Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 05:01 PM EDT

PDB ID	:	1DW9
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.

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 (i) 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 (i)) were used in the production of this report:

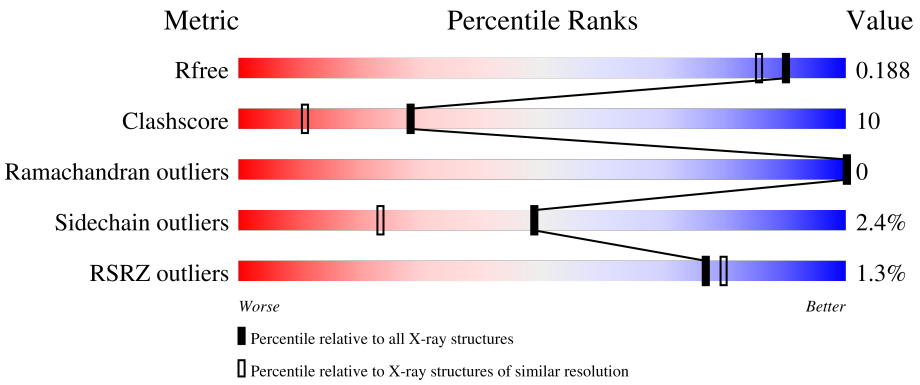
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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}	130704	1827 (1.66-1.66)
Clashscore	141614	1931 (1.66-1.66)
Ramachandran outliers	138981	1891 (1.66-1.66)
Sidechain outliers	138945	1891 (1.66-1.66)
RSRZ outliers	127900	1791 (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 <=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	2% 82% 15% •
1	B	156	% 79% 19% •
1	C	156	% 77% 19% • •
1	D	156	79% 19% • •
1	E	156	76% 20% • •

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Mol	Chain	Length	Quality of chain
1	F	156	81% 17%
1	G	156	82% 14%
1	H	156	4% 78% 17%
1	I	156	83% 16%
1	J	156	2% 79% 17%

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

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

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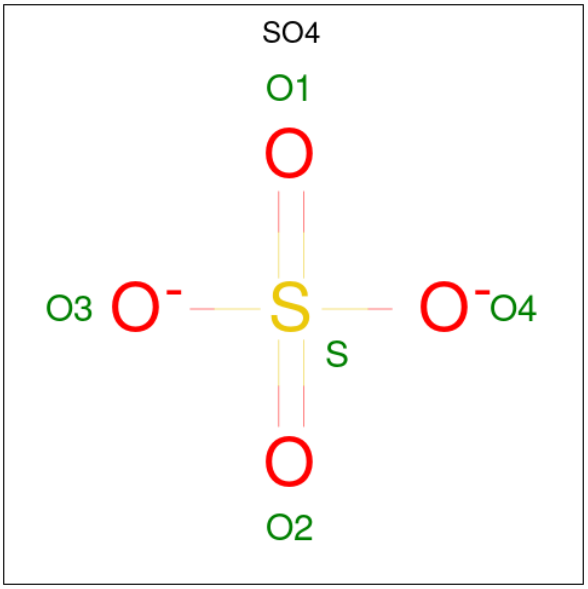
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
2	E	1	1	1	0	0
2	F	1	1	1	0	0
2	G	1	1	1	0	0
2	H	1	1	1	0	0
2	I	1	1	1	0	0
2	J	1	1	1	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
3	A	1	5	4	1	0	0
3	A	1	10	8	2	0	1
3	B	1	5	4	1	0	0
3	B	1	5	4	1	0	0
3	C	1	5	4	1	0	0

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

- Molecule 4 is water.

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

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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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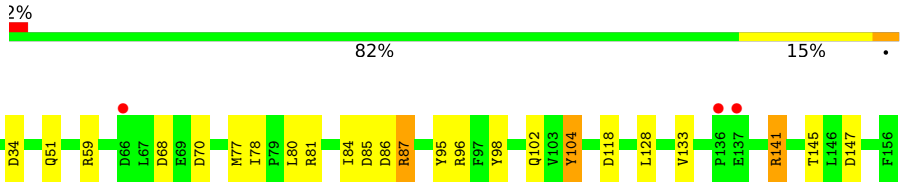
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	I	2	Total O 2 2	0	0
4	J	188	Total O 188 188	0	0
4	J	3	Total O 3 3	0	0

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.

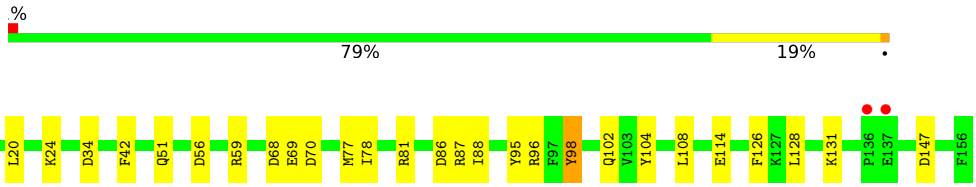
• Molecule 1: CYANATE LYASE

Chain A:



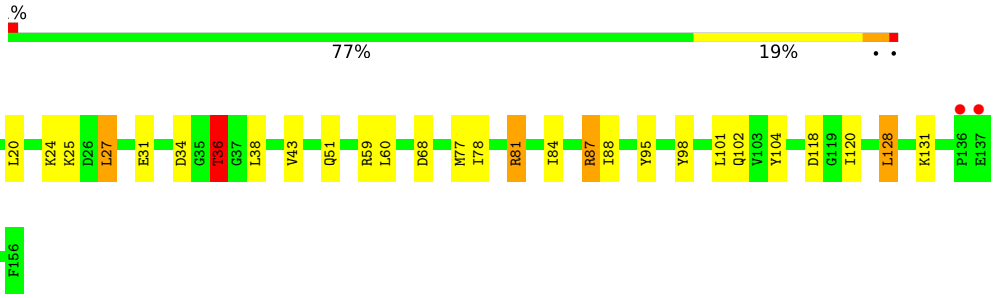
• Molecule 1: CYANATE LYASE

Chain B:



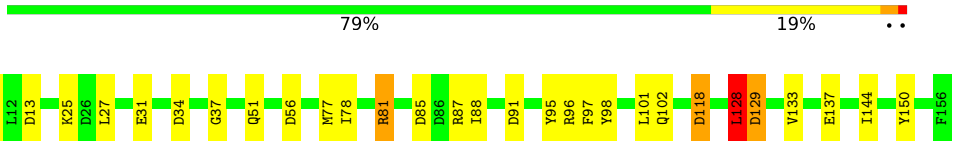
• Molecule 1: CYANATE LYASE

Chain C:



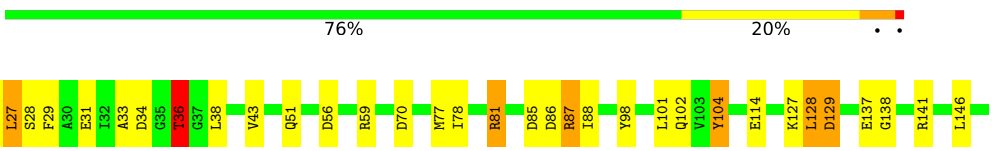
• Molecule 1: CYANATE LYASE

Chain D:



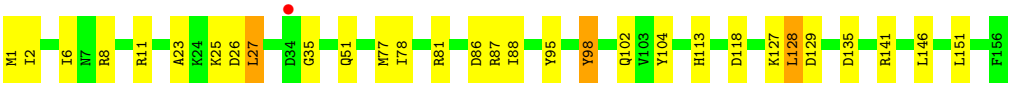
• Molecule 1: CYANATE LYASE

Chain E:



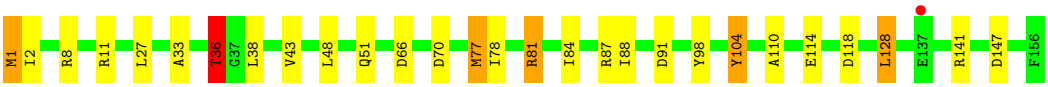
• Molecule 1: CYANATE LYASE

Chain F:



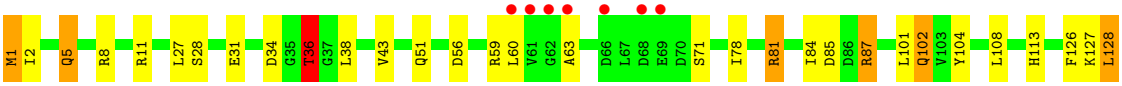
• Molecule 1: CYANATE LYASE

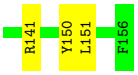
Chain G:



• Molecule 1: CYANATE LYASE

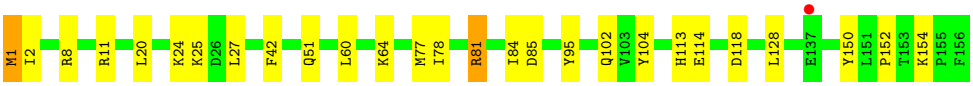
Chain H:





• Molecule 1: CYANATE LYASE

Chain I:



• Molecule 1: CYANATE LYASE

Chain J:

4 Data and refinement statistics (i)

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 20.58 – 1.65	Depositor EDS
% Data completeness (in resolution range)	94.2 (20.00-1.65) 94.0 (20.58-1.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$< I/\sigma(I) >$ [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 , 58.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.84	1/1301 (0.1%)	1.65	23/1754 (1.3%)
1	B	0.88	1/1276 (0.1%)	1.62	23/1721 (1.3%)
1	C	0.84	2/1277 (0.2%)	1.57	19/1723 (1.1%)
1	D	0.87	0/1250	1.63	21/1687 (1.2%)
1	E	0.86	0/1269	1.61	23/1712 (1.3%)
1	F	0.85	0/1252	1.58	15/1689 (0.9%)
1	G	0.84	1/1260 (0.1%)	1.63	18/1699 (1.1%)
1	H	0.89	0/1253	1.76	26/1690 (1.5%)
1	I	0.81	1/1243 (0.1%)	1.44	12/1676 (0.7%)
1	J	0.87	1/1252 (0.1%)	1.60	24/1689 (1.4%)
All	All	0.86	7/12633 (0.1%)	1.61	204/17040 (1.2%)

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 (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	1	MSE	SE-CE	-9.52	1.39	1.95
1	B	1	MSE	CG-SE	-6.96	1.71	1.95
1	C	1	MSE	CG-SE	-6.76	1.72	1.95
1	A	1	MSE	CG-SE	-6.52	1.73	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	1	MSE	CG-SE	-6.30	1.74	1.95
1	I	1	MSE	CG-SE	-5.95	1.75	1.95
1	C	1	MSE	SE-CE	-5.04	1.65	1.95

All (204) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	1	MSE	CG-SE-CE	18.51	139.62	98.90
1	H	11	ARG	NE-CZ-NH1	17.26	128.93	120.30
1	B	1	MSE	CG-SE-CE	15.09	132.09	98.90
1	G	81	ARG	NE-CZ-NH1	15.06	127.83	120.30
1	G	8	ARG	NE-CZ-NH2	-14.81	112.90	120.30
1	G	1	MSE	CG-SE-CE	14.22	130.18	98.90
1	F	8	ARG	NE-CZ-NH1	13.05	126.83	120.30
1	A	96	ARG	NE-CZ-NH2	-12.77	113.92	120.30
1	H	141	ARG	NE-CZ-NH1	12.28	126.44	120.30
1	A	8	ARG	NE-CZ-NH1	12.05	126.33	120.30
1	A	1	MSE	CG-SE-CE	11.87	125.02	98.90
1	F	8	ARG	NE-CZ-NH2	-11.80	114.40	120.30
1	J	1	MSE	CG-SE-CE	11.68	124.60	98.90
1	E	81	ARG	NE-CZ-NH1	11.37	125.98	120.30
1	E	104	TYR	CB-CG-CD1	-11.32	114.21	121.00
1	H	59	ARG	NE-CZ-NH1	11.14	125.87	120.30
1	G	81	ARG	NE-CZ-NH2	-11.00	114.80	120.30
1	F	141	ARG	NE-CZ-NH1	10.97	125.79	120.30
1	D	81	ARG	NE-CZ-NH2	-10.74	114.93	120.30
1	A	141	ARG	NE-CZ-NH2	-10.70	114.95	120.30
1	E	81	ARG	NE-CZ-NH2	-10.63	114.98	120.30
1	D	129	ASP	CB-CG-OD1	-10.58	108.78	118.30
1	B	126	PHE	CB-CG-CD1	-10.32	113.58	120.80
1	D	11	ARG	NE-CZ-NH2	-10.18	115.21	120.30
1	A	59	ARG	NE-CZ-NH2	-10.06	115.27	120.30
1	I	8	ARG	NE-CZ-NH1	9.98	125.29	120.30
1	H	56	ASP	CB-CG-OD2	-9.91	109.38	118.30
1	J	104	TYR	CB-CG-CD1	-9.59	115.25	121.00
1	H	141	ARG	NE-CZ-NH2	-9.54	115.53	120.30
1	D	11	ARG	NE-CZ-NH1	9.37	124.99	120.30
1	A	34[A]	ASP	CB-CG-OD1	9.19	126.57	118.30
1	A	34[B]	ASP	CB-CG-OD1	9.19	126.57	118.30
1	G	104	TYR	CB-CG-CD1	-9.17	115.50	121.00
1	F	95	TYR	CB-CG-CD1	-9.12	115.53	121.00
1	J	11	ARG	NE-CZ-NH1	9.10	124.85	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	36	THR	N-CA-CB	-9.04	93.13	110.30
1	F	104	TYR	CB-CG-CD1	-8.92	115.65	121.00
1	E	141	ARG	NE-CZ-NH2	-8.83	115.89	120.30
1	J	36	THR	N-CA-CB	-8.82	93.54	110.30
1	I	150	TYR	CB-CG-CD1	8.81	126.29	121.00
1	E	59	ARG	NE-CZ-NH2	-8.77	115.91	120.30
1	B	34	ASP	CB-CG-OD1	-8.76	110.42	118.30
1	E	59	ARG	NE-CZ-NH1	8.75	124.68	120.30
1	G	118	ASP	CB-CG-OD2	-8.75	110.42	118.30
1	J	36	THR	OG1-CB-CG2	8.74	130.11	110.00
1	B	68	ASP	CB-CG-OD1	8.62	126.06	118.30
1	B	42	PHE	CB-CG-CD1	-8.61	114.77	120.80
1	H	85	ASP	CB-CG-OD1	-8.53	110.62	118.30
1	A	8	ARG	NE-CZ-NH2	-8.51	116.04	120.30
1	J	118	ASP	CB-CG-OD2	-8.49	110.66	118.30
1	C	36	THR	N-CA-CB	-8.46	94.23	110.30
1	H	81	ARG	NE-CZ-NH2	-8.41	116.09	120.30
1	G	11	ARG	NE-CZ-NH2	-8.36	116.12	120.30
1	C	104	TYR	CB-CG-CD1	-8.27	116.04	121.00
1	A	95	TYR	CB-CG-CD1	-8.20	116.08	121.00
1	D	150	TYR	CB-CG-CD2	-8.09	116.15	121.00
1	C	36	THR	OG1-CB-CG2	8.05	128.52	110.00
1	H	59	ARG	NE-CZ-NH2	-8.04	116.28	120.30
1	A	141	ARG	NE-CZ-NH1	8.02	124.31	120.30
1	D	150	TYR	CB-CG-CD1	8.01	125.80	121.00
1	E	36	THR	OG1-CB-CG2	7.98	128.34	110.00
1	B	59	ARG	NE-CZ-NH1	7.97	124.29	120.30
1	E	36	THR	N-CA-CB	-7.94	95.22	110.30
1	G	147	ASP	CB-CG-OD1	7.87	125.38	118.30
1	D	128[A]	LEU	N-CA-CB	7.84	126.09	110.40
1	D	128[B]	LEU	N-CA-CB	7.84	126.09	110.40
1	B	96	ARG	NE-CZ-NH2	7.79	124.20	120.30
1	C	81	ARG	NE-CZ-NH2	-7.78	116.41	120.30
1	F	141	ARG	NE-CZ-NH2	-7.75	116.43	120.30
1	J	141	ARG	NE-CZ-NH2	-7.55	116.52	120.30
1	H	81	ARG	NE-CZ-NH1	7.53	124.06	120.30
1	E	56	ASP	CB-CG-OD2	-7.46	111.59	118.30
1	H	36	THR	O-C-N	-7.43	110.56	123.20
1	E	150	TYR	CB-CG-CD1	7.40	125.44	121.00
1	H	104	TYR	CB-CG-CD1	-7.37	116.58	121.00
1	J	81	ARG	NE-CZ-NH1	7.37	123.98	120.30
1	B	59	ARG	NE-CZ-NH2	-7.33	116.64	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	85	ASP	CB-CG-OD1	-7.31	111.72	118.30
1	B	8	ARG	NE-CZ-NH1	7.29	123.95	120.30
1	B	104	TYR	CB-CG-CD1	-7.22	116.67	121.00
1	I	81	ARG	NE-CZ-NH2	-7.22	116.69	120.30
1	D	81	ARG	NE-CZ-NH1	7.21	123.91	120.30
1	G	147	ASP	CB-CG-OD2	-7.18	111.84	118.30
1	B	87	ARG	NE-CZ-NH1	-7.10	116.75	120.30
1	H	150	TYR	CZ-CE2-CD2	6.98	126.08	119.80
1	C	34	ASP	CB-CG-OD2	6.96	124.56	118.30
1	D	31	GLU	OE1-CD-OE2	6.95	131.64	123.30
1	G	36	THR	OG1-CB-CG2	6.94	125.97	110.00
1	C	68	ASP	CB-CG-OD1	6.93	124.54	118.30
1	D	91	ASP	CB-CG-OD2	-6.87	112.11	118.30
1	D	31	GLU	CA-CB-CG	6.85	128.46	113.40
1	E	129	ASP	CB-CG-OD1	-6.84	112.15	118.30
1	C	34	ASP	CB-CG-OD1	-6.80	112.18	118.30
1	E	137	GLU	CB-CG-CD	6.79	132.54	114.20
1	I	104	TYR	CB-CG-CD1	-6.79	116.92	121.00
1	F	95	TYR	CG-CD1-CE1	-6.71	115.94	121.30
1	I	1	MSE	CG-SE-CE	6.68	113.61	98.90
1	G	91	ASP	CB-CG-OD2	-6.66	112.31	118.30
1	B	126	PHE	CB-CG-CD2	6.63	125.44	120.80
1	C	141	ARG	NE-CZ-NH2	-6.62	116.99	120.30
1	H	36	THR	N-CA-CB	-6.58	97.79	110.30
1	H	36	THR	C-N-CA	6.56	136.07	122.30
1	G	11	ARG	NE-CZ-NH1	6.53	123.57	120.30
1	D	118	ASP	CB-CG-OD2	-6.50	112.45	118.30
1	E	8	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	A	11	ARG	NE-CZ-NH2	-6.49	117.06	120.30
1	B	8	ARG	NE-CZ-NH2	-6.48	117.06	120.30
1	J	98	TYR	CG-CD1-CE1	-6.48	116.12	121.30
1	J	56	ASP	CB-CG-OD1	6.46	124.11	118.30
1	B	147	ASP	CB-CG-OD2	-6.44	112.50	118.30
1	J	126	PHE	CB-CG-CD2	-6.41	116.32	120.80
1	H	127	LYS	CA-CB-CG	6.38	127.44	113.40
1	F	135	ASP	CB-CG-OD2	6.37	124.03	118.30
1	F	86	ASP	CB-CG-OD1	6.37	124.03	118.30
1	J	129	ASP	CB-CG-OD1	-6.34	112.60	118.30
1	A	96	ARG	NE-CZ-NH1	6.32	123.46	120.30
1	E	150	TYR	CB-CG-CD2	-6.31	117.22	121.00
1	J	118	ASP	CB-CG-OD1	6.29	123.97	118.30
1	H	11	ARG	NH1-CZ-NH2	-6.25	112.53	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	59	ARG	CD-NE-CZ	6.25	132.34	123.60
1	A	147	ASP	CB-CG-OD1	6.22	123.90	118.30
1	F	98	TYR	CB-CG-CD1	-6.22	117.27	121.00
1	J	81	ARG	NE-CZ-NH2	-6.19	117.21	120.30
1	D	34	ASP	CB-CG-OD1	-6.14	112.77	118.30
1	D	8	ARG	NE-CZ-NH1	6.13	123.37	120.30
1	D	56	ASP	CB-CG-OD1	6.09	123.78	118.30
1	E	87	ARG	CD-NE-CZ	-6.07	115.11	123.60
1	C	59	ARG	NE-CZ-NH2	-6.01	117.30	120.30
1	B	70	ASP	CB-CG-OD1	5.98	123.69	118.30
1	B	86	ASP	CB-CG-OD1	5.95	123.65	118.30
1	J	85	ASP	CB-CG-OD1	-5.94	112.95	118.30
1	D	95	TYR	CB-CG-CD1	-5.92	117.45	121.00
1	J	126	PHE	CB-CG-CD1	5.92	124.94	120.80
1	C	95	TYR	CG-CD1-CE1	-5.90	116.58	121.30
1	H	71	SER	O-C-N	-5.90	113.26	122.70
1	F	23	ALA	O-C-N	5.88	132.11	122.70
1	I	104	TYR	CB-CG-CD2	5.88	124.53	121.00
1	I	11	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	E	85	ASP	CB-CG-OD1	-5.86	113.03	118.30
1	B	87	ARG	CD-NE-CZ	-5.84	115.43	123.60
1	A	95	TYR	CB-CG-CD2	5.83	124.50	121.00
1	H	34	ASP	CB-CG-OD1	-5.82	113.07	118.30
1	C	118	ASP	CB-CG-OD2	-5.79	113.08	118.30
1	G	8	ARG	NE-CZ-NH1	5.79	123.19	120.30
1	B	98	TYR	CZ-CE2-CD2	-5.79	114.59	119.80
1	C	141	ARG	NE-CZ-NH1	5.77	123.18	120.30
1	H	1	MSE	CG-SE-CE	5.75	111.56	98.90
1	C	8	ARG	NE-CZ-NH1	5.73	123.17	120.30
1	B	147	ASP	CB-CG-OD1	5.71	123.44	118.30
1	E	26	ASP	CB-CG-OD1	5.71	123.44	118.30
1	E	138	GLY	O-C-N	5.70	132.89	123.20
1	A	87	ARG	CD-NE-CZ	-5.69	115.64	123.60
1	G	77	MSE	CG-SE-CE	-5.68	86.40	98.90
1	B	56	ASP	CB-CG-OD1	5.67	123.40	118.30
1	C	150	TYR	CB-CG-CD2	5.62	124.37	121.00
1	D	96	ARG	NE-CZ-NH1	-5.60	117.50	120.30
1	I	118	ASP	CB-CG-OD2	-5.58	113.28	118.30
1	C	140	GLU	O-C-N	5.58	131.62	122.70
1	I	85	ASP	CB-CG-OD2	5.57	123.31	118.30
1	J	98	TYR	CB-CG-CD1	-5.56	117.66	121.00
1	H	87	ARG	CD-NE-CZ	-5.55	115.82	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	141	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	A	34[A]	ASP	CB-CG-OD2	-5.49	113.36	118.30
1	A	34[B]	ASP	CB-CG-OD2	-5.49	113.36	118.30
1	J	141	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	E	127	LYS	CA-CB-CG	5.45	125.39	113.40
1	G	8	ARG	CD-NE-CZ	-5.45	115.97	123.60
1	E	104	TYR	CG-CD2-CE2	-5.45	116.94	121.30
1	H	8	ARG	NE-CZ-NH1	5.45	123.02	120.30
1	A	86	ASP	CB-CG-OD1	5.44	123.19	118.30
1	F	11	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	I	8	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	H	126	PHE	CB-CG-CD2	-5.39	117.03	120.80
1	I	95	TYR	CZ-CE2-CD2	-5.38	114.96	119.80
1	A	98	TYR	CG-CD1-CE1	-5.38	117.00	121.30
1	F	118	ASP	CB-CG-OD1	5.37	123.13	118.30
1	A	85	ASP	CB-CG-OD1	-5.34	113.49	118.30
1	H	5	GLN	CB-CA-C	-5.32	99.76	110.40
1	B	95	TYR	CG-CD1-CE1	-5.30	117.06	121.30
1	A	118	ASP	CB-CG-OD2	-5.28	113.55	118.30
1	E	104	TYR	CD1-CG-CD2	5.27	123.69	117.90
1	E	87	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	H	102	GLN	OE1-CD-NE2	-5.25	109.83	121.90
1	C	87	ARG	CD-NE-CZ	-5.23	116.28	123.60
1	A	59	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	F	95	TYR	CD1-CG-CD2	5.22	123.64	117.90
1	H	56	ASP	CB-CG-OD1	5.20	122.98	118.30
1	J	99	GLU	OE1-CD-OE2	5.18	129.52	123.30
1	G	66	ASP	CB-CG-OD1	5.17	122.95	118.30
1	C	95	TYR	CB-CG-CD1	-5.16	117.91	121.00
1	C	16	ASP	CB-CG-OD1	5.15	122.93	118.30
1	E	86	ASP	CB-CG-OD1	5.11	122.90	118.30
1	I	42	PHE	CB-CG-CD1	-5.11	117.22	120.80
1	B	95	TYR	CB-CG-CD1	-5.10	117.94	121.00
1	J	87	ARG	CA-CB-CG	-5.08	102.22	113.40
1	D	95	TYR	CG-CD1-CE1	-5.06	117.25	121.30
1	B	104	TYR	CG-CD2-CE2	-5.04	117.27	121.30
1	D	13	ASP	CB-CG-OD1	5.03	122.83	118.30
1	F	26	ASP	CB-CG-OD1	5.03	122.83	118.30
1	J	57	ALA	O-C-N	-5.03	114.66	122.70
1	J	11	ARG	NH1-CZ-NH2	-5.02	113.88	119.40
1	J	13	ASP	CB-CG-OD1	5.01	122.81	118.30
1	A	104	TYR	CG-CD2-CE2	-5.01	117.29	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	J	59	ARG	NE-CZ-NH2	-5.01	117.80	120.30

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	21	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	36	0
1	H	1215	0	1268	43	0
1	I	1210	0	1271	22	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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	248	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 (248) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:E:27[B]:LEU:HD23	1:E:31[B]:GLU:CD	1.93	0.88
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
1:C:27[A]:LEU:HD12	1:C:31:GLU:CD	1.96	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:25:LYS:HB3	1:I:27[B]:LEU:HD13	1.86	0.56
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
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:E:27[B]:LEU:CD2	1:E:31[B]:GLU:CD	2.74	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:80:LEU:HD13	1:A:80:LEU:C	2.41	0.41
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 (i)

5.3.1 Protein backbone (i)

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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 (i)

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%)	137 (99%)	1 (1%)	84	73
1	B	135/123 (110%)	132 (98%)	3 (2%)	52	27
1	C	135/123 (110%)	129 (96%)	6 (4%)	28	7
1	D	132/123 (107%)	127 (96%)	5 (4%)	33	10
1	E	134/123 (109%)	127 (95%)	7 (5%)	23	5
1	F	132/123 (107%)	128 (97%)	4 (3%)	41	15
1	G	133/123 (108%)	130 (98%)	3 (2%)	50	25
1	H	132/123 (107%)	127 (96%)	5 (4%)	33	10
1	I	131/123 (106%)	128 (98%)	3 (2%)	50	25
1	J	132/123 (107%)	127 (96%)	5 (4%)	33	10
All	All	1334/1230 (108%)	1292 (97%)	42 (3%)	49	14

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	102	GLN
1	B	102	GLN
1	B	128[A]	LEU
1	B	128[B]	LEU

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Mol	Chain	Res	Type
1	C	1	MSE
1	C	27[A]	LEU
1	C	27[B]	LEU
1	C	36	THR
1	C	128[A]	LEU
1	C	128[B]	LEU
1	D	102	GLN
1	D	128[A]	LEU
1	D	128[B]	LEU
1	D	129	ASP
1	D	137	GLU
1	E	27[A]	LEU
1	E	27[B]	LEU
1	E	36	THR
1	E	102	GLN
1	E	128[A]	LEU
1	E	128[B]	LEU
1	E	129	ASP
1	F	27	LEU
1	F	102	GLN
1	F	128[A]	LEU
1	F	128[B]	LEU
1	G	36	THR
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	102	GLN
1	I	128[A]	LEU
1	I	128[B]	LEU
1	J	36	THR
1	J	102	GLN
1	J	128[A]	LEU
1	J	128[B]	LEU
1	J	129	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	GLN
1	A	102	GLN
1	B	51	GLN
1	B	102	GLN
1	C	51	GLN
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 monosaccharides 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	D	1159	-	4,4,4	0.49	0	6,6,6	1.22	1 (16%)
3	SO4	H	1159	-	4,4,4	0.57	0	6,6,6	0.90	0
3	SO4	H	1158	-	4,4,4	0.66	0	6,6,6	0.39	0
3	SO4	J	1158	-	4,4,4	0.63	0	6,6,6	0.94	0
3	SO4	J	1160	-	4,4,4	0.55	0	6,6,6	0.57	0
3	SO4	E	1160	-	4,4,4	0.57	0	6,6,6	0.35	0
3	SO4	F	1159	-	4,4,4	0.56	0	6,6,6	0.64	0
3	SO4	I	1159	-	4,4,4	0.56	0	6,6,6	0.52	0
3	SO4	I	1158	-	4,4,4	0.57	0	6,6,6	0.68	0
3	SO4	H	1160	-	4,4,4	0.58	0	6,6,6	0.29	0
3	SO4	A	1159[A]	-	4,4,4	8.30	4 (100%)	6,6,6	8.81	4 (66%)
3	SO4	E	1159	-	4,4,4	0.81	0	6,6,6	1.07	0
3	SO4	B	1158	-	4,4,4	0.60	0	6,6,6	0.48	0
3	SO4	E	1158	-	4,4,4	0.59	0	6,6,6	0.38	0
3	SO4	B	1159	-	4,4,4	0.44	0	6,6,6	1.13	0
3	SO4	A	1158	-	4,4,4	0.56	0	6,6,6	0.74	0
3	SO4	C	1158	-	4,4,4	0.56	0	6,6,6	0.45	0
3	SO4	G	1158	-	4,4,4	0.64	0	6,6,6	0.48	0
3	SO4	J	1159	-	4,4,4	0.56	0	6,6,6	0.82	0
3	SO4	G	1159	-	4,4,4	0.54	0	6,6,6	0.39	0
3	SO4	F	1158	-	4,4,4	0.65	0	6,6,6	0.41	0
3	SO4	A	1159[B]	-	4,4,4	0.59	0	6,6,6	0.80	0
3	SO4	D	1158	-	4,4,4	0.61	0	6,6,6	0.48	0
3	SO4	D	1160	-	4,4,4	0.61	0	6,6,6	0.46	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	-13.15	0.39	1.47
3	A	1159[A]	SO4	O1-S	-7.48	1.05	1.46
3	A	1159[A]	SO4	O3-S	6.29	1.99	1.47
3	A	1159[A]	SO4	O2-S	2.74	1.60	1.46

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1159[A]	SO4	O4-S-O3	-14.81	45.86	109.06
3	A	1159[A]	SO4	O4-S-O1	-12.62	43.45	109.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1159[A]	SO4	O4-S-O2	7.26	147.21	109.31
3	A	1159[A]	SO4	O3-S-O1	-5.69	79.64	109.31
3	D	1159	SO4	O3-S-O2	2.11	120.33	109.31

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	H	1159	SO4	2	0
3	F	1159	SO4	1	0
3	A	1159[A]	SO4	6	0
3	E	1159	SO4	2	0
3	B	1159	SO4	1	0
3	J	1159	SO4	1	0
3	D	1160	SO4	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	152/156 (97%)	-0.30	3 (1%)	65	67	8, 14, 24, 42	0
1	B	152/156 (97%)	-0.36	2 (1%)	77	80	8, 13, 24, 45	0
1	C	152/156 (97%)	-0.39	2 (1%)	77	80	8, 13, 25, 41	0
1	D	152/156 (97%)	-0.37	0	100	100	8, 14, 25, 37	0
1	E	152/156 (97%)	-0.36	0	100	100	8, 14, 23, 31	0
1	F	152/156 (97%)	-0.26	1 (0%)	87	89	8, 15, 26, 35	0
1	G	152/156 (97%)	-0.29	1 (0%)	87	89	8, 15, 26, 43	0
1	H	152/156 (97%)	-0.09	7 (4%)	32	31	8, 16, 33, 41	0
1	I	152/156 (97%)	-0.30	1 (0%)	87	89	8, 15, 28, 41	0
1	J	152/156 (97%)	-0.31	3 (1%)	65	67	8, 14, 23, 44	0
All	All	1520/1560 (97%)	-0.30	20 (1%)	77	80	8, 14, 26, 45	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	136	PRO	3.5
1	J	137	GLU	3.4
1	H	66	ASP	3.2
1	H	60	LEU	3.1
1	C	137	GLU	3.0
1	G	137	GLU	2.8
1	A	136	PRO	2.8
1	F	34	ASP	2.7
1	J	66	ASP	2.6
1	A	137	GLU	2.6
1	C	136	PRO	2.6
1	A	66[A]	ASP	2.5
1	J	136	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	H	63	ALA	2.4
1	H	61	VAL	2.4
1	H	68	ASP	2.4
1	I	137	GLU	2.1
1	H	69	GLU	2.1
1	B	137	GLU	2.1
1	H	62	GLY	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (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	0.80	0.23	55,55,56,57	0
3	SO4	D	1160	5/5	0.88	0.18	55,56,57,57	0
3	SO4	I	1159	5/5	0.89	0.19	56,56,57,58	0
3	SO4	F	1159	5/5	0.90	0.26	57,57,58,58	0
3	SO4	J	1160	5/5	0.91	0.21	51,52,52,53	0
3	SO4	H	1160	5/5	0.93	0.22	58,59,59,60	0
3	SO4	H	1158	5/5	0.95	0.22	51,51,52,52	0
3	SO4	E	1159	5/5	0.96	0.22	33,36,37,38	0
3	SO4	J	1158	5/5	0.96	0.22	39,41,42,43	0
3	SO4	G	1159	5/5	0.96	0.12	42,43,43,44	0
3	SO4	F	1158	5/5	0.97	0.18	46,46,48,48	0
3	SO4	B	1158	5/5	0.97	0.17	42,44,45,45	0
3	SO4	G	1158	5/5	0.97	0.18	42,43,46,47	0
3	SO4	C	1158	5/5	0.97	0.20	39,40,41,42	0
3	SO4	D	1158	5/5	0.97	0.21	34,36,38,39	0
3	SO4	H	1159	5/5	0.97	0.17	34,39,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	SO4	D	1159	5/5	0.97	0.16	32,37,38,39	0
3	SO4	I	1158	5/5	0.97	0.21	39,39,42,43	0
3	SO4	A	1158	5/5	0.97	0.19	36,37,40,41	0
3	SO4	A	1159[A]	5/5	0.97	0.13	16,36,41,46	5
3	SO4	A	1159[B]	5/5	0.97	0.13	28,31,32,32	5
3	SO4	E	1158	5/5	0.98	0.23	41,42,44,44	0
3	SO4	J	1159	5/5	0.98	0.22	32,37,38,39	0
3	SO4	B	1159	5/5	0.98	0.18	32,38,39,39	0
2	CL	B	1157	1/1	0.99	0.03	15,15,15,15	0
2	CL	C	1157	1/1	0.99	0.03	14,14,14,14	0
2	CL	E	1157	1/1	0.99	0.02	17,17,17,17	0
2	CL	F	1157	1/1	0.99	0.02	17,17,17,17	0
2	CL	G	1157	1/1	0.99	0.03	15,15,15,15	0
2	CL	J	1157	1/1	0.99	0.03	15,15,15,15	0
2	CL	A	1157	1/1	1.00	0.03	16,16,16,16	0
2	CL	H	1157	1/1	1.00	0.02	15,15,15,15	0
2	CL	I	1157	1/1	1.00	0.03	15,15,15,15	0
2	CL	D	1157	1/1	1.00	0.04	15,15,15,15	0

6.5 Other polymers (i)

There are no such residues in this entry.