (3%)
All	All	1520/1560 (97%)	-0.47	12 (0%) 82 87	7, 14, 26, 45	62 (4%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	63	ALA	4.1
1	H	66	ASP	3.7
1	H	62	GLY	3.6
1	H	60	LEU	3.6
1	F	34	ASP	3.0
1	H	35	GLY	2.9
1	H	61	VAL	2.8
1	D	137	GLU	2.5
1	H	68	ASP	2.3
1	H	56	ASP	2.2
1	E	137	GLU	2.1
1	H	69	GLU	2.1

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	E	1160	5/5	0.79	0.17	55,55,56,57	0
3	SO4	D	1160	5/5	0.86	0.17	55,56,57,57	0
3	SO4	H	1160	5/5	0.86	0.12	58,59,59,60	0
3	SO4	A	1159[B]	5/5	0.88	0.16	28,31,32,32	5
3	SO4	F	1159	5/5	0.88	0.12	57,57,58,58	0
3	SO4	A	1159[A]	5/5	0.88	0.16	16,36,41,46	5
3	SO4	I	1159	5/5	0.89	0.10	56,56,57,58	0
3	SO4	J	1160	5/5	0.90	0.13	51,52,52,53	0
3	SO4	J	1158	5/5	0.93	0.15	39,41,42,43	0
3	SO4	H	1158	5/5	0.93	0.09	51,51,52,52	0
3	SO4	E	1159	5/5	0.94	0.16	33,36,37,38	0
3	SO4	G	1158	5/5	0.95	0.09	42,43,46,47	0
3	SO4	G	1159	5/5	0.95	0.10	42,43,43,44	0
3	SO4	E	1158	5/5	0.95	0.15	41,42,44,44	0
3	SO4	H	1159	5/5	0.95	0.15	34,39,40,40	0
3	SO4	B	1159	5/5	0.95	0.13	32,38,39,39	0
3	SO4	D	1159	5/5	0.95	0.14	32,37,38,39	0
3	SO4	F	1158	5/5	0.95	0.08	46,46,48,48	0
3	SO4	B	1158	5/5	0.95	0.10	42,44,45,45	0
3	SO4	I	1158	5/5	0.96	0.12	39,39,42,43	0
3	SO4	A	1158	5/5	0.96	0.10	36,37,40,41	0
3	SO4	C	1158	5/5	0.96	0.08	39,40,41,42	0
3	SO4	J	1159	5/5	0.96	0.17	32,37,38,39	0
3	SO4	D	1158	5/5	0.96	0.12	34,36,38,39	0
2	CL	A	1157	1/1	0.99	0.05	16,16,16,16	0
2	CL	B	1157	1/1	0.99	0.07	15,15,15,15	0
2	CL	C	1157	1/1	0.99	0.04	14,14,14,14	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CL	E	1157	1/1	0.99	0.05	17,17,17,17	0
2	CL	F	1157	1/1	0.99	0.05	17,17,17,17	0
2	CL	G	1157	1/1	0.99	0.07	15,15,15,15	0
2	CL	I	1157	1/1	0.99	0.05	15,15,15,15	0
2	CL	J	1157	1/1	0.99	0.05	15,15,15,15	0
2	CL	D	1157	1/1	1.00	0.03	15,15,15,15	0
2	CL	H	1157	1/1	1.00	0.05	15,15,15,15	0

6.5 Other polymers [i](#)

There are no such residues in this entry.