Full wwPDB X-ray Structure Validation Report (i)

Jun 19, 2024 – 12:53 AM EDT

PDB ID	:	4NFW
Title	:	Structure and atypical hydrolysis mechanism of the Nudix hydrolase Orf153 (YmfB) from Escherichia coli
Authors	:	Hong, M.K.; Kim, J.K.; Kang, L.W.
Deposited on	:	2013-11-01
Resolution	:	2.30 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:

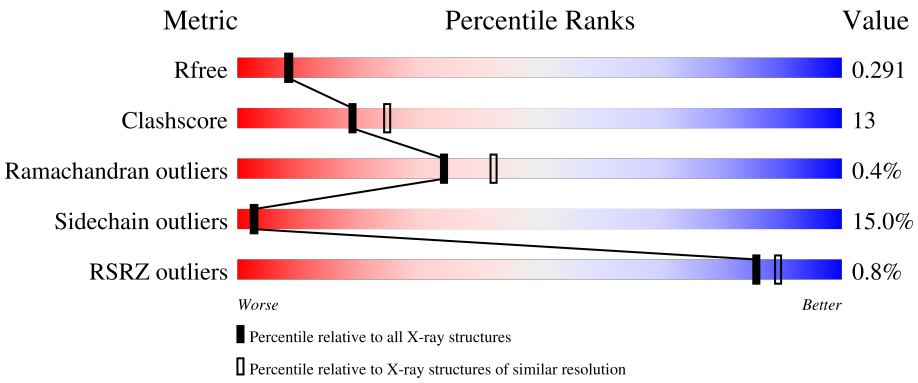
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	153	65% 27% 6% •
1	B	153	73% 19% 6% •
1	C	153	% 64% 29% 5% •
1	D	153	% 62% 33% • •
1	E	153	71% 24% • • •

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Mol	Chain	Length	Quality of chain
1	F	153	2% 63% 33%
1	G	153	% 67% 25% 5%
1	H	153	% 65% 29%
1	I	153	2% 48% 39% 10%
1	J	153	% 64% 30% 5%
1	K	153	68% 28%
1	L	153	% 58% 29% 5% 8%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 14906 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 Putative Nudix hydrolase ymfB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	150	1208	773	206	221	8	0	0	0
1	B	150	1208	773	206	221	8	0	0	0
1	C	150	1208	773	206	221	8	0	0	0
1	D	150	1208	773	206	221	8	0	0	0
1	E	150	1208	773	206	221	8	0	0	0
1	F	153	1227	786	209	224	8	0	0	0
1	G	150	1208	773	206	221	8	0	0	0
1	H	150	1208	773	206	221	8	0	0	0
1	I	138	1122	723	192	200	7	0	0	0
1	J	152	1219	780	208	223	8	0	0	0
1	K	150	1208	773	206	221	8	0	0	0
1	L	141	1143	734	195	206	8	0	0	0

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mn		
2	A	2	2	2	0	0
2	B	2	2	2	0	0

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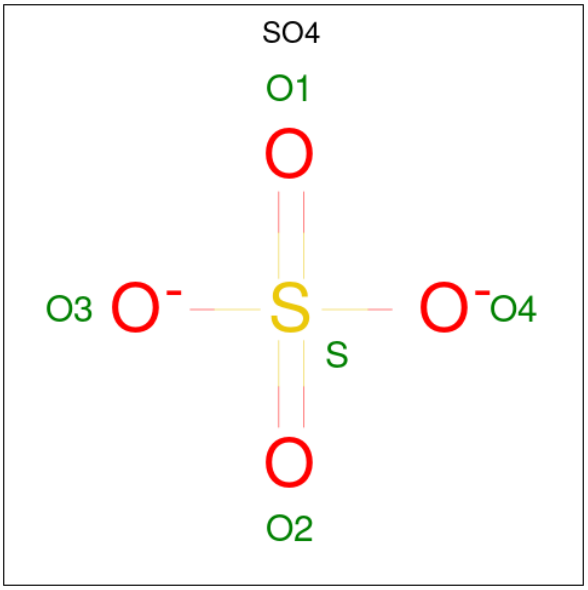
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mn		
2	C	2	2	2	0	0
2	D	2	2	2	0	0
2	E	2	2	2	0	0
2	F	2	2	2	0	0
2	G	2	2	2	0	0
2	H	2	2	2	0	0
2	I	1	1	1	0	0
2	J	2	2	2	0	0
2	K	2	2	2	0	0
2	L	1	1	1	0	0

- 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

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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	H	1	Total O S 5 4 1	0	0
3	H	1	Total O S 5 4 1	0	0
3	I	1	Total O S 5 4 1	0	0
3	I	1	Total O S 5 4 1	0	0
3	J	1	Total O S 5 4 1	0	0
3	J	1	Total O S 5 4 1	0	0
3	J	1	Total O S 5 4 1	0	0
3	K	1	Total O S 5 4 1	0	0
3	K	1	Total O S 5 4 1	0	0
3	K	1	Total O S 5 4 1	0	0
3	L	1	Total O S 5 4 1	0	0
3	L	1	Total O S 5 4 1	0	0
3	L	1	Total O S 5 4 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	42	Total O 42 42	0	0
4	B	34	Total O 34 34	0	0
4	C	36	Total O 36 36	0	0
4	D	23	Total O 23 23	0	0
4	E	37	Total O 37 37	0	0
4	F	17	Total O 17 17	0	0

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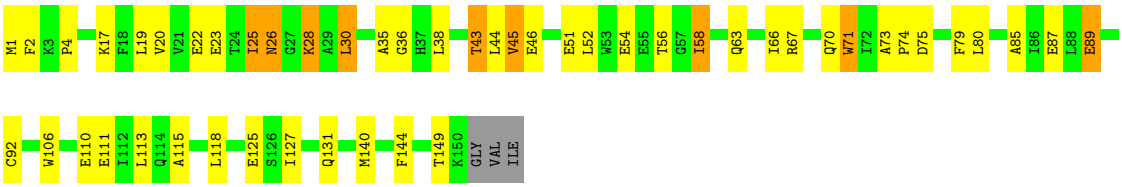
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	G	29	29	29	0	0
			Total	O		
4	H	25	25	25	0	0
			Total	O		
4	I	19	19	19	0	0
			Total	O		
4	J	17	17	17	0	0
			Total	O		
4	K	37	37	37	0	0
			Total	O		
4	L	18	18	18	0	0

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.

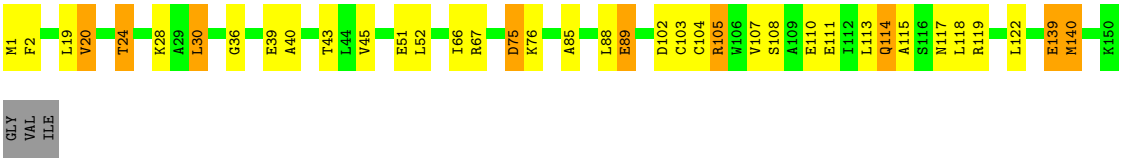
• Molecule 1: Putative Nudix hydrolase ymfB

Chain A:



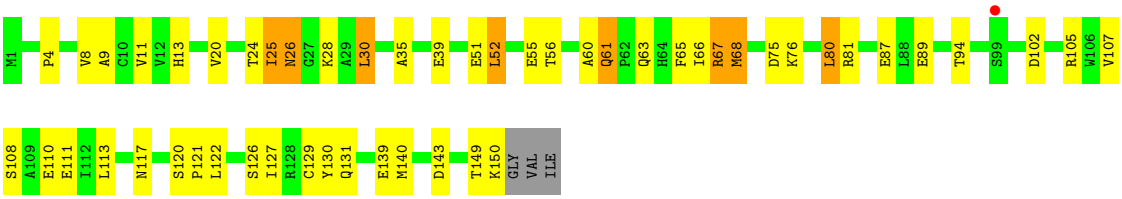
• Molecule 1: Putative Nudix hydrolase ymfB

Chain B:



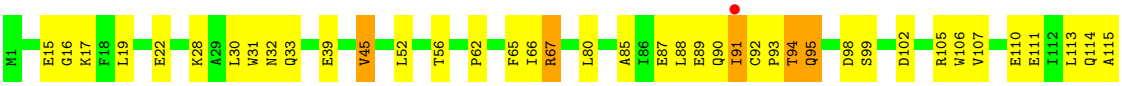
• Molecule 1: Putative Nudix hydrolase ymfB

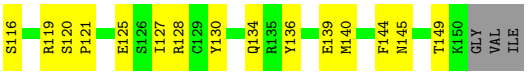
Chain C:



• Molecule 1: Putative Nudix hydrolase ymfB

Chain D:



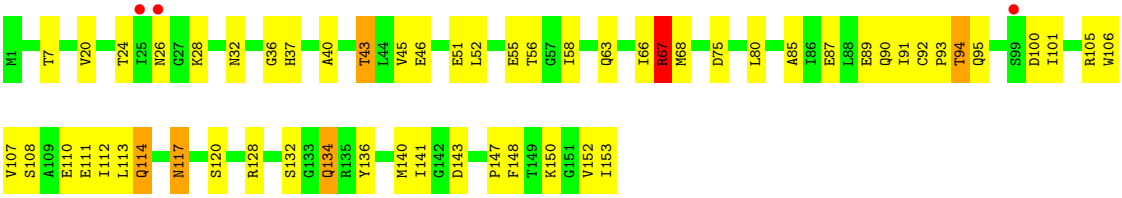


• Molecule 1: Putative Nudix hydrolase ymfB

Chain E:

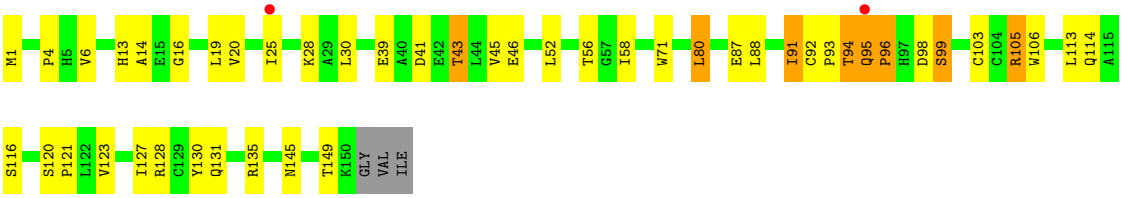
• Molecule 1: Putative Nudix hydrolase ymfB

Chain F:



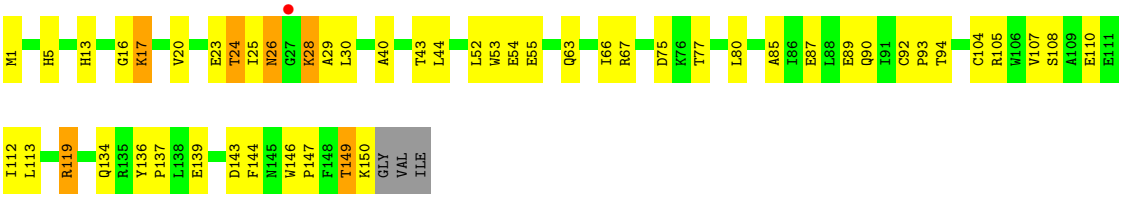
• Molecule 1: Putative Nudix hydrolase ymfB

Chain G:



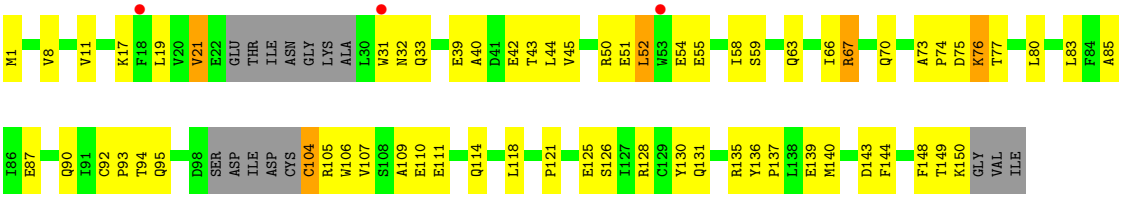
• Molecule 1: Putative Nudix hydrolase ymfB

Chain H:



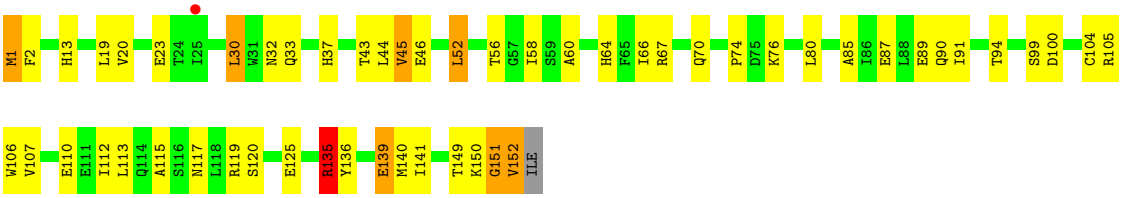
• Molecule 1: Putative Nudix hydrolase ymfB

Chain I:



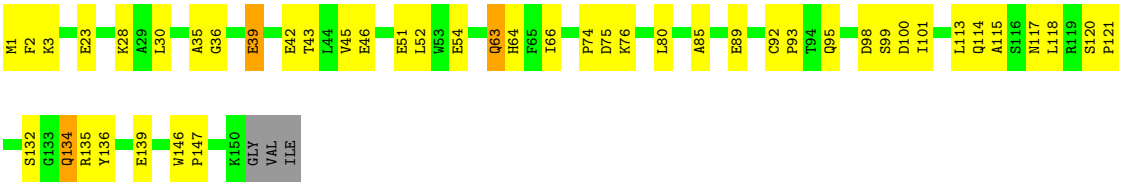
• Molecule 1: Putative Nudix hydrolase ymfB

Chain J:



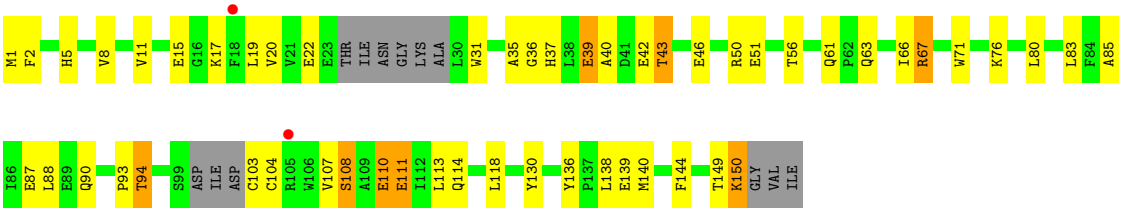
• Molecule 1: Putative Nudix hydrolase ymfB

Chain K:



• Molecule 1: Putative Nudix hydrolase ymfB

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α, β, γ	111.39Å 111.39Å 247.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.42 – 2.30 32.39 – 2.30	Depositor EDS
% Data completeness (in resolution range)	96.8 (32.42-2.30) 96.9 (32.39-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.94 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.240 , 0.289 0.243 , 0.291	Depositor DCC
R_{free} test set	6505 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	22.6	Xtriage
Anisotropy	0.108	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 15.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.478 for h,-k,-l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	14906	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.75% 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: SO4, MN

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	0.94	0/1243	0.91	0/1693
1	B	0.91	0/1243	0.96	2/1693 (0.1%)
1	C	0.77	0/1243	0.84	0/1693
1	D	0.86	0/1243	0.91	1/1693 (0.1%)
1	E	0.83	0/1243	0.89	2/1693 (0.1%)
1	F	0.78	0/1262	0.86	0/1719
1	G	0.77	0/1243	0.92	2/1693 (0.1%)
1	H	0.76	0/1243	0.84	1/1693 (0.1%)
1	I	0.80	0/1155	0.87	0/1571
1	J	0.82	0/1254	0.91	1/1708 (0.1%)
1	K	0.80	0/1243	0.84	0/1693
1	L	0.82	0/1176	0.86	0/1599
All	All	0.82	0/14791	0.89	9/20141 (0.0%)

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	E	0	1
1	I	0	1
1	J	0	1
All	All	0	3

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	128	ARG	NE-CZ-NH2	-6.27	117.17	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	128	ARG	NE-CZ-NH2	-6.23	117.18	120.30
1	E	67	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	J	135	ARG	NE-CZ-NH1	5.69	123.14	120.30
1	B	75	ASP	N-CA-CB	-5.61	100.50	110.60
1	G	94	THR	N-CA-C	5.57	126.03	111.00
1	B	119	ARG	NE-CZ-NH1	5.35	122.98	120.30
1	H	104	CYS	CA-CB-SG	-5.31	104.44	114.00
1	E	83	LEU	CB-CG-CD2	-5.15	102.25	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	25	ILE	Peptide
1	I	21	VAL	Peptide
1	J	151	GLY	Peptide

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	1208	0	1167	31	0
1	B	1208	0	1167	24	0
1	C	1208	0	1167	35	0
1	D	1208	0	1167	41	0
1	E	1208	0	1167	24	0
1	F	1227	0	1190	32	0
1	G	1208	0	1167	39	0
1	H	1208	0	1167	34	0
1	I	1122	0	1085	43	0
1	J	1219	0	1179	35	0
1	K	1208	0	1167	29	0
1	L	1143	0	1101	40	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
2	I	1	0	0	0	0
2	J	2	0	0	0	0
2	K	2	0	0	0	0
2	L	1	0	0	0	0
3	A	15	0	0	1	0
3	B	15	0	0	1	0
3	C	15	0	0	1	0
3	D	15	0	0	0	0
3	E	15	0	0	1	0
3	F	15	0	0	0	0
3	G	15	0	0	0	0
3	H	15	0	0	1	0
3	I	10	0	0	0	0
3	J	15	0	0	1	0
3	K	15	0	0	0	0
3	L	15	0	0	2	0
4	A	42	0	0	3	0
4	B	34	0	0	0	0
4	C	36	0	0	2	0
4	D	23	0	0	0	0
4	E	37	0	0	1	0
4	F	17	0	0	0	0
4	G	29	0	0	3	0
4	H	25	0	0	2	0
4	I	19	0	0	3	0
4	J	17	0	0	0	0
4	K	37	0	0	5	0
4	L	18	0	0	1	0
All	All	14906	0	13891	370	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 13.

All (370) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:15:GLU:OE2	1:D:91:ILE:N	1.73	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:25:ILE:HD12	1:H:119:ARG:NH2	1.66	1.10
1:D:92:CYS:HB2	1:D:93:PRO:HD2	1.32	1.06
1:C:25:ILE:HG22	1:C:26:ASN:H	1.20	1.02
1:H:66:ILE:HD11	1:H:85:ALA:HB2	1.42	1.00
1:H:25:ILE:CD1	1:H:119:ARG:NH2	2.26	0.98
1:D:17:LYS:CE	1:D:106:TRP:O	2.12	0.97
1:C:25:ILE:CG2	1:C:26:ASN:N	2.30	0.95
1:D:17:LYS:HE2	1:D:106:TRP:O	1.68	0.94
1:H:25:ILE:HD12	1:H:119:ARG:HH22	1.35	0.91
1:G:92:CYS:HB2	1:G:93:PRO:HD2	1.53	0.89
1:J:151:GLY:O	1:J:152:VAL:HG22	1.71	0.89
1:G:93:PRO:O	1:G:94:THR:HG22	1.73	0.88
1:A:43:THR:HG22	1:A:46:GLU:H	1.39	0.87
1:B:88:LEU:HA	1:F:153:ILE:HD11	1.56	0.87
1:C:25:ILE:HG22	1:C:26:ASN:N	1.87	0.85
1:H:149:THR:O	4:H:309:HOH:O	1.92	0.85
1:K:98:ASP:HB3	1:K:101:ILE:HG12	1.60	0.84
1:G:93:PRO:C	1:G:94:THR:HG22	1.99	0.83
1:F:66:ILE:HD11	1:F:85:ALA:HB2	1.63	0.80
1:D:17:LYS:HE3	1:D:106:TRP:O	1.83	0.78
1:G:93:PRO:O	1:G:94:THR:CG2	2.30	0.78
1:D:92:CYS:HB2	1:D:93:PRO:CD	2.11	0.78
1:G:92:CYS:CB	1:G:93:PRO:HD2	2.09	0.77
1:B:110:GLU:O	1:B:114:GLN:HG2	1.87	0.74
1:B:140:MET:HE1	1:L:140:MET:SD	2.28	0.73
1:K:100:ASP:O	4:K:326:HOH:O	2.06	0.73
1:I:136:TYR:HB3	1:I:140:MET:HE3	1.70	0.72
1:H:24:THR:HA	1:H:29:ALA:HA	1.69	0.72
1:H:25:ILE:CD1	1:H:119:ARG:HH22	1.99	0.72
1:A:35:ALA:O	3:A:204:SO4:O1	2.09	0.70
1:I:73:ALA:HB1	1:I:74:PRO:HD2	1.72	0.70
1:G:91:ILE:HG22	1:G:92:CYS:N	2.06	0.69
1:B:2:PHE:CD1	1:L:40:ALA:HB2	2.27	0.69
1:J:66:ILE:HD11	1:J:85:ALA:HB2	1.73	0.69
1:G:92:CYS:HB2	1:G:93:PRO:CD	2.22	0.69
1:J:74:PRO:C	1:J:76:LYS:H	1.96	0.68
1:J:43:THR:HG22	1:J:45:VAL:H	1.58	0.68
1:A:36:GLY:HA3	1:A:51:GLU:CD	2.14	0.68
1:K:54:GLU:CB	4:K:322:HOH:O	2.41	0.68
1:J:117:ASN:OD1	1:J:117:ASN:N	2.26	0.67
1:G:91:ILE:HD13	1:G:106:TRP:CD2	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:94:THR:OG1	4:L:318:HOH:O	2.13	0.66
1:H:25:ILE:HA	4:H:304:HOH:O	1.96	0.66
1:C:63:GLN:NE2	1:C:87:GLU:H	1.94	0.66
1:D:92:CYS:CB	1:D:93:PRO:HD2	2.06	0.66
1:F:152:VAL:O	1:F:153:ILE:HB	1.96	0.65
3:B:203:SO4:O4	3:B:204:SO4:O4	2.16	0.64
1:F:24:THR:HG23	1:F:28:LYS:O	1.97	0.64
1:C:25:ILE:HG23	1:C:26:ASN:N	2.11	0.64
1:D:15:GLU:OE2	1:D:91:ILE:CG1	2.46	0.64
1:D:15:GLU:OE2	1:D:91:ILE:HG13	1.98	0.64
1:L:11:VAL:HG23	1:L:83:LEU:HD11	1.81	0.63
1:F:40:ALA:HB2	1:K:2:PHE:CD1	2.34	0.63
1:A:25:ILE:HG13	1:A:25:ILE:O	1.99	0.62
1:H:25:ILE:HG23	1:H:26:ASN:N	2.14	0.62
1:C:108:SER:OG	1:C:111:GLU:HG3	2.00	0.62
1:D:16:GLY:HA2	1:I:114:GLN:HE22	1.65	0.62
1:K:98:ASP:HB3	1:K:101:ILE:CG1	2.29	0.62
1:D:31:TRP:CH2	1:D:107:VAL:HG11	2.35	0.62
1:K:132:SER:OG	1:K:134:GLN:HG2	2.00	0.62
1:B:2:PHE:CD1	1:L:40:ALA:CB	2.83	0.62
1:C:81:ARG:HD3	1:C:122:LEU:HD13	1.83	0.60
1:A:54:GLU:OE1	4:A:329:HOH:O	2.16	0.60
1:K:132:SER:OG	1:K:134:GLN:CG	2.50	0.60
1:K:66:ILE:HD11	1:K:85:ALA:HB2	1.84	0.59
1:H:13:HIS:HD2	1:H:87:GLU:OE2	1.86	0.59
1:G:91:ILE:HG22	1:G:92:CYS:H	1.65	0.59
1:F:67:ARG:HG3	1:F:68:MET:N	2.18	0.59
1:K:54:GLU:HB3	4:K:322:HOH:O	2.00	0.59
1:K:54:GLU:HB2	4:K:322:HOH:O	2.01	0.59
1:F:117:ASN:OD1	1:F:117:ASN:N	2.36	0.59
1:F:43:THR:HG22	1:F:46:GLU:H	1.68	0.59
1:I:66:ILE:HG22	1:I:67:ARG:HB2	1.85	0.58
1:L:37:HIS:CD2	3:L:202:SO4:S	2.96	0.58
1:F:107:VAL:HG13	1:F:111:GLU:HB2	1.86	0.58
1:D:130:TYR:OH	1:I:128:ARG:NH1	2.36	0.58
1:G:19:LEU:HD13	1:G:106:TRP:CE2	2.39	0.58
1:D:66:ILE:O	1:D:67:ARG:HB2	2.03	0.58
1:J:43:THR:HG22	1:J:44:LEU:N	2.18	0.58
1:B:36:GLY:HA3	1:B:51:GLU:CD	2.24	0.58
1:L:136:TYR:HB3	1:L:140:MET:CE	2.34	0.57
1:E:24:THR:HA	1:E:28:LYS:O	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:109:ALA:HB2	1:I:131:GLN:NE2	2.19	0.57
1:L:42:GLU:OE1	1:L:50:ARG:NE	2.35	0.57
1:I:66:ILE:HD11	1:I:85:ALA:HB2	1.85	0.57
1:L:36:GLY:HA3	1:L:51:GLU:HG3	1.86	0.57
1:A:19:LEU:HD21	1:A:56:THR:HG21	1.87	0.57
1:A:2:PHE:CD1	1:I:40:ALA:HB2	2.40	0.57
1:E:81:ARG:HD2	1:E:122:LEU:HD13	1.86	0.57
1:K:114:GLN:OE1	1:K:114:GLN:HA	2.04	0.57
1:L:66:ILE:HG22	1:L:67:ARG:HB2	1.85	0.57
1:J:64:HIS:CG	1:J:135:ARG:HG2	2.40	0.57
1:F:20:VAL:HG23	1:F:32:ASN:O	2.04	0.57
1:J:151:GLY:O	1:J:152:VAL:CG2	2.51	0.57
1:A:125:GLU:OE1	1:K:135:ARG:NH2	2.33	0.56
1:F:66:ILE:O	1:F:67:ARG:HB3	2.05	0.56
1:G:41:ASP:OD1	1:K:76:LYS:NZ	2.39	0.56
1:B:1:MET:SD	1:L:5:HIS:CE1	2.99	0.56
1:H:55:GLU:OE2	3:H:204:SO4:O4	2.24	0.56
1:E:81:ARG:HD3	4:E:302:HOH:O	2.05	0.55
1:A:58:ILE:HD13	1:A:92:CYS:SG	2.46	0.55
1:C:51:GLU:O	1:C:55:GLU:HG3	2.06	0.55
1:G:91:ILE:HD13	1:G:106:TRP:CE3	2.42	0.55
1:K:35:ALA:O	1:K:51:GLU:HB3	2.06	0.55
1:A:58:ILE:CD1	1:A:92:CYS:SG	2.95	0.55
1:H:66:ILE:CD1	1:H:85:ALA:HB2	2.27	0.55
1:J:37:HIS:ND1	3:J:203:SO4:O1	2.35	0.55
1:K:115:ALA:HB3	1:K:118:LEU:HD21	1.88	0.55
1:F:91:ILE:HG23	1:F:106:TRP:CE2	2.42	0.55
1:B:75:ASP:O	1:B:76:LYS:HB2	2.06	0.55
1:L:130:TYR:CD2	1:L:130:TYR:C	2.79	0.55
1:A:115:ALA:HB3	1:A:118:LEU:HD21	1.89	0.55
1:I:144:PHE:HA	4:I:313:HOH:O	2.07	0.55
1:A:140:MET:SD	1:I:136:TYR:CE2	3.00	0.54
1:C:11:VAL:HG11	1:C:130:TYR:CD1	2.42	0.54
1:H:144:PHE:CE1	1:J:125:GLU:HG3	2.43	0.54
1:A:43:THR:HA	1:I:70:GLN:OE1	2.08	0.53
1:E:30:LEU:HD23	1:E:119:ARG:HA	1.91	0.53
1:K:63:GLN:O	1:K:64:HIS:CG	2.61	0.53
1:L:110:GLU:H	1:L:110:GLU:CD	2.12	0.53
1:A:63:GLN:NE2	4:A:323:HOH:O	2.42	0.53
1:F:128:ARG:HD3	4:I:318:HOH:O	2.08	0.53
1:J:74:PRO:C	1:J:76:LYS:N	2.63	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:136:TYR:HB3	1:L:140:MET:HE3	1.89	0.53
1:D:15:GLU:CD	1:D:91:ILE:HG13	2.30	0.52
1:D:95:GLN:HA	1:D:95:GLN:NE2	2.25	0.52
1:L:19:LEU:HD21	1:L:56:THR:HG21	1.91	0.52
1:E:91:ILE:HG23	1:E:106:TRP:CE2	2.45	0.52
1:G:91:ILE:CG2	1:G:92:CYS:N	2.72	0.52
1:J:56:THR:OG1	1:J:58:ILE:HG12	2.10	0.52
1:D:120:SER:HB2	1:D:121:PRO:HD2	1.92	0.52
1:A:25:ILE:HG23	1:A:30:LEU:HD22	1.92	0.52
1:C:61:GLN:HA	1:C:61:GLN:NE2	2.25	0.52
1:C:30:LEU:HD22	1:C:30:LEU:N	2.25	0.51
1:C:61:GLN:HG2	1:J:89:GLU:HG3	1.92	0.51
1:F:56:THR:OG1	1:F:58:ILE:HG12	2.10	0.51
1:D:15:GLU:CG	1:D:91:ILE:HG13	2.41	0.51
1:L:66:ILE:HD11	1:L:85:ALA:HB2	1.93	0.51
1:D:95:GLN:HA	1:D:95:GLN:HE21	1.76	0.51
1:J:20:VAL:HG23	1:J:32:ASN:O	2.11	0.51
1:F:110:GLU:O	1:F:114:GLN:HG2	2.10	0.51
1:H:63:GLN:HE22	1:H:87:GLU:H	1.59	0.51
1:L:15:GLU:OE2	1:L:90:GLN:HB2	2.11	0.51
1:D:65:PHE:HE2	1:E:140:MET:HE3	1.76	0.51
1:G:43:THR:HG22	1:G:46:GLU:H	1.77	0.51
1:H:25:ILE:CG2	1:H:26:ASN:N	2.73	0.51
1:G:13:HIS:HD2	1:G:87:GLU:OE2	1.94	0.50
1:J:43:THR:HG22	1:J:45:VAL:N	2.26	0.50
1:J:115:ALA:HB1	1:J:117:ASN:OD1	2.11	0.50
1:L:107:VAL:CG1	1:L:111:GLU:CB	2.89	0.50
1:G:98:ASP:OD1	1:G:99:SER:N	2.44	0.50
1:I:109:ALA:HB2	1:I:131:GLN:HE22	1.75	0.50
1:D:87:GLU:O	1:D:88:LEU:HD23	2.12	0.50
1:D:127:ILE:HD12	1:D:127:ILE:N	2.27	0.50
1:I:110:GLU:CD	1:I:110:GLU:H	2.14	0.50
1:A:73:ALA:HB1	1:A:74:PRO:HD2	1.92	0.50
1:I:125:GLU:O	1:I:126:SER:C	2.50	0.50
1:J:13:HIS:HD2	1:J:87:GLU:OE2	1.95	0.50
1:D:45:VAL:HB	1:D:62:PRO:HG2	1.94	0.49
1:G:149:THR:HG23	4:G:325:HOH:O	2.12	0.49
1:D:19:LEU:HD13	1:D:106:TRP:CE2	2.46	0.49
1:I:42:GLU:OE1	1:I:50:ARG:NE	2.36	0.49
1:G:103:CYS:SG	4:G:322:HOH:O	2.60	0.49
1:B:19:LEU:HD11	1:B:104:CYS:HB3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:43:THR:HG22	1:H:44:LEU:N	2.28	0.49
1:J:56:THR:OG1	1:J:58:ILE:CG1	2.61	0.49
1:I:52:LEU:CD1	1:I:58:ILE:O	2.61	0.49
1:K:114:GLN:OE1	1:K:114:GLN:CA	2.61	0.49
1:F:147:PRO:HG2	1:F:148:PHE:CD1	2.48	0.49
1:D:15:GLU:CG	1:D:91:ILE:CG1	2.91	0.48
1:I:51:GLU:O	1:I:55:GLU:HG3	2.13	0.48
1:L:36:GLY:HA3	1:L:51:GLU:CG	2.43	0.48
1:G:130:TYR:C	1:G:130:TYR:CD2	2.86	0.48
1:B:111:GLU:O	1:B:115:ALA:HB2	2.14	0.48
1:G:16:GLY:HA2	1:L:114:GLN:HE22	1.78	0.48
1:I:136:TYR:CB	1:I:140:MET:HE3	2.40	0.48
1:J:136:TYR:HB3	1:J:140:MET:HE3	1.96	0.48
1:B:103:CYS:SG	1:B:105:ARG:NH1	2.86	0.48
1:C:149:THR:O	1:C:150:LYS:HB2	2.13	0.48
3:E:203:SO4:O3	3:E:204:SO4:O2	2.32	0.48
1:G:91:ILE:CG2	1:G:92:CYS:H	2.26	0.48
1:B:89:GLU:OE1	1:G:145:ASN:ND2	2.43	0.47
1:B:115:ALA:HB3	1:B:118:LEU:HD21	1.96	0.47
1:L:110:GLU:CD	1:L:110:GLU:N	2.68	0.47
1:I:92:CYS:HB2	1:I:93:PRO:CD	2.44	0.47
1:A:66:ILE:HD11	1:A:85:ALA:HB2	1.94	0.47
1:C:25:ILE:HD12	1:C:25:ILE:HA	1.70	0.47
1:C:105:ARG:NH2	4:C:333:HOH:O	2.48	0.47
1:D:91:ILE:HG23	1:D:106:TRP:CE2	2.49	0.47
1:B:40:ALA:HB2	1:L:2:PHE:CD1	2.50	0.47
1:H:25:ILE:HD12	1:H:119:ARG:CZ	2.42	0.47
1:I:92:CYS:HB2	1:I:93:PRO:HD2	1.95	0.47
1:I:130:TYR:CD2	1:I:130:TYR:C	2.88	0.47
1:L:63:GLN:NE2	1:L:87:GLU:H	2.13	0.47
1:G:56:THR:OG1	1:G:58:ILE:HG13	2.13	0.47
1:H:92:CYS:HB2	1:H:93:PRO:CD	2.45	0.47
1:A:144:PHE:CE1	1:I:125:GLU:HG3	2.50	0.47
1:B:20:VAL:HG12	1:B:105:ARG:HG2	1.96	0.47
1:C:25:ILE:HG23	1:C:26:ASN:ND2	2.30	0.47
1:D:91:ILE:HG23	1:D:106:TRP:CD2	2.49	0.47
1:F:92:CYS:O	1:F:94:THR:HG22	2.15	0.47
1:J:43:THR:CG2	1:J:44:LEU:N	2.78	0.47
1:D:111:GLU:O	1:D:115:ALA:HB2	2.15	0.47
1:H:25:ILE:HG23	1:H:26:ASN:H	1.80	0.47
1:E:103:CYS:SG	1:E:105:ARG:NH1	2.89	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:75:ASP:O	1:I:76:LYS:HB2	2.15	0.46
1:K:46:GLU:HB3	4:K:313:HOH:O	2.15	0.46
1:D:94:THR:O	1:D:94:THR:OG1	2.29	0.46
1:G:103:CYS:N	4:G:322:HOH:O	2.49	0.46
1:C:8:VAL:O	1:C:35:ALA:HB1	2.15	0.46
1:C:35:ALA:O	3:C:204:SO4:O3	2.33	0.46
1:G:105:ARG:HH11	1:G:105:ARG:HG2	1.81	0.46
1:H:75:ASP:OD1	1:H:77:THR:OG1	2.27	0.46
1:A:111:GLU:O	1:A:115:ALA:HB2	2.14	0.46
1:C:66:ILE:HG22	1:C:67:ARG:HB2	1.97	0.46
1:G:120:SER:HB2	1:G:121:PRO:HD2	1.97	0.46
1:C:13:HIS:HD2	1:C:87:GLU:OE2	1.99	0.46
1:K:120:SER:HB2	1:K:121:PRO:HD2	1.97	0.46
1:K:117:ASN:OD1	1:K:117:ASN:N	2.48	0.46
1:I:21:VAL:HG12	1:I:104:CYS:HB3	1.97	0.46
1:C:61:GLN:CA	1:C:61:GLN:HE21	2.28	0.46
1:F:92:CYS:HB2	1:F:93:PRO:HD2	1.98	0.46
1:L:94:THR:HB	1:L:104:CYS:SG	2.56	0.46
1:C:30:LEU:HA	1:C:117:ASN:O	2.17	0.45
1:G:94:THR:O	1:G:94:THR:OG1	2.29	0.45
1:I:11:VAL:HG23	1:I:83:LEU:HD11	1.97	0.45
1:I:136:TYR:HB3	1:I:137:PRO:HD2	1.97	0.45
1:E:61:GLN:HG2	1:F:89:GLU:HG3	1.98	0.45
1:L:35:ALA:C	3:L:203:SO4:O3	2.55	0.45
1:B:122:LEU:HD21	1:L:144:PHE:CD2	2.52	0.45
1:C:52:LEU:HD22	1:C:56:THR:OG1	2.17	0.45
1:D:136:TYR:CE2	1:E:140:MET:HG3	2.52	0.45
1:H:25:ILE:CG2	1:H:26:ASN:H	2.28	0.45
1:C:4:PRO:CG	1:G:6:VAL:HG21	2.47	0.45
1:F:7:THR:HG22	1:F:37:HIS:HA	1.98	0.45
1:A:71:TRP:CD1	1:A:79:PHE:HB2	2.52	0.45
1:D:110:GLU:O	1:D:114:GLN:HB2	2.16	0.45
1:E:11:VAL:HG11	1:E:130:TYR:CD1	2.52	0.45
1:D:89:GLU:OE1	1:I:121:PRO:HG3	2.17	0.45
1:D:22:GLU:HG2	1:D:31:TRP:NE1	2.32	0.45
1:G:105:ARG:HH11	1:G:105:ARG:CG	2.30	0.45
1:J:52:LEU:CD1	1:J:60:ALA:HB3	2.47	0.45
1:L:19:LEU:HD12	1:L:20:VAL:H	1.81	0.45
1:G:127:ILE:N	1:G:127:ILE:HD12	2.32	0.45
1:C:68:MET:SD	1:C:80:LEU:HG	2.57	0.44
1:F:107:VAL:HG13	1:F:111:GLU:CB	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:19:LEU:HD11	1:I:104:CYS:HB2	1.98	0.44
1:H:24:THR:HA	1:H:28:LYS:O	2.17	0.44
1:C:61:GLN:NE2	1:C:61:GLN:CA	2.80	0.44
1:D:140:MET:HE3	1:E:67:ARG:HA	1.99	0.44
1:F:143:ASP:OD1	1:F:143:ASP:N	2.50	0.44
1:H:40:ALA:HA	1:J:2:PHE:CE1	2.52	0.44
1:C:25:ILE:HB	1:C:30:LEU:CD2	2.48	0.44
1:G:14:ALA:HB2	1:G:88:LEU:HB2	2.00	0.44
1:K:92:CYS:HB2	1:K:93:PRO:HD2	2.00	0.44
1:J:19:LEU:HD11	1:J:104:CYS:HB3	2.00	0.44
1:L:31:TRP:HB2	1:L:118:LEU:HD23	2.00	0.44
1:L:107:VAL:CG1	1:L:111:GLU:HB3	2.47	0.44
1:A:43:THR:CG2	1:A:45:VAL:HG13	2.48	0.44
1:E:65:PHE:CD2	1:E:140:MET:HE2	2.53	0.44
1:L:46:GLU:OE1	1:L:150:LYS:HG3	2.18	0.44
1:L:63:GLN:HE22	1:L:87:GLU:H	1.65	0.44
1:A:38:LEU:HD22	1:A:44:LEU:HD23	1.99	0.44
1:A:19:LEU:HD13	1:A:106:TRP:CE2	2.53	0.43
1:B:24:THR:HG23	1:B:102:ASP:OD2	2.18	0.43
1:D:125:GLU:HG3	1:E:144:PHE:CZ	2.53	0.43
1:I:17:LYS:HB3	1:I:106:TRP:HB3	2.00	0.43
1:J:91:ILE:HG23	1:J:106:TRP:CE2	2.53	0.43
1:L:138:LEU:C	1:L:140:MET:H	2.22	0.43
1:G:4:PRO:HG2	1:G:80:LEU:HD22	1.99	0.43
1:L:35:ALA:O	1:L:51:GLU:HB3	2.17	0.43
1:L:107:VAL:HG12	1:L:108:SER:N	2.32	0.43
1:K:36:GLY:HA3	1:K:51:GLU:CD	2.38	0.43
1:D:93:PRO:C	1:D:94:THR:HG22	2.38	0.43
1:F:55:GLU:HG2	1:F:101:ILE:HD11	2.01	0.43
1:H:53:TRP:O	1:H:54:GLU:C	2.57	0.43
1:K:39:GLU:HB2	1:K:42:GLU:OE2	2.18	0.43
1:F:63:GLN:HE21	1:F:63:GLN:HB2	1.60	0.43
1:I:135:ARG:NH1	4:I:303:HOH:O	2.50	0.43
1:A:144:PHE:CZ	1:I:125:GLU:HG3	2.53	0.43
1:E:95:GLN:O	1:E:96:PRO:C	2.56	0.43
1:F:141:ILE:C	1:F:141:ILE:HD12	2.39	0.43
1:I:52:LEU:HD13	1:I:58:ILE:O	2.19	0.43
1:K:132:SER:OG	1:K:134:GLN:HG3	2.18	0.43
1:I:63:GLN:HE22	1:I:87:GLU:H	1.67	0.43
1:A:127:ILE:O	1:A:131:GLN:HG3	2.19	0.43
1:G:88:LEU:HD23	1:G:88:LEU:HA	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:108:SER:O	1:H:112:ILE:HG13	2.19	0.43
1:K:74:PRO:C	1:K:76:LYS:H	2.22	0.43
1:B:76:LYS:HA	1:B:76:LYS:HD2	1.83	0.43
1:F:136:TYR:HB3	1:F:140:MET:HE3	2.01	0.43
1:A:43:THR:O	1:A:46:GLU:HB2	2.19	0.43
1:B:2:PHE:CD2	1:L:39:GLU:O	2.72	0.43
1:D:66:ILE:HD11	1:D:85:ALA:HB2	2.00	0.43
1:I:31:TRP:HZ3	1:I:111:GLU:O	2.02	0.43
1:L:43:THR:HG22	1:L:46:GLU:H	1.84	0.43
1:L:107:VAL:HG12	1:L:108:SER:O	2.18	0.43
1:D:15:GLU:HG2	1:D:91:ILE:HG12	2.00	0.42
1:I:21:VAL:HG22	1:I:32:ASN:O	2.19	0.42
1:I:32:ASN:ND2	1:I:33:GLN:O	2.46	0.42
1:J:64:HIS:CG	1:J:135:ARG:CG	3.01	0.42
1:A:89:GLU:OE1	1:D:145:ASN:ND2	2.52	0.42
1:E:107:VAL:HG11	1:E:112:ILE:HG13	2.02	0.42
1:G:19:LEU:HD13	1:G:106:TRP:NE1	2.35	0.42
1:G:127:ILE:O	1:G:131:GLN:HG3	2.19	0.42
1:I:11:VAL:HG11	1:I:130:TYR:CD1	2.54	0.42
1:I:73:ALA:HB1	1:I:74:PRO:CD	2.45	0.42
1:A:70:GLN:O	1:I:143:ASP:HA	2.19	0.42
1:C:9:ALA:CB	1:C:35:ALA:HB2	2.49	0.42
1:E:130:TYR:CD2	1:E:130:TYR:C	2.92	0.42
1:I:107:VAL:CG1	1:I:111:GLU:HB3	2.50	0.42
1:J:107:VAL:CG1	1:J:112:ILE:HG13	2.49	0.42
1:D:22:GLU:HG2	1:D:31:TRP:HE1	1.84	0.42
1:B:30:LEU:HA	1:B:117:ASN:O	2.20	0.42
1:J:32:ASN:OD1	1:J:33:GLN:N	2.52	0.42
1:E:108:SER:OG	1:E:111:GLU:HB2	2.20	0.42
1:I:43:THR:HG22	1:I:45:VAL:H	1.84	0.42
1:H:63:GLN:NE2	1:H:87:GLU:H	2.17	0.42
1:C:9:ALA:HB2	1:C:35:ALA:HB2	2.01	0.42
1:C:127:ILE:O	1:C:131:GLN:HG3	2.19	0.42
1:I:106:TRP:C	1:I:107:VAL:HG23	2.40	0.42
1:L:136:TYR:HB3	1:L:140:MET:HE1	2.00	0.42
1:L:107:VAL:HG11	1:L:111:GLU:HB3	2.01	0.42
1:J:139:GLU:O	1:J:139:GLU:HG3	2.19	0.41
1:C:126:SER:O	1:C:129:CYS:HB2	2.20	0.41
1:E:19:LEU:HD11	1:E:104:CYS:HB3	2.02	0.41
1:G:4:PRO:CG	1:G:80:LEU:HD22	2.50	0.41
1:H:16:GLY:C	1:H:17:LYS:HG2	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:THR:HG22	1:B:45:VAL:H	1.86	0.41
1:C:65:PHE:CE2	1:C:140:MET:HE2	2.55	0.41
1:E:65:PHE:CE2	1:E:140:MET:HE2	2.55	0.41
1:F:36:GLY:HA3	1:F:51:GLU:HG3	2.01	0.41
1:A:63:GLN:NE2	1:A:87:GLU:H	2.19	0.41
1:B:66:ILE:HD11	1:B:85:ALA:HB2	2.01	0.41
1:C:120:SER:OG	1:C:122:LEU:HB2	2.20	0.41
1:G:13:HIS:CD2	1:G:87:GLU:OE2	2.73	0.41
1:F:140:MET:HE2	1:K:136:TYR:CE2	2.56	0.41
1:F:63:GLN:NE2	1:F:87:GLU:H	2.18	0.41
1:F:108:SER:O	1:F:112:ILE:HG13	2.21	0.41
1:H:5:HIS:CE1	1:J:1:MET:SD	3.13	0.41
1:K:75:ASP:C	1:K:75:ASP:OD1	2.58	0.41
1:H:26:ASN:O	1:H:26:ASN:ND2	2.43	0.41
1:J:151:GLY:C	1:J:152:VAL:HG22	2.35	0.41
1:A:28:LYS:NZ	4:A:317:HOH:O	2.49	0.41
1:B:140:MET:SD	1:L:136:TYR:CE2	3.14	0.41
1:E:17:LYS:HD3	1:E:107:VAL:N	2.36	0.41
1:E:28:LYS:O	1:E:30:LEU:HD12	2.21	0.41
1:E:122:LEU:HD23	1:E:122:LEU:HA	1.94	0.41
1:F:75:ASP:OD2	1:F:75:ASP:N	2.44	0.41
1:H:110:GLU:CD	1:H:110:GLU:H	2.24	0.41
1:J:30:LEU:HA	1:J:117:ASN:O	2.21	0.41
1:K:43:THR:HG22	1:K:45:VAL:H	1.86	0.41
1:B:89:GLU:CD	1:C:121:PRO:HB3	2.40	0.41
1:F:132:SER:OG	1:F:134:GLN:HG2	2.21	0.41
1:G:95:GLN:HA	1:G:96:PRO:HD2	1.94	0.41
1:G:123:VAL:O	1:G:127:ILE:HD13	2.21	0.41
1:J:151:GLY:O	1:J:152:VAL:HG13	2.21	0.41
1:D:32:ASN:OD1	1:D:33:GLN:N	2.53	0.40
1:C:60:ALA:HA	4:C:309:HOH:O	2.22	0.40
1:H:136:TYR:HB3	1:H:137:PRO:CD	2.52	0.40
1:E:91:ILE:HG23	1:E:106:TRP:CD2	2.57	0.40
1:H:146:TRP:HA	1:H:147:PRO:HD3	1.95	0.40
1:I:43:THR:HG22	1:I:44:LEU:N	2.37	0.40
1:J:46:GLU:OE1	1:J:150:LYS:HD2	2.21	0.40
1:A:22:GLU:HA	1:A:30:LEU:O	2.22	0.40
1:D:144:PHE:CE1	1:E:125:GLU:HG2	2.57	0.40
1:H:143:ASP:HA	1:J:70:GLN:HB3	2.02	0.40
1:H:144:PHE:CE1	1:J:125:GLU:CG	3.05	0.40
1:K:146:TRP:HA	1:K:147:PRO:HD3	1.87	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	148/153 (97%)	139 (94%)	7 (5%)	2 (1%)	11	11
1	B	148/153 (97%)	138 (93%)	9 (6%)	1 (1%)	22	26
1	C	148/153 (97%)	135 (91%)	13 (9%)	0	100	100
1	D	148/153 (97%)	132 (89%)	16 (11%)	0	100	100
1	E	148/153 (97%)	142 (96%)	5 (3%)	1 (1%)	22	26
1	F	151/153 (99%)	138 (91%)	12 (8%)	1 (1%)	22	26
1	G	148/153 (97%)	135 (91%)	12 (8%)	1 (1%)	22	26
1	H	148/153 (97%)	140 (95%)	8 (5%)	0	100	100
1	I	132/153 (86%)	120 (91%)	12 (9%)	0	100	100
1	J	150/153 (98%)	138 (92%)	12 (8%)	0	100	100
1	K	148/153 (97%)	135 (91%)	13 (9%)	0	100	100
1	L	135/153 (88%)	122 (90%)	12 (9%)	1 (1%)	22	26
All	All	1752/1836 (95%)	1614 (92%)	131 (8%)	7 (0%)	34	42

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	PRO
1	A	26	ASN
1	F	67	ARG
1	G	96	PRO
1	L	93	PRO
1	B	139	GLU
1	E	96	PRO

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	130/132 (98%)	110 (85%)	20 (15%)	2	2
1	B	130/132 (98%)	115 (88%)	15 (12%)	5	6
1	C	130/132 (98%)	108 (83%)	22 (17%)	2	2
1	D	130/132 (98%)	108 (83%)	22 (17%)	2	2
1	E	130/132 (98%)	112 (86%)	18 (14%)	3	3
1	F	132/132 (100%)	115 (87%)	17 (13%)	4	4
1	G	130/132 (98%)	111 (85%)	19 (15%)	3	3
1	H	130/132 (98%)	108 (83%)	22 (17%)	2	2
1	I	120/132 (91%)	100 (83%)	20 (17%)	2	2
1	J	131/132 (99%)	110 (84%)	21 (16%)	2	2
1	K	130/132 (98%)	115 (88%)	15 (12%)	5	6
1	L	123/132 (93%)	102 (83%)	21 (17%)	2	2
All	All	1546/1584 (98%)	1314 (85%)	232 (15%)	3	3

All (232) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	17	LYS
1	A	20	VAL
1	A	23	GLU
1	A	25	ILE
1	A	26	ASN
1	A	28	LYS
1	A	30	LEU
1	A	43	THR
1	A	45	VAL
1	A	52	LEU
1	A	58	ILE
1	A	67	ARG
1	A	71	TRP

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Mol	Chain	Res	Type
1	A	75	ASP
1	A	80	LEU
1	A	89	GLU
1	A	110	GLU
1	A	113	LEU
1	A	149	THR
1	B	20	VAL
1	B	24	THR
1	B	28	LYS
1	B	30	LEU
1	B	39	GLU
1	B	52	LEU
1	B	67	ARG
1	B	89	GLU
1	B	105	ARG
1	B	107	VAL
1	B	108	SER
1	B	113	LEU
1	B	114	GLN
1	B	139	GLU
1	B	140	MET
1	C	20	VAL
1	C	24	THR
1	C	25	ILE
1	C	26	ASN
1	C	28	LYS
1	C	30	LEU
1	C	39	GLU
1	C	52	LEU
1	C	61	GLN
1	C	67	ARG
1	C	68	MET
1	C	75	ASP
1	C	76	LYS
1	C	80	LEU
1	C	89	GLU
1	C	94	THR
1	C	102	ASP
1	C	107	VAL
1	C	110	GLU
1	C	113	LEU
1	C	139	GLU

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Mol	Chain	Res	Type
1	C	143	ASP
1	D	28	LYS
1	D	30	LEU
1	D	39	GLU
1	D	45	VAL
1	D	52	LEU
1	D	56	THR
1	D	67	ARG
1	D	80	LEU
1	D	90	GLN
1	D	91	ILE
1	D	94	THR
1	D	95	GLN
1	D	98	ASP
1	D	99	SER
1	D	102	ASP
1	D	105	ARG
1	D	113	LEU
1	D	116	SER
1	D	119	ARG
1	D	134	GLN
1	D	139	GLU
1	D	149	THR
1	E	1	MET
1	E	20	VAL
1	E	25	ILE
1	E	26	ASN
1	E	28	LYS
1	E	43	THR
1	E	52	LEU
1	E	61	GLN
1	E	62	PRO
1	E	67	ARG
1	E	68	MET
1	E	80	LEU
1	E	92	CYS
1	E	93	PRO
1	E	94	THR
1	E	105	ARG
1	E	113	LEU
1	E	120	SER
1	F	26	ASN

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Mol	Chain	Res	Type
1	F	43	THR
1	F	45	VAL
1	F	52	LEU
1	F	67	ARG
1	F	80	LEU
1	F	90	GLN
1	F	94	THR
1	F	95	GLN
1	F	100	ASP
1	F	105	ARG
1	F	113	LEU
1	F	114	GLN
1	F	117	ASN
1	F	120	SER
1	F	134	GLN
1	F	150	LYS
1	G	1	MET
1	G	20	VAL
1	G	25	ILE
1	G	28	LYS
1	G	30	LEU
1	G	39	GLU
1	G	43	THR
1	G	45	VAL
1	G	52	LEU
1	G	71	TRP
1	G	80	LEU
1	G	91	ILE
1	G	95	GLN
1	G	99	SER
1	G	105	ARG
1	G	113	LEU
1	G	114	GLN
1	G	116	SER
1	G	135	ARG
1	H	1	MET
1	H	17	LYS
1	H	20	VAL
1	H	23	GLU
1	H	24	THR
1	H	26	ASN
1	H	28	LYS

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Mol	Chain	Res	Type
1	H	30	LEU
1	H	52	LEU
1	H	67	ARG
1	H	80	LEU
1	H	89	GLU
1	H	90	GLN
1	H	94	THR
1	H	105	ARG
1	H	107	VAL
1	H	113	LEU
1	H	119	ARG
1	H	134	GLN
1	H	139	GLU
1	H	149	THR
1	H	150	LYS
1	I	1	MET
1	I	8	VAL
1	I	39	GLU
1	I	52	LEU
1	I	54	GLU
1	I	59	SER
1	I	67	ARG
1	I	76	LYS
1	I	77	THR
1	I	80	LEU
1	I	90	GLN
1	I	94	THR
1	I	95	GLN
1	I	104	CYS
1	I	105	ARG
1	I	118	LEU
1	I	139	GLU
1	I	148	PHE
1	I	149	THR
1	I	150	LYS
1	J	1	MET
1	J	23	GLU
1	J	30	LEU
1	J	45	VAL
1	J	52	LEU
1	J	67	ARG
1	J	80	LEU

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Mol	Chain	Res	Type
1	J	90	GLN
1	J	94	THR
1	J	99	SER
1	J	100	ASP
1	J	105	ARG
1	J	110	GLU
1	J	113	LEU
1	J	119	ARG
1	J	120	SER
1	J	135	ARG
1	J	139	GLU
1	J	141	ILE
1	J	149	THR
1	J	152	VAL
1	K	1	MET
1	K	3	LYS
1	K	23	GLU
1	K	28	LYS
1	K	30	LEU
1	K	39	GLU
1	K	52	LEU
1	K	63	GLN
1	K	80	LEU
1	K	89	GLU
1	K	95	GLN
1	K	99	SER
1	K	113	LEU
1	K	134	GLN
1	K	139	GLU
1	L	1	MET
1	L	8	VAL
1	L	17	LYS
1	L	22	GLU
1	L	39	GLU
1	L	43	THR
1	L	61	GLN
1	L	67	ARG
1	L	71	TRP
1	L	76	LYS
1	L	80	LEU
1	L	88	LEU
1	L	94	THR

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Mol	Chain	Res	Type
1	L	103	CYS
1	L	108	SER
1	L	110	GLU
1	L	111	GLU
1	L	113	LEU
1	L	139	GLU
1	L	149	THR
1	L	150	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	GLN
1	A	63	GLN
1	B	26	ASN
1	B	61	GLN
1	B	63	GLN
1	B	95	GLN
1	B	134	GLN
1	C	13	HIS
1	C	26	ASN
1	C	61	GLN
1	C	63	GLN
1	C	95	GLN
1	D	61	GLN
1	D	63	GLN
1	D	95	GLN
1	D	97	HIS
1	D	114	GLN
1	D	134	GLN
1	E	61	GLN
1	E	63	GLN
1	E	134	GLN
1	F	63	GLN
1	F	97	HIS
1	F	134	GLN
1	G	13	HIS
1	G	26	ASN
1	G	61	GLN
1	G	63	GLN
1	H	13	HIS
1	H	63	GLN

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Mol	Chain	Res	Type
1	H	95	GLN
1	H	134	GLN
1	H	145	ASN
1	I	63	GLN
1	I	97	HIS
1	I	114	GLN
1	I	131	GLN
1	J	13	HIS
1	K	95	GLN
1	L	5	HIS
1	L	37	HIS
1	L	63	GLN
1	L	114	GLN
1	L	131	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 57 ligands modelled in this entry, 22 are monoatomic - leaving 35 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	A	205	-	4,4,4	0.53	0	6,6,6	0.47	0
3	SO4	B	204	-	4,4,4	0.55	0	6,6,6	0.32	0
3	SO4	D	205	-	4,4,4	0.58	0	6,6,6	0.51	0
3	SO4	H	205	-	4,4,4	0.71	0	6,6,6	0.47	0
3	SO4	E	204	2	4,4,4	0.50	0	6,6,6	0.29	0
3	SO4	E	205	-	4,4,4	0.52	0	6,6,6	0.32	0
3	SO4	I	202	2	4,4,4	0.48	0	6,6,6	0.10	0
3	SO4	G	204	-	4,4,4	0.58	0	6,6,6	0.44	0
3	SO4	B	203	2	4,4,4	0.60	0	6,6,6	0.54	0
3	SO4	L	203	-	4,4,4	0.50	0	6,6,6	0.31	0
3	SO4	B	205	-	4,4,4	0.67	0	6,6,6	0.58	0
3	SO4	F	203	2	4,4,4	0.42	0	6,6,6	0.26	0
3	SO4	A	204	2	4,4,4	0.54	0	6,6,6	0.45	0
3	SO4	C	205	-	4,4,4	0.52	0	6,6,6	0.31	0
3	SO4	H	203	2	4,4,4	0.42	0	6,6,6	0.76	0
3	SO4	G	205	-	4,4,4	0.52	0	6,6,6	0.24	0
3	SO4	K	203	2	4,4,4	0.36	0	6,6,6	0.63	0
3	SO4	L	204	-	4,4,4	0.49	0	6,6,6	0.38	0
3	SO4	A	203	2	4,4,4	0.73	0	6,6,6	0.31	0
3	SO4	L	202	2	4,4,4	0.43	0	6,6,6	0.18	0
3	SO4	J	205	-	4,4,4	0.61	0	6,6,6	0.43	0
3	SO4	D	203	2	4,4,4	0.48	0	6,6,6	0.73	0
3	SO4	E	203	-	4,4,4	0.51	0	6,6,6	0.35	0
3	SO4	I	203	-	4,4,4	0.48	0	6,6,6	0.19	0
3	SO4	F	204	-	4,4,4	0.54	0	6,6,6	0.18	0
3	SO4	G	203	2	4,4,4	0.40	0	6,6,6	0.54	0
3	SO4	C	203	2	4,4,4	0.51	0	6,6,6	0.50	0
3	SO4	C	204	-	4,4,4	0.47	0	6,6,6	0.47	0
3	SO4	K	204	2	4,4,4	0.45	0	6,6,6	0.26	0
3	SO4	K	205	-	4,4,4	0.58	0	6,6,6	0.41	0
3	SO4	D	204	-	4,4,4	0.51	0	6,6,6	0.25	0
3	SO4	J	203	2	4,4,4	0.47	0	6,6,6	0.52	0
3	SO4	H	204	-	4,4,4	0.56	0	6,6,6	0.28	0
3	SO4	F	205	-	4,4,4	0.75	0	6,6,6	0.30	0
3	SO4	J	204	2	4,4,4	0.45	0	6,6,6	0.20	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	204	SO4	1	0
3	E	204	SO4	1	0
3	B	203	SO4	1	0
3	L	203	SO4	1	0
3	A	204	SO4	1	0
3	L	202	SO4	1	0
3	E	203	SO4	1	0
3	C	204	SO4	1	0
3	J	203	SO4	1	0
3	H	204	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	150/153 (98%)	-0.36	0	100	100	12, 21, 40, 62	2 (1%)
1	B	150/153 (98%)	-0.35	0	100	100	12, 21, 42, 60	2 (1%)
1	C	150/153 (98%)	-0.26	1 (0%)	87	91	13, 27, 58, 74	2 (1%)
1	D	150/153 (98%)	-0.08	1 (0%)	87	91	15, 32, 69, 78	2 (1%)
1	E	150/153 (98%)	-0.26	0	100	100	14, 25, 61, 80	2 (1%)
1	F	153/153 (100%)	-0.09	3 (1%)	65	71	13, 30, 72, 107	2 (1%)
1	G	150/153 (98%)	-0.10	2 (1%)	77	81	16, 33, 69, 82	2 (1%)
1	H	150/153 (98%)	-0.24	1 (0%)	87	91	14, 30, 52, 78	2 (1%)
1	I	138/153 (90%)	0.02	3 (2%)	62	69	15, 39, 72, 89	2 (1%)
1	J	152/153 (99%)	-0.06	1 (0%)	87	91	15, 29, 71, 83	2 (1%)
1	K	150/153 (98%)	-0.25	0	100	100	12, 30, 54, 70	2 (1%)
1	L	141/153 (92%)	0.07	2 (1%)	75	80	17, 40, 78, 96	2 (1%)
All	All	1784/1836 (97%)	-0.17	14 (0%)	86	89	12, 29, 66, 107	24 (1%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	25	ILE	4.8
1	H	27	GLY	3.7
1	I	18	PHE	2.7
1	D	91	ILE	2.6
1	C	99	SER	2.6
1	G	25	ILE	2.6
1	L	105	ARG	2.6
1	F	26	ASN	2.6
1	I	31	TRP	2.5
1	L	18	PHE	2.5
1	G	95	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	99	SER	2.5
1	I	53	TRP	2.5
1	J	25	ILE	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 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
2	MN	D	201	1/1	0.62	0.23	100,100,100,100	0
3	SO4	L	203	5/5	0.71	0.19	106,109,118,119	0
3	SO4	H	204	5/5	0.73	0.27	102,104,111,116	0
2	MN	G	202	1/1	0.79	0.08	86,86,86,86	0
3	SO4	L	202	5/5	0.80	0.26	119,119,121,126	0
3	SO4	G	205	5/5	0.80	0.16	78,82,96,101	0
3	SO4	D	204	5/5	0.82	0.24	93,98,106,107	0
3	SO4	K	204	5/5	0.82	0.22	97,98,105,106	0
2	MN	E	202	1/1	0.85	0.12	96,96,96,96	0
3	SO4	F	204	5/5	0.85	0.39	104,110,116,123	0
3	SO4	I	202	5/5	0.85	0.23	129,131,135,137	0
3	SO4	E	204	5/5	0.86	0.30	87,95,104,105	0
3	SO4	J	204	5/5	0.90	0.24	97,99,104,104	0
3	SO4	C	204	5/5	0.90	0.24	91,96,101,103	0
2	MN	J	201	1/1	0.91	0.08	87,87,87,87	0
2	MN	H	201	1/1	0.91	0.14	101,101,101,101	0
3	SO4	B	204	5/5	0.92	0.17	61,63,71,79	0
3	SO4	A	204	5/5	0.92	0.21	60,61,71,75	0
2	MN	C	201	1/1	0.93	0.12	95,95,95,95	0
3	SO4	F	203	5/5	0.93	0.14	72,73,78,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MN	D	202	1/1	0.93	0.12	87,87,87,87	0
3	SO4	I	203	5/5	0.93	0.23	103,110,116,116	0
2	MN	C	202	1/1	0.94	0.07	92,92,92,92	0
2	MN	H	202	1/1	0.94	0.07	87,87,87,87	0
3	SO4	G	203	5/5	0.94	0.13	56,60,63,66	0
3	SO4	G	204	5/5	0.94	0.13	44,46,53,53	0
3	SO4	L	204	5/5	0.94	0.35	85,89,93,98	0
2	MN	F	201	1/1	0.95	0.11	86,86,86,86	0
2	MN	G	201	1/1	0.95	0.04	88,88,88,88	0
3	SO4	B	205	5/5	0.95	0.11	41,43,48,48	0
3	SO4	C	203	5/5	0.95	0.10	66,68,74,77	0
2	MN	E	201	1/1	0.95	0.09	82,82,82,82	0
2	MN	J	202	1/1	0.95	0.12	112,112,112,112	0
3	SO4	E	203	5/5	0.95	0.08	55,58,62,66	0
3	SO4	J	205	5/5	0.96	0.10	51,52,62,64	0
2	MN	K	201	1/1	0.96	0.04	81,81,81,81	0
2	MN	K	202	1/1	0.96	0.04	72,72,72,72	0
2	MN	L	201	1/1	0.96	0.05	77,77,77,77	0
2	MN	I	201	1/1	0.96	0.08	87,87,87,87	0
2	MN	F	202	1/1	0.97	0.11	82,82,82,82	0
3	SO4	D	203	5/5	0.97	0.08	53,54,62,63	0
3	SO4	A	203	5/5	0.97	0.07	45,45,48,50	0
3	SO4	D	205	5/5	0.97	0.10	46,46,52,56	0
2	MN	B	202	1/1	0.97	0.04	60,60,60,60	0
3	SO4	B	203	5/5	0.98	0.08	45,46,49,51	0
3	SO4	J	203	5/5	0.98	0.14	60,66,68,68	0
3	SO4	E	205	5/5	0.98	0.08	52,56,58,61	0
3	SO4	C	205	5/5	0.98	0.11	49,50,51,53	0
3	SO4	H	203	5/5	0.98	0.09	38,45,49,51	0
3	SO4	K	205	5/5	0.98	0.12	31,33,37,39	0
2	MN	A	201	1/1	0.98	0.08	78,78,78,78	0
3	SO4	H	205	5/5	0.98	0.09	26,29,31,31	0
3	SO4	F	205	5/5	0.98	0.08	38,41,46,48	0
2	MN	B	201	1/1	0.99	0.05	75,75,75,75	0
2	MN	A	202	1/1	0.99	0.04	65,65,65,65	0
3	SO4	K	203	5/5	0.99	0.07	43,46,48,49	0
3	SO4	A	205	5/5	0.99	0.10	36,36,37,38	0

6.5 Other polymers (i)

There are no such residues in this entry.