



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 04:09 PM UTC

PDB ID : 3SHD / pdb_00003shd
Title : Crystal structure of Nudix hydrolase Orf153, ymfB, from Escherichia coli K-1
Authors : Hong, M.K.; Kim, J.K.; Kang, L.W.
Deposited on : 2011-06-16
Resolution : 2.50 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

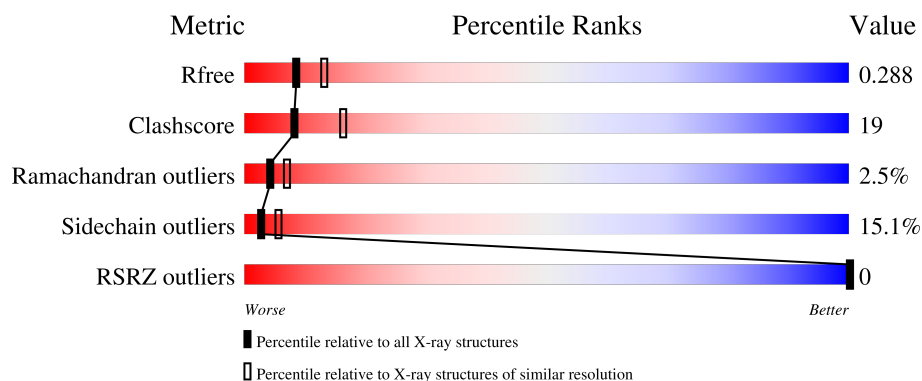
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	153	
1	B	153	
1	C	153	
1	D	153	
1	E	153	

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Mol	Chain	Length	Quality of chain
1	F	153	
1	G	153	
1	H	153	
1	I	153	
1	J	153	
1	K	153	
1	L	153	

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	157	-	-	X	-
3	SO4	B	156	-	-	X	-
3	SO4	B	157	-	-	X	-
3	SO4	C	157	-	-	X	-
3	SO4	D	156	-	-	X	-
3	SO4	D	157	-	-	X	-
3	SO4	E	157	-	-	X	-
3	SO4	G	156	-	-	X	-
3	SO4	G	158	-	-	X	-
3	SO4	H	157	-	-	X	-
3	SO4	L	157	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 14985 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 Phosphatase nudJ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	150	Total	C	N	O	S	0	0	0
			1208	773	206	221	8			
1	B	150	Total	C	N	O	S	0	0	0
			1208	773	206	221	8			
1	C	150	Total	C	N	O	S	0	0	0
			1208	773	206	221	8			
1	D	150	Total	C	N	O	S	0	0	0
			1208	773	206	221	8			
1	E	150	Total	C	N	O	S	0	0	0
			1208	773	206	221	8			
1	F	150	Total	C	N	O	S	0	0	0
			1208	773	206	221	8			
1	G	150	Total	C	N	O	S	0	0	0
			1208	773	206	221	8			
1	H	150	Total	C	N	O	S	0	0	0
			1208	773	206	221	8			
1	I	150	Total	C	N	O	S	0	0	0
			1208	773	206	221	8			
1	J	150	Total	C	N	O	S	0	0	0
			1208	773	206	221	8			
1	K	150	Total	C	N	O	S	0	0	0
			1208	773	206	221	8			
1	L	150	Total	C	N	O	S	0	0	0
			1208	773	206	221	8			

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

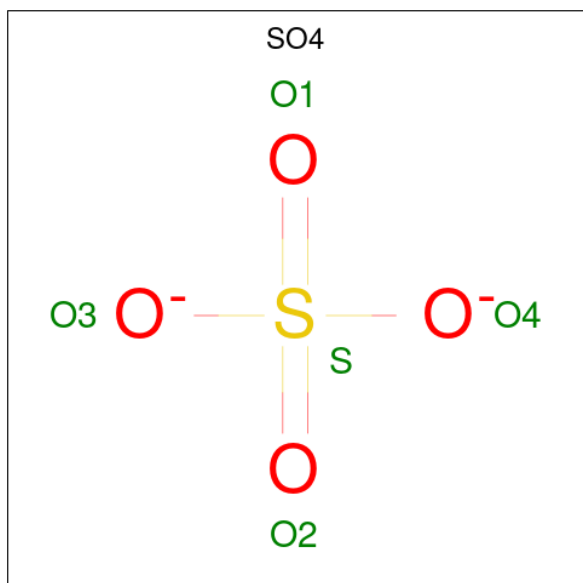
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Mn	0	0
			2	2		
2	B	2	Total	Mn	0	0
			2	2		

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

- 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		

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

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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	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	35	Total O 35 35	0	0
4	B	30	Total O 30 30	0	0
4	C	33	Total O 33 33	0	0
4	D	18	Total O 18 18	0	0
4	E	35	Total O 35 35	0	0

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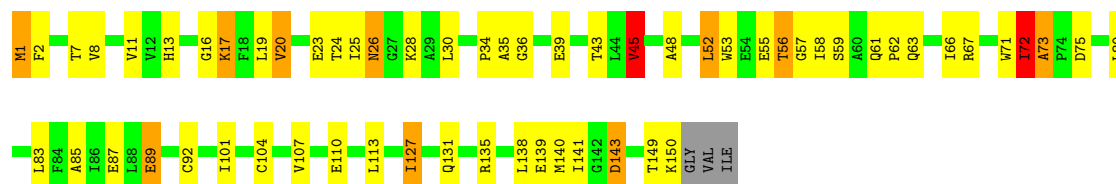
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	F	11	Total 11	O 11	0	0
4	G	27	Total 27	O 27	0	0
4	H	17	Total 17	O 17	0	0
4	I	18	Total 18	O 18	0	0
4	J	14	Total 14	O 14	0	0
4	K	31	Total 31	O 31	0	0
4	L	16	Total 16	O 16	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

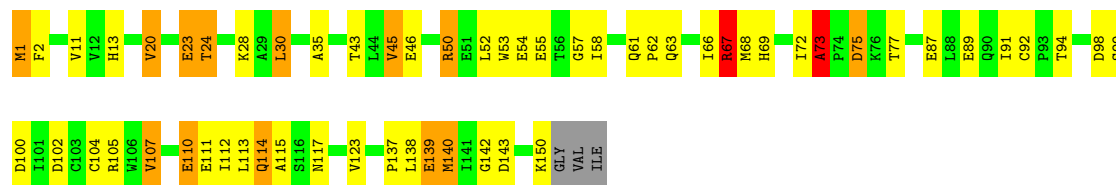
• Molecule 1: Phosphatase nudJ

Chain A: 



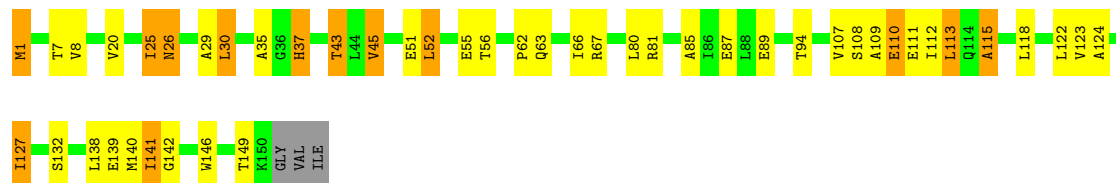
• Molecule 1: Phosphatase nudJ

Chain B: 

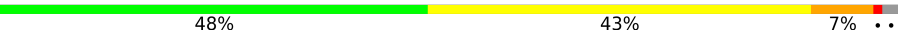


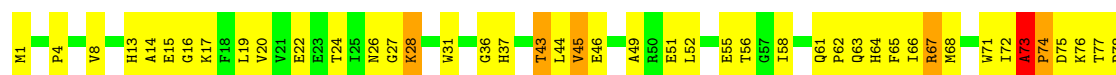
• Molecule 1: Phosphatase nudJ

Chain C: 



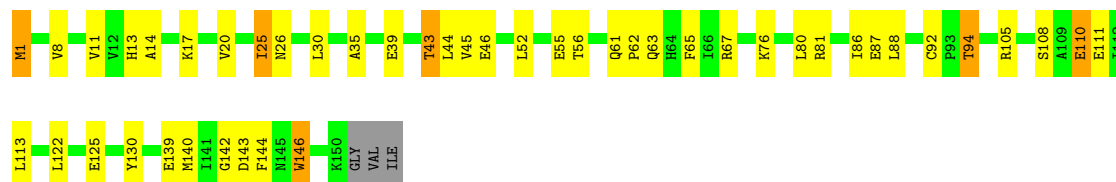
• Molecule 1: Phosphatase nudJ

Chain D: 

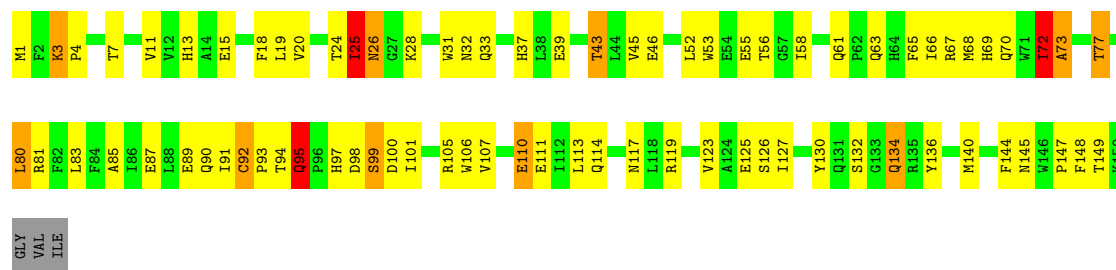




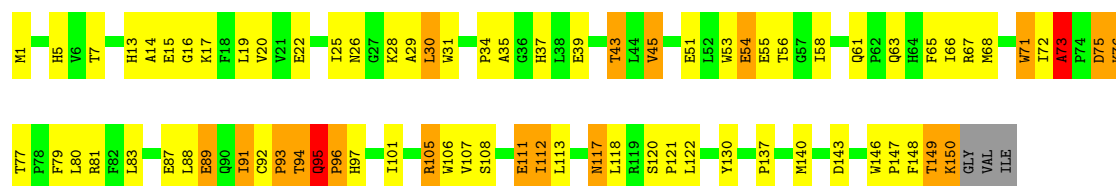
• Molecule 1: Phosphatase nudJ



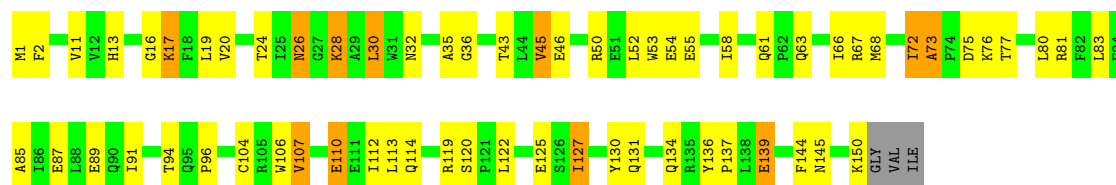
• Molecule 1: Phosphatase nudJ



• Molecule 1: Phosphatase nudJ

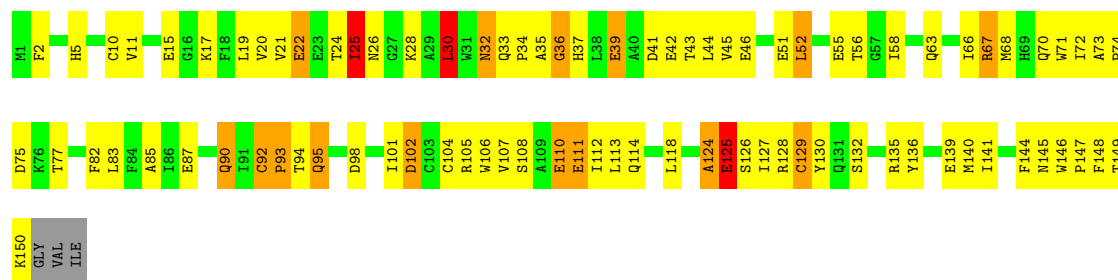


• Molecule 1: Phosphatase nudJ



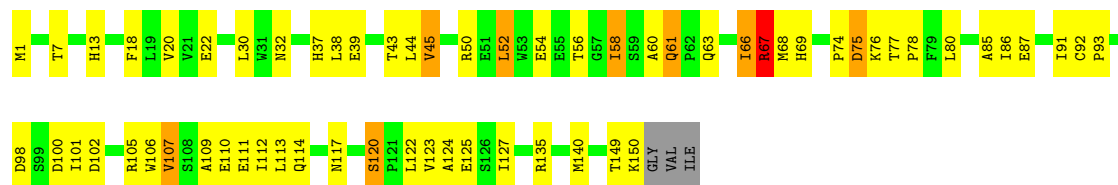
• Molecule 1: Phosphatase nudJ





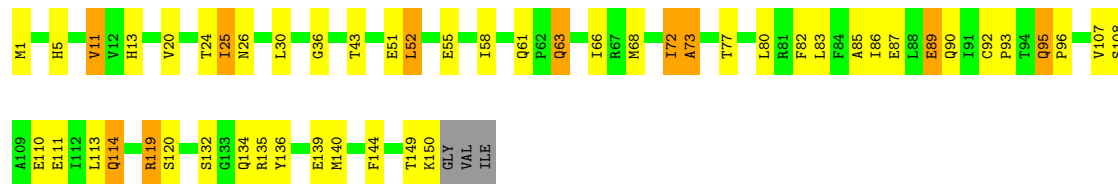
• Molecule 1: Phosphatase nudJ

Chain J: 58% 35% 5% ..



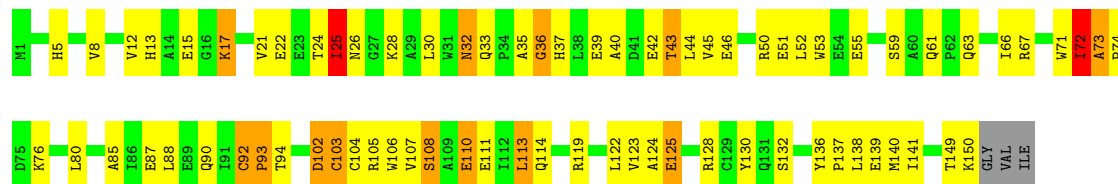
• Molecule 1: Phosphatase nudJ

Chain K: 65% 27% 7% .



• Molecule 1: Phosphatase nudJ

Chain L: 49% 39% 8% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α , β , γ	111.13Å 111.13Å 247.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.50 30.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	95.7 (30.00-2.50) 95.7 (30.00-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.89 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.226 , 0.291 0.224 , 0.288	Depositor DCC
R_{free} test set	4946 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å ²)	36.0	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 18.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.438 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14985	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.73% 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, 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	1.04	0/1243	1.21	6/1693 (0.4%)
1	B	1.05	1/1243 (0.1%)	1.21	8/1693 (0.5%)
1	C	0.96	1/1243 (0.1%)	1.16	5/1693 (0.3%)
1	D	0.96	0/1243	1.17	3/1693 (0.2%)
1	E	0.93	0/1243	1.19	4/1693 (0.2%)
1	F	0.97	2/1243 (0.2%)	1.20	10/1693 (0.6%)
1	G	0.97	0/1243	1.19	5/1693 (0.3%)
1	H	0.95	0/1243	1.09	4/1693 (0.2%)
1	I	0.92	0/1243	1.16	8/1693 (0.5%)
1	J	0.98	1/1243 (0.1%)	1.16	3/1693 (0.2%)
1	K	0.93	0/1243	1.12	7/1693 (0.4%)
1	L	0.94	2/1243 (0.2%)	1.17	8/1693 (0.5%)
All	All	0.97	7/14916 (0.0%)	1.17	71/20316 (0.3%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	101	ILE	CA-CB	5.67	1.60	1.53
1	L	12	VAL	CA-CB	-5.58	1.47	1.54
1	L	25	ILE	CA-CB	5.37	1.61	1.54
1	F	25	ILE	CA-CB	5.34	1.61	1.54
1	C	123	VAL	CA-CB	-5.29	1.48	1.54
1	B	104	CYS	CA-C	-5.16	1.46	1.52
1	J	101	ILE	CA-CB	5.07	1.60	1.54

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	146	TRP	CA-C-N	9.76	130.02	119.28
1	E	146	TRP	C-N-CA	9.76	130.02	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	132	SER	N-CA-C	-8.87	101.89	112.89
1	I	30	LEU	N-CA-C	8.44	119.39	108.34
1	K	52	LEU	N-CA-C	-8.14	101.99	111.03
1	H	120	SER	CA-C-N	-7.95	111.60	119.87
1	H	120	SER	C-N-CA	-7.95	111.60	119.87
1	C	146	TRP	CA-C-N	7.90	127.62	119.56
1	C	146	TRP	C-N-CA	7.90	127.62	119.56
1	G	97	HIS	N-CA-C	-7.81	100.85	110.61
1	L	125	GLU	N-CA-C	-7.69	104.50	114.04
1	B	73	ALA	CA-C-N	7.55	129.28	119.84
1	B	73	ALA	C-N-CA	7.55	129.28	119.84
1	G	73	ALA	CA-C-N	7.28	128.94	119.84
1	G	73	ALA	C-N-CA	7.28	128.94	119.84
1	A	56	THR	CB-CA-C	-7.07	100.03	109.16
1	L	92	CYS	CA-C-N	6.83	128.38	119.84
1	L	92	CYS	C-N-CA	6.83	128.38	119.84
1	C	149	THR	CB-CA-C	-6.73	105.98	114.40
1	A	45	VAL	CB-CA-C	6.62	120.08	111.81
1	I	92	CYS	CA-C-N	6.57	128.05	119.84
1	I	92	CYS	C-N-CA	6.57	128.05	119.84
1	G	89	GLU	N-CA-C	-6.46	103.48	112.45
1	G	117	ASN	N-CA-C	6.40	120.40	112.59
1	I	36	GLY	N-CA-C	6.35	119.13	110.69
1	J	120	SER	CA-C-N	-6.05	113.58	119.87
1	J	120	SER	C-N-CA	-6.05	113.58	119.87
1	B	123	VAL	N-CA-C	-6.03	104.43	111.00
1	D	73	ALA	CA-C-N	5.99	127.32	119.84
1	D	73	ALA	C-N-CA	5.99	127.32	119.84
1	F	95	GLN	CA-C-N	5.97	127.30	119.84
1	F	95	GLN	C-N-CA	5.97	127.30	119.84
1	E	25	ILE	CB-CA-C	5.95	118.16	110.96
1	L	72	ILE	CB-CA-C	5.82	120.83	111.29
1	L	92	CYS	N-CA-C	5.80	114.98	108.25
1	B	142	GLY	N-CA-C	5.75	121.30	112.51
1	A	72	ILE	N-CA-C	5.73	117.65	111.58
1	K	95	GLN	CA-C-N	5.67	126.92	119.84
1	K	95	GLN	C-N-CA	5.67	126.92	119.84
1	L	32	ASN	N-CA-C	5.63	116.97	108.46
1	I	32	ASN	N-CA-C	5.63	117.08	108.52
1	H	45	VAL	N-CA-CB	5.61	117.11	110.55
1	K	58	ILE	N-CA-C	5.60	116.83	109.21
1	I	129	CYS	N-CA-C	-5.56	105.28	112.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	115	ALA	N-CA-C	5.49	118.76	109.76
1	F	33	GLN	N-CA-C	-5.46	102.19	110.39
1	K	11	VAL	N-CA-C	-5.42	99.44	107.51
1	I	132	SER	N-CA-C	-5.38	105.97	112.54
1	F	3	LYS	N-CA-C	-5.33	103.91	110.31
1	F	136	TYR	CA-C-N	5.33	125.09	119.76
1	F	136	TYR	C-N-CA	5.33	125.09	119.76
1	J	66	ILE	N-CA-C	-5.33	106.49	111.45
1	A	20	VAL	N-CA-CB	-5.29	102.77	111.44
1	F	92	CYS	N-CA-C	5.24	112.94	108.22
1	B	11	VAL	CA-C-N	-5.22	116.22	122.90
1	B	11	VAL	C-N-CA	-5.22	116.22	122.90
1	F	123	VAL	N-CA-C	-5.21	105.30	110.62
1	F	72	ILE	N-CA-C	5.19	117.08	111.58
1	A	24	THR	CA-C-N	-5.18	116.76	123.19
1	A	24	THR	C-N-CA	-5.18	116.76	123.19
1	L	36	GLY	N-CA-C	5.18	117.73	110.38
1	E	56	THR	N-CA-C	-5.14	108.27	114.75
1	H	36	GLY	N-CA-C	5.10	117.98	110.80
1	B	23	GLU	CA-C-N	-5.09	115.01	122.19
1	B	23	GLU	C-N-CA	-5.09	115.01	122.19
1	D	115	ALA	N-CA-C	5.08	117.68	109.40
1	I	10	CYS	N-CA-C	5.08	116.69	108.26
1	F	77	THR	N-CA-C	5.06	116.90	109.42
1	C	37	HIS	N-CA-C	5.05	117.56	110.23
1	K	120	SER	CA-C-N	-5.03	114.89	119.82
1	K	120	SER	C-N-CA	-5.03	114.89	119.82

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1208	0	1167	41	0
1	B	1208	0	1167	45	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1208	0	1167	34	0
1	D	1208	0	1167	65	0
1	E	1208	0	1167	34	0
1	F	1208	0	1167	63	0
1	G	1208	0	1167	71	0
1	H	1208	0	1167	41	0
1	I	1208	0	1167	71	0
1	J	1208	0	1167	38	0
1	K	1208	0	1167	35	0
1	L	1208	0	1167	59	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
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	2	0	0	0	0
2	J	2	0	0	0	0
2	K	2	0	0	0	0
2	L	2	0	0	0	0
3	A	15	0	0	6	0
3	B	15	0	0	6	0
3	C	15	0	0	4	0
3	D	15	0	0	3	0
3	E	15	0	0	4	0
3	F	15	0	0	1	0
3	G	15	0	0	7	0
3	H	15	0	0	6	0
3	I	15	0	0	1	0
3	J	15	0	0	1	0
3	K	15	0	0	2	0
3	L	15	0	0	3	0
4	A	35	0	0	1	0
4	B	30	0	0	0	0
4	C	33	0	0	0	0
4	D	18	0	0	0	0
4	E	35	0	0	1	0
4	F	11	0	0	0	0
4	G	27	0	0	1	0
4	H	17	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	I	18	0	0	2	0
4	J	14	0	0	0	0
4	K	31	0	0	0	0
4	L	16	0	0	0	0
All	All	14985	0	14004	554	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 19.

All (554) 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:64:HIS:CE1	1:D:135:ARG:HH21	1.73	1.06
1:L:136:TYR:HB3	1:L:140:MET:HE1	1.38	1.01
1:I:136:TYR:HB3	1:I:140:MET:HE1	1.46	0.97
1:F:43:THR:HG22	1:F:46:GLU:H	1.26	0.95
1:K:132:SER:OG	1:K:134:GLN:HG2	1.68	0.94
1:K:119:ARG:HG2	1:K:119:ARG:HH11	1.30	0.93
1:F:149:THR:HG22	1:G:149:THR:HG23	1.52	0.92
1:A:35:ALA:O	3:A:157:SO4:S	2.28	0.91
1:K:114:GLN:OE1	1:K:114:GLN:HA	1.71	0.90
1:L:51:GLU:O	1:L:55:GLU:HG3	1.71	0.90
1:F:110:GLU:O	1:F:114:GLN:HG2	1.72	0.89
1:D:65:PHE:HE2	1:E:140:MET:HE3	1.38	0.88
1:C:63:GLN:NE2	1:C:87:GLU:H	1.72	0.87
1:D:64:HIS:CE1	1:D:135:ARG:NH2	2.41	0.87
1:B:35:ALA:O	3:B:157:SO4:S	2.33	0.87
1:L:25:ILE:HG22	1:L:28:LYS:HB2	1.57	0.86
1:H:55:GLU:OE2	3:H:157:SO4:O4	1.92	0.85
1:B:72:ILE:O	1:B:73:ALA:HB3	1.76	0.85
1:B:72:ILE:O	1:B:73:ALA:CB	2.25	0.84
1:H:35:ALA:O	3:H:157:SO4:S	2.37	0.82
1:K:72:ILE:O	1:K:73:ALA:CB	2.28	0.81
1:D:56:THR:OG1	1:D:58:ILE:HD12	1.81	0.81
1:F:20:VAL:HG23	1:F:32:ASN:O	1.81	0.80
1:G:25:ILE:HG22	1:G:26:ASN:HD22	1.46	0.79
1:D:37:HIS:CD2	1:E:1:MET:HE1	2.17	0.79
1:E:43:THR:HG22	1:E:46:GLU:H	1.45	0.79
1:I:21:VAL:HG22	1:I:32:ASN:O	1.83	0.78
1:B:24:THR:HG23	1:B:102:ASP:OD2	1.82	0.78
1:H:110:GLU:CD	1:H:110:GLU:H	1.91	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:136:TYR:HB3	1:L:140:MET:CE	2.14	0.78
1:I:136:TYR:HB3	1:I:140:MET:CE	2.13	0.78
1:I:51:GLU:O	1:I:55:GLU:HG3	1.84	0.77
1:I:107:VAL:CG1	1:I:111:GLU:HB3	2.13	0.77
1:G:13:HIS:HD2	1:G:87:GLU:OE2	1.67	0.77
1:G:72:ILE:O	1:G:73:ALA:HB3	1.83	0.76
1:I:136:TYR:CB	1:I:140:MET:HE1	2.16	0.76
1:B:63:GLN:NE2	1:B:87:GLU:H	1.83	0.76
1:I:92:CYS:HB2	1:I:93:PRO:HD2	1.68	0.76
1:B:43:THR:HB	1:B:46:GLU:HB2	1.69	0.75
1:D:123:VAL:O	1:D:127:ILE:CD1	2.35	0.75
1:H:72:ILE:O	1:H:77:THR:O	2.04	0.74
1:A:143:ASP:OD2	1:A:150:LYS:NZ	2.18	0.74
1:C:35:ALA:O	3:C:157:SO4:S	2.46	0.74
1:F:63:GLN:HE22	1:F:87:GLU:H	1.34	0.74
1:G:91:ILE:HG22	1:G:92:CYS:H	1.51	0.73
1:I:107:VAL:HG13	1:I:111:GLU:HB3	1.69	0.73
1:C:140:MET:HE3	1:G:65:PHE:HE2	1.54	0.73
1:L:107:VAL:HG12	1:L:108:SER:O	1.88	0.73
1:F:132:SER:OG	1:F:134:GLN:HG3	1.88	0.73
1:K:72:ILE:O	1:K:73:ALA:HB2	1.88	0.73
1:H:66:ILE:HD11	1:H:85:ALA:HB2	1.70	0.73
1:K:119:ARG:HG2	1:K:119:ARG:NH1	1.99	0.72
1:J:43:THR:HG22	1:J:44:LEU:N	2.03	0.71
1:B:35:ALA:O	3:B:157:SO4:O2	2.08	0.71
1:E:35:ALA:O	3:E:157:SO4:S	2.48	0.71
1:G:35:ALA:O	3:G:158:SO4:S	2.48	0.71
1:D:123:VAL:O	1:D:127:ILE:HD12	1.91	0.71
1:B:63:GLN:HE22	1:B:87:GLU:H	1.37	0.71
1:L:130:TYR:CD2	1:L:130:TYR:C	2.69	0.71
1:B:55:GLU:OE2	3:B:157:SO4:S	2.48	0.71
1:L:72:ILE:O	1:L:73:ALA:HB2	1.90	0.71
1:E:63:GLN:HE22	1:E:87:GLU:H	1.39	0.70
1:D:43:THR:HG22	1:D:46:GLU:H	1.56	0.69
1:A:55:GLU:OE2	3:A:157:SO4:S	2.50	0.69
1:G:43:THR:HG22	1:G:45:VAL:H	1.58	0.69
1:L:63:GLN:HE22	1:L:87:GLU:H	1.40	0.69
1:B:110:GLU:O	1:B:114:GLN:HG2	1.93	0.69
1:H:72:ILE:O	1:H:73:ALA:CB	2.39	0.69
1:A:13:HIS:HD2	1:A:87:GLU:OE2	1.74	0.69
1:F:63:GLN:NE2	1:F:87:GLU:H	1.90	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:GLU:OE2	3:A:157:SO4:O1	2.11	0.69
1:L:63:GLN:NE2	1:L:87:GLU:H	1.90	0.69
1:G:92:CYS:O	1:G:93:PRO:O	2.11	0.69
1:C:1:MET:HE1	1:G:37:HIS:CD2	2.28	0.69
1:F:107:VAL:HG13	1:F:111:GLU:HB2	1.74	0.68
1:L:105:ARG:HG2	1:L:106:TRP:H	1.58	0.68
1:L:136:TYR:CB	1:L:140:MET:HE1	2.18	0.68
1:D:92:CYS:HB2	1:D:93:PRO:HD2	1.74	0.68
1:A:11:VAL:HG23	1:A:83:LEU:HD11	1.74	0.68
1:A:35:ALA:O	3:A:157:SO4:O1	2.12	0.68
1:E:108:SER:OG	1:E:111:GLU:HB2	1.93	0.68
1:B:43:THR:HG22	1:B:45:VAL:H	1.59	0.68
1:C:108:SER:OG	1:C:111:GLU:HG3	1.92	0.67
1:J:20:VAL:HG23	1:J:32:ASN:O	1.92	0.67
1:B:24:THR:CG2	1:B:102:ASP:OD2	2.43	0.67
1:L:43:THR:HG21	1:L:45:VAL:HG22	1.76	0.67
1:G:43:THR:HG22	1:G:45:VAL:N	2.09	0.67
1:F:67:ARG:HG2	1:F:68:MET:N	2.09	0.66
1:F:25:ILE:HG23	1:F:26:ASN:N	2.10	0.66
1:H:55:GLU:OE2	3:H:157:SO4:S	2.53	0.66
1:L:43:THR:HG22	1:L:45:VAL:N	2.10	0.66
1:L:107:VAL:HG13	1:L:111:GLU:CB	2.26	0.66
1:F:66:ILE:HD11	1:F:85:ALA:HB2	1.77	0.66
1:F:149:THR:HG23	1:G:149:THR:HA	1.77	0.66
1:D:17:LYS:HD3	1:D:106:TRP:O	1.96	0.65
1:G:15:GLU:OE2	1:G:91:ILE:HG12	1.96	0.65
1:E:63:GLN:NE2	1:E:87:GLU:H	1.94	0.65
1:B:53:TRP:O	1:B:57:GLY:N	2.30	0.65
1:I:145:ASN:ND2	1:K:89:GLU:OE1	2.28	0.65
1:L:92:CYS:HB2	1:L:93:PRO:HD2	1.77	0.65
1:A:63:GLN:NE2	1:A:87:GLU:H	1.95	0.65
3:D:156:SO4:O2	3:D:157:SO4:O4	2.14	0.65
1:D:71:TRP:CZ3	1:D:73:ALA:HB2	2.31	0.65
1:D:66:ILE:O	1:D:67:ARG:HB2	1.97	0.65
1:G:55:GLU:OE2	3:G:158:SO4:O2	2.15	0.64
1:B:137:PRO:HB2	1:B:139:GLU:HG2	1.80	0.64
1:F:140:MET:SD	1:K:140:MET:HE2	2.37	0.64
1:E:55:GLU:OE2	3:E:157:SO4:O2	2.16	0.64
1:B:43:THR:HG22	1:B:45:VAL:N	2.13	0.64
1:L:55:GLU:OE2	3:L:157:SO4:O1	2.16	0.64
1:L:13:HIS:CD2	1:L:130:TYR:OH	2.51	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:43:THR:HG21	1:I:45:VAL:HG22	1.81	0.63
1:D:19:LEU:HD21	1:D:56:THR:HG21	1.81	0.63
1:G:16:GLY:HA2	1:L:114:GLN:HE22	1.62	0.63
1:F:149:THR:CG2	1:G:149:THR:HG23	2.25	0.63
1:J:66:ILE:HD11	1:J:85:ALA:HB2	1.81	0.63
1:I:125:GLU:HA	1:I:125:GLU:OE1	1.97	0.62
1:D:140:MET:HE2	1:E:140:MET:HE1	1.80	0.62
1:D:65:PHE:CE2	1:E:140:MET:HE3	2.27	0.62
1:H:13:HIS:HD2	1:H:87:GLU:OE2	1.83	0.62
1:I:52:LEU:HD13	1:I:58:ILE:O	1.99	0.62
1:H:35:ALA:O	3:H:157:SO4:O2	2.17	0.62
1:B:66:ILE:O	1:B:67:ARG:HB2	1.99	0.62
1:B:98:ASP:OD1	1:B:100:ASP:HB2	2.00	0.62
1:E:35:ALA:O	3:E:157:SO4:O2	2.19	0.61
1:I:33:GLN:O	1:I:35:ALA:N	2.33	0.61
1:A:72:ILE:O	1:A:73:ALA:HB3	2.01	0.61
1:B:50:ARG:HD2	1:B:54:GLU:OE2	2.01	0.61
1:I:110:GLU:C	1:I:112:ILE:H	2.08	0.61
1:B:137:PRO:O	1:B:140:MET:HB2	2.02	0.60
1:K:132:SER:OG	1:K:134:GLN:CG	2.47	0.60
1:L:72:ILE:O	1:L:73:ALA:CB	2.49	0.60
1:C:110:GLU:CD	1:C:110:GLU:H	2.10	0.60
1:J:68:MET:HG2	1:J:69:HIS:N	2.17	0.60
1:L:124:ALA:O	1:L:128:ARG:HG3	2.01	0.60
1:K:66:ILE:HD11	1:K:85:ALA:HB2	1.84	0.60
1:A:63:GLN:HE22	1:A:87:GLU:H	1.49	0.60
1:J:56:THR:OG1	1:J:58:ILE:HG12	2.02	0.60
1:I:15:GLU:OE2	1:I:90:GLN:HB2	2.01	0.59
1:I:22:GLU:HA	1:I:30:LEU:O	2.02	0.59
1:L:15:GLU:OE2	1:L:90:GLN:HB2	2.02	0.59
1:D:17:LYS:CD	1:D:106:TRP:O	2.51	0.58
1:G:72:ILE:O	1:G:77:THR:O	2.21	0.58
1:H:127:ILE:O	1:H:131:GLN:HG3	2.03	0.58
1:K:110:GLU:O	1:K:114:GLN:HG2	2.03	0.58
1:H:72:ILE:O	1:H:73:ALA:HB3	2.03	0.58
1:G:17:LYS:HD3	1:G:106:TRP:C	2.28	0.58
1:B:1:MET:SD	1:L:5:HIS:CE1	2.97	0.58
1:D:22:GLU:OE1	1:D:105:ARG:NH1	2.36	0.58
1:L:103:CYS:SG	1:L:104:CYS:N	2.76	0.58
1:G:71:TRP:CH2	1:G:121:PRO:HD2	2.38	0.58
1:C:51:GLU:O	1:C:55:GLU:HG3	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:94:THR:O	1:D:95:GLN:HB3	2.04	0.58
1:I:41:ASP:HB3	1:I:148:PHE:CE1	2.39	0.58
1:A:43:THR:HG22	1:A:45:VAL:H	1.68	0.58
1:I:107:VAL:HG12	1:I:108:SER:O	2.04	0.58
3:G:156:SO4:O3	3:G:158:SO4:O2	2.22	0.58
1:A:2:PHE:C	1:A:2:PHE:CD2	2.82	0.57
1:B:55:GLU:OE2	3:B:157:SO4:O2	2.21	0.57
1:C:7:THR:HG22	1:C:37:HIS:HA	1.86	0.57
3:G:156:SO4:O3	3:G:158:SO4:S	2.62	0.57
1:K:36:GLY:HA2	3:K:156:SO4:O1	2.03	0.57
1:F:117:ASN:OD1	1:F:117:ASN:N	2.32	0.57
1:D:24:THR:HA	1:D:28:LYS:O	2.04	0.57
1:J:43:THR:HG22	1:J:45:VAL:H	1.69	0.57
1:E:81:ARG:HD3	4:E:162:HOH:O	2.04	0.57
1:I:130:TYR:C	1:I:130:TYR:CD2	2.82	0.57
1:L:21:VAL:HG22	1:L:32:ASN:O	2.05	0.57
1:K:68:MET:HG3	1:K:82:PHE:CD2	2.39	0.56
1:L:35:ALA:O	1:L:51:GLU:HB3	2.05	0.56
1:B:58:ILE:HD11	1:B:94:THR:HG22	1.86	0.56
1:I:75:ASP:OD1	1:I:77:THR:OG1	2.23	0.56
1:I:71:TRP:CZ3	1:I:73:ALA:HA	2.40	0.56
1:D:67:ARG:NH2	1:E:142:GLY:O	2.39	0.56
1:C:25:ILE:HB	1:C:30:LEU:HD23	1.86	0.56
1:F:125:GLU:HG3	1:K:144:PHE:CE1	2.41	0.56
1:A:135:ARG:NH2	1:E:125:GLU:OE1	2.33	0.56
1:I:25:ILE:HD13	1:I:26:ASN:H	1.71	0.56
1:A:55:GLU:OE2	3:A:157:SO4:O2	2.24	0.56
1:B:75:ASP:HB3	1:B:77:THR:H	1.70	0.56
1:G:30:LEU:HD12	1:G:117:ASN:HB2	1.88	0.56
1:L:102:ASP:OD1	1:L:102:ASP:N	2.39	0.56
1:G:71:TRP:CZ3	1:G:121:PRO:HG2	2.41	0.55
1:L:107:VAL:HG13	1:L:111:GLU:HB3	1.88	0.55
1:L:43:THR:CG2	1:L:45:VAL:HG22	2.36	0.55
1:D:87:GLU:O	1:D:88:LEU:HG	2.06	0.55
1:E:92:CYS:O	1:E:94:THR:HG22	2.05	0.55
1:L:43:THR:HG22	1:L:45:VAL:H	1.70	0.55
1:D:135:ARG:NH1	1:I:128:ARG:HB2	2.20	0.55
1:G:71:TRP:CE2	1:G:73:ALA:HB2	2.42	0.55
1:G:77:THR:OG1	4:G:198:HOH:O	2.18	0.55
1:H:32:ASN:HD21	1:H:35:ALA:HB3	1.72	0.55
1:B:13:HIS:HD2	1:B:87:GLU:OE2	1.90	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:110:GLU:H	1:E:110:GLU:CD	2.14	0.55
1:F:144:PHE:O	1:F:145:ASN:HB2	2.06	0.55
1:L:110:GLU:HA	1:L:113:LEU:HB2	1.87	0.55
1:C:109:ALA:HB3	1:C:110:GLU:OE1	2.06	0.55
1:G:81:ARG:HD3	1:G:122:LEU:HD13	1.87	0.55
1:D:14:ALA:HB3	1:D:106:TRP:CZ3	2.41	0.55
1:B:2:PHE:C	1:B:2:PHE:CD2	2.85	0.54
1:G:17:LYS:HD3	1:G:107:VAL:N	2.22	0.54
1:J:43:THR:CG2	1:J:44:LEU:N	2.69	0.54
1:L:36:GLY:HA2	3:L:157:SO4:O2	2.08	0.54
1:G:72:ILE:O	1:G:73:ALA:CB	2.49	0.54
1:J:13:HIS:HD2	1:J:87:GLU:OE2	1.90	0.54
1:G:31:TRP:HE1	1:G:105:ARG:HH12	1.55	0.54
1:G:120:SER:HB2	1:G:121:PRO:HD2	1.89	0.54
1:J:66:ILE:O	1:J:67:ARG:HB2	2.07	0.54
1:A:43:THR:HA	1:I:70:GLN:OE1	2.08	0.54
1:G:71:TRP:C	1:G:71:TRP:CD1	2.85	0.54
3:H:156:SO4:O1	3:H:157:SO4:O4	2.26	0.54
1:D:55:GLU:OE2	3:D:157:SO4:O4	2.25	0.53
1:L:107:VAL:CG1	1:L:111:GLU:HB2	2.39	0.53
1:A:1:MET:HE1	1:I:5:HIS:CE1	2.43	0.53
1:A:23:GLU:HG3	1:A:101:ILE:HD13	1.88	0.53
1:A:43:THR:CG2	1:A:45:VAL:HG13	2.38	0.53
1:C:55:GLU:OE2	3:C:157:SO4:O3	2.25	0.53
1:F:107:VAL:CG1	1:F:111:GLU:HB2	2.38	0.53
1:H:136:TYR:HB3	1:H:137:PRO:HD2	1.89	0.53
1:B:2:PHE:CD1	1:L:40:ALA:HB2	2.43	0.53
1:H:43:THR:HG22	1:H:45:VAL:H	1.72	0.53
1:I:43:THR:HG22	1:I:44:LEU:N	2.23	0.53
1:L:107:VAL:HG13	1:L:111:GLU:HB2	1.91	0.53
1:F:55:GLU:OE2	3:F:157:SO4:O3	2.25	0.53
1:L:107:VAL:CG1	1:L:111:GLU:CB	2.85	0.53
1:F:25:ILE:HG12	1:F:26:ASN:H	1.72	0.53
1:F:119:ARG:O	1:F:119:ARG:HG3	2.09	0.53
1:G:71:TRP:HZ3	1:G:121:PRO:HG2	1.74	0.53
1:I:11:VAL:HG23	1:I:83:LEU:HD11	1.90	0.53
1:G:35:ALA:O	3:G:158:SO4:O1	2.27	0.53
1:J:117:ASN:OD1	1:J:117:ASN:N	2.40	0.53
1:I:19:LEU:HD11	1:I:104:CYS:HB2	1.91	0.53
1:I:24:THR:HA	1:I:28:LYS:O	2.09	0.53
1:L:92:CYS:CB	1:L:93:PRO:HD2	2.36	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:35:ALA:O	3:C:157:SO4:O3	2.26	0.52
1:D:62:PRO:HA	1:D:86:ILE:HG12	1.90	0.52
1:F:13:HIS:HD2	1:F:87:GLU:OE2	1.91	0.52
1:A:58:ILE:CD1	1:A:92:CYS:SG	2.97	0.52
1:H:107:VAL:CG1	1:H:112:ILE:HG13	2.40	0.52
1:D:135:ARG:HH12	1:I:128:ARG:HB2	1.75	0.52
1:G:94:THR:OG1	1:G:95:GLN:N	2.42	0.52
1:I:95:GLN:HB3	4:I:164:HOH:O	2.08	0.52
1:I:110:GLU:CD	1:I:110:GLU:H	2.18	0.52
1:J:107:VAL:CG1	1:J:112:ILE:HG13	2.39	0.52
1:G:71:TRP:HD1	1:G:79:PHE:HB2	1.75	0.52
1:C:81:ARG:HD3	1:C:122:LEU:HD13	1.92	0.52
1:F:24:THR:HA	1:F:28:LYS:O	2.09	0.52
1:G:14:ALA:HB2	1:G:88:LEU:HB2	1.92	0.52
1:F:68:MET:HG2	1:F:69:HIS:N	2.24	0.51
1:D:125:GLU:HG3	1:E:144:PHE:CZ	2.45	0.51
1:H:144:PHE:O	1:H:145:ASN:C	2.53	0.51
1:F:70:GLN:OE1	1:K:43:THR:HA	2.11	0.51
1:E:8:VAL:O	1:E:35:ALA:HB1	2.10	0.51
1:I:73:ALA:HB1	1:I:74:PRO:HD2	1.92	0.51
1:B:72:ILE:O	1:B:77:THR:O	2.28	0.51
1:L:32:ASN:ND2	1:L:33:GLN:O	2.44	0.51
1:E:55:GLU:OE2	3:E:157:SO4:S	2.69	0.51
1:H:110:GLU:O	1:H:114:GLN:HG2	2.11	0.51
1:C:140:MET:HE1	1:G:140:MET:HE2	1.93	0.51
1:I:144:PHE:HA	4:I:224:HOH:O	2.11	0.51
1:D:130:TYR:OH	1:I:128:ARG:NH1	2.44	0.51
1:J:107:VAL:HG12	1:J:112:ILE:HG13	1.91	0.51
1:L:63:GLN:HE22	1:L:87:GLU:HB2	1.76	0.51
1:B:53:TRP:O	1:B:57:GLY:HA2	2.10	0.50
1:D:136:TYR:CE2	1:E:140:MET:HG3	2.46	0.50
1:H:63:GLN:HE22	1:H:87:GLU:H	1.59	0.50
1:L:13:HIS:HD2	1:L:87:GLU:OE1	1.95	0.50
1:F:7:THR:HG22	1:F:37:HIS:HA	1.93	0.50
1:I:124:ALA:O	1:I:125:GLU:C	2.53	0.50
1:L:42:GLU:OE1	1:L:50:ARG:NE	2.41	0.50
1:C:140:MET:HE3	1:G:65:PHE:CE2	2.42	0.50
1:F:70:GLN:HG3	1:F:80:LEU:HD12	1.93	0.50
1:G:91:ILE:HG23	1:G:106:TRP:CE2	2.46	0.50
1:H:30:LEU:HD23	1:H:119:ARG:HD2	1.92	0.50
1:I:63:GLN:HE22	1:I:87:GLU:H	1.60	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:91:ILE:O	1:F:53:TRP:CH2	2.65	0.50
1:D:135:ARG:HD3	1:I:128:ARG:O	2.11	0.50
1:G:25:ILE:HG22	1:G:26:ASN:ND2	2.23	0.50
1:B:138:LEU:C	1:B:140:MET:H	2.18	0.50
1:F:25:ILE:HG23	1:F:26:ASN:H	1.75	0.49
1:H:136:TYR:HB3	1:H:137:PRO:CD	2.43	0.49
1:I:36:GLY:HA3	1:I:51:GLU:HG3	1.94	0.49
1:I:66:ILE:HG22	1:I:67:ARG:HB2	1.93	0.49
1:A:43:THR:HG21	1:A:45:VAL:HG13	1.93	0.49
1:H:75:ASP:OD1	1:H:75:ASP:C	2.54	0.49
1:C:8:VAL:O	1:C:35:ALA:HB1	2.11	0.49
1:H:53:TRP:C	1:H:55:GLU:H	2.20	0.49
1:H:91:ILE:HG23	1:H:106:TRP:CE2	2.48	0.49
1:H:139:GLU:HG2	1:L:137:PRO:HB3	1.93	0.49
1:B:58:ILE:HD13	1:B:92:CYS:SG	2.51	0.49
1:D:125:GLU:CG	1:E:144:PHE:CZ	2.95	0.49
1:F:147:PRO:HG2	1:F:148:PHE:CD1	2.47	0.49
1:F:149:THR:HG22	1:G:149:THR:CG2	2.34	0.49
1:G:55:GLU:OE1	3:G:158:SO4:O1	2.30	0.49
1:L:25:ILE:N	1:L:28:LYS:O	2.44	0.49
1:D:72:ILE:O	1:D:73:ALA:HB3	2.11	0.49
1:E:25:ILE:HB	1:E:30:LEU:HD22	1.95	0.49
1:E:61:GLN:HG2	1:F:89:GLU:HG3	1.94	0.49
1:E:139:GLU:CD	1:E:139:GLU:H	2.21	0.49
1:L:36:GLY:HA3	1:L:51:GLU:HG3	1.93	0.49
1:L:130:TYR:CD2	1:L:130:TYR:O	2.65	0.49
1:C:141:ILE:HG22	1:G:68:MET:HB3	1.94	0.49
1:F:147:PRO:HG2	1:F:148:PHE:CE1	2.47	0.49
1:K:92:CYS:HB2	1:K:93:PRO:HD2	1.94	0.49
1:I:21:VAL:HG12	1:I:104:CYS:HB3	1.94	0.49
1:F:20:VAL:CG2	1:F:31:TRP:HB3	2.43	0.48
1:K:25:ILE:HG22	1:K:26:ASN:N	2.28	0.48
1:L:107:VAL:CG1	1:L:111:GLU:HB3	2.43	0.48
1:D:14:ALA:O	1:D:15:GLU:C	2.55	0.48
1:B:53:TRP:O	1:B:57:GLY:CA	2.62	0.48
1:J:63:GLN:NE2	1:J:87:GLU:H	2.12	0.48
1:L:138:LEU:C	1:L:140:MET:H	2.22	0.48
1:I:17:LYS:HB3	1:I:106:TRP:HB3	1.96	0.48
1:A:35:ALA:O	3:A:157:SO4:O2	2.31	0.48
1:D:135:ARG:NH1	1:I:128:ARG:CB	2.76	0.48
1:J:61:GLN:HA	1:J:61:GLN:NE2	2.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:107:VAL:HG22	1:K:108:SER:N	2.28	0.48
1:I:43:THR:CG2	1:I:45:VAL:HG22	2.43	0.48
1:J:74:PRO:C	1:J:76:LYS:H	2.21	0.48
1:A:53:TRP:O	1:A:57:GLY:N	2.45	0.48
1:C:112:ILE:HG21	1:C:127:ILE:HD13	1.96	0.48
1:D:43:THR:HG22	1:D:45:VAL:N	2.29	0.48
1:J:120:SER:O	1:J:123:VAL:HG23	2.14	0.48
1:L:44:LEU:HD12	1:L:141:ILE:HD13	1.95	0.48
1:F:67:ARG:CG	1:F:68:MET:N	2.76	0.48
1:H:35:ALA:O	3:H:157:SO4:O4	2.31	0.47
1:I:43:THR:HG22	1:I:45:VAL:H	1.78	0.47
1:I:19:LEU:HD21	1:I:56:THR:HG21	1.97	0.47
1:H:53:TRP:C	1:H:55:GLU:N	2.71	0.47
1:L:66:ILE:HD11	1:L:85:ALA:HB2	1.97	0.47
1:J:92:CYS:HB2	1:J:93:PRO:HD2	1.97	0.47
1:A:87:GLU:HB3	4:A:218:HOH:O	2.14	0.47
1:A:138:LEU:O	1:A:140:MET:N	2.47	0.47
1:B:68:MET:HG2	1:B:69:HIS:N	2.29	0.47
1:F:18:PHE:N	1:F:107:VAL:O	2.43	0.47
1:G:22:GLU:OE1	1:G:29:ALA:HB1	2.15	0.47
1:G:75:ASP:O	1:G:76:LYS:HB3	2.15	0.47
1:J:63:GLN:HE22	1:J:87:GLU:H	1.61	0.47
1:K:119:ARG:HH11	1:K:119:ARG:CG	2.15	0.47
1:D:13:HIS:HD2	1:D:87:GLU:OE2	1.98	0.47
1:D:127:ILE:O	1:D:131:GLN:HG3	2.14	0.47
1:D:81:ARG:HD2	1:D:122:LEU:HD13	1.97	0.47
1:L:139:GLU:CD	1:L:139:GLU:O	2.58	0.47
1:F:72:ILE:HD13	1:F:72:ILE:HA	1.79	0.47
1:H:2:PHE:C	1:H:2:PHE:CD2	2.92	0.47
1:A:13:HIS:CD2	1:A:87:GLU:OE2	2.62	0.46
1:F:20:VAL:HG21	1:F:31:TRP:HB3	1.97	0.46
1:A:52:LEU:HD13	1:A:58:ILE:HB	1.96	0.46
1:C:63:GLN:HE22	1:C:87:GLU:H	1.60	0.46
1:I:98:ASP:O	1:I:101:ILE:HG12	2.15	0.46
1:I:33:GLN:HE21	1:I:127:ILE:HD11	1.80	0.46
1:I:87:GLU:OE1	1:I:130:TYR:OH	2.20	0.46
1:D:46:GLU:O	1:D:49:ALA:HB3	2.16	0.46
1:I:129:CYS:O	1:I:130:TYR:C	2.59	0.46
1:A:127:ILE:O	1:A:131:GLN:HG3	2.15	0.46
1:D:92:CYS:HB2	1:D:93:PRO:CD	2.44	0.46
1:J:68:MET:HG2	1:J:69:HIS:H	1.78	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:71:TRP:HH2	1:G:121:PRO:HD2	1.79	0.46
1:B:111:GLU:O	1:B:115:ALA:HB2	2.16	0.46
1:C:118:LEU:CD1	1:C:124:ALA:HB2	2.45	0.46
1:D:64:HIS:HB2	1:D:85:ALA:HB3	1.97	0.46
1:I:11:VAL:O	1:I:11:VAL:HG12	2.15	0.46
1:A:7:THR:HA	1:A:36:GLY:O	2.15	0.46
1:D:16:GLY:HA2	1:I:114:GLN:HE22	1.81	0.46
1:G:96:PRO:HG3	1:G:101:ILE:HG22	1.98	0.46
1:J:91:ILE:HG23	1:J:106:TRP:CE2	2.51	0.46
1:C:111:GLU:O	1:C:115:ALA:HB2	2.16	0.46
1:C:138:LEU:C	1:C:140:MET:H	2.24	0.46
1:F:65:PHE:CE2	1:K:140:MET:HE3	2.51	0.46
1:H:16:GLY:C	1:H:17:LYS:HG2	2.41	0.46
1:I:125:GLU:OE1	1:I:125:GLU:CA	2.64	0.46
1:B:140:MET:HE1	1:L:140:MET:SD	2.56	0.45
1:B:138:LEU:C	1:B:140:MET:N	2.71	0.45
1:H:75:ASP:O	1:H:76:LYS:HB2	2.16	0.45
1:B:139:GLU:HG3	1:G:137:PRO:HB3	1.97	0.45
1:E:62:PRO:HA	1:E:86:ILE:HG12	1.98	0.45
1:K:114:GLN:OE1	1:K:114:GLN:CA	2.50	0.45
1:F:43:THR:CG2	1:F:46:GLU:H	2.14	0.45
1:G:66:ILE:HD12	1:G:83:LEU:HG	1.98	0.45
1:I:127:ILE:C	1:I:129:CYS:H	2.23	0.45
1:K:36:GLY:HA3	1:K:51:GLU:CD	2.41	0.45
1:B:110:GLU:CD	1:B:110:GLU:H	2.23	0.45
3:D:156:SO4:S	3:D:157:SO4:O4	2.75	0.45
1:F:19:LEU:HB2	1:F:106:TRP:CZ3	2.51	0.45
1:G:19:LEU:HD23	1:G:34:PRO:HG2	1.99	0.45
1:L:130:TYR:C	1:L:130:TYR:HD2	2.23	0.45
1:G:105:ARG:HH11	1:G:105:ARG:HG2	1.81	0.45
1:C:113:LEU:HD12	1:C:113:LEU:HA	1.83	0.45
1:E:11:VAL:HG11	1:E:130:TYR:CD1	2.52	0.45
1:F:125:GLU:CD	1:I:135:ARG:HH22	2.25	0.45
1:J:107:VAL:HG13	1:J:111:GLU:HB2	1.98	0.45
1:C:35:ALA:O	3:C:157:SO4:O4	2.35	0.45
1:D:22:GLU:HG2	1:D:31:TRP:CD1	2.52	0.45
1:G:95:GLN:HA	1:G:96:PRO:HD2	1.63	0.45
3:J:156:SO4:O4	3:J:157:SO4:O2	2.35	0.45
1:D:73:ALA:HA	1:D:74:PRO:HD2	1.72	0.44
1:E:81:ARG:HD3	1:E:81:ARG:HH11	1.66	0.44
1:L:72:ILE:HG22	1:L:73:ALA:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:ASP:OD2	1:B:150:LYS:NZ	2.46	0.44
1:C:25:ILE:HD12	1:C:25:ILE:HA	1.78	0.44
1:G:71:TRP:CZ2	1:G:73:ALA:HB2	2.52	0.44
1:H:19:LEU:HD11	1:H:104:CYS:HB3	1.98	0.44
1:G:150:LYS:HB3	1:G:150:LYS:HE3	1.79	0.44
1:J:61:GLN:NE2	1:J:61:GLN:CA	2.80	0.44
1:I:35:ALA:O	1:I:51:GLU:HB3	2.18	0.44
1:F:70:GLN:HG3	1:F:80:LEU:CD1	2.48	0.44
1:L:15:GLU:O	1:L:17:LYS:HE3	2.18	0.44
1:D:94:THR:O	1:D:95:GLN:CB	2.65	0.44
1:G:140:MET:HE3	1:G:140:MET:HB3	1.85	0.44
1:I:102:ASP:OD1	1:I:102:ASP:N	2.51	0.44
1:I:110:GLU:C	1:I:112:ILE:N	2.75	0.44
1:L:43:THR:HG22	1:L:46:GLU:H	1.83	0.44
1:D:125:GLU:HG3	1:E:144:PHE:CE1	2.53	0.44
1:I:66:ILE:HD11	1:I:85:ALA:HB2	1.99	0.44
1:C:43:THR:HG22	1:C:45:VAL:N	2.33	0.43
1:C:52:LEU:HD22	1:C:56:THR:OG1	2.18	0.43
1:G:7:THR:HG22	1:G:37:HIS:HA	2.00	0.43
1:G:130:TYR:CD2	1:G:130:TYR:C	2.96	0.43
1:I:124:ALA:O	1:I:126:SER:N	2.51	0.43
1:A:89:GLU:OE1	1:D:145:ASN:ND2	2.51	0.43
1:D:26:ASN:O	1:D:28:LYS:N	2.51	0.43
1:E:143:ASP:OD2	1:E:146:TRP:HB2	2.18	0.43
1:G:53:TRP:C	1:G:55:GLU:H	2.26	0.43
1:H:28:LYS:HD2	1:H:28:LYS:HA	1.85	0.43
1:J:38:LEU:HD13	1:J:44:LEU:HD23	2.00	0.43
1:K:11:VAL:HG23	1:K:83:LEU:HD11	2.00	0.43
1:J:7:THR:HG22	1:J:37:HIS:HA	2.00	0.43
1:J:52:LEU:CD1	1:J:60:ALA:HB3	2.48	0.43
1:D:91:ILE:HG12	1:D:106:TRP:CE3	2.53	0.43
1:F:92:CYS:HB2	1:F:93:PRO:HD2	2.00	0.43
1:J:18:PHE:CE2	1:J:109:ALA:HB2	2.53	0.43
1:J:124:ALA:O	1:J:127:ILE:N	2.51	0.43
1:K:25:ILE:HG22	1:K:26:ASN:H	1.82	0.43
1:B:30:LEU:HA	1:B:117:ASN:O	2.19	0.43
1:B:107:VAL:CG1	1:B:112:ILE:HG13	2.48	0.43
1:D:71:TRP:CZ2	1:D:73:ALA:HA	2.53	0.43
1:E:13:HIS:HA	1:E:17:LYS:O	2.19	0.43
1:I:141:ILE:HD12	1:I:141:ILE:O	2.19	0.43
1:K:95:GLN:HA	1:K:96:PRO:HD2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:VAL:HG21	1:A:48:ALA:N	2.34	0.43
1:J:77:THR:HA	1:J:78:PRO:HD3	1.88	0.43
1:L:122:LEU:HA	1:L:125:GLU:HB3	2.00	0.43
1:H:53:TRP:O	1:H:55:GLU:N	2.52	0.43
1:I:72:ILE:HD13	1:I:72:ILE:HA	1.91	0.43
1:B:140:MET:HE3	1:B:140:MET:HB3	1.48	0.43
1:F:3:LYS:HE2	1:K:5:HIS:CD2	2.54	0.43
1:G:92:CYS:C	1:G:93:PRO:O	2.61	0.43
1:K:13:HIS:HD2	1:K:87:GLU:OE2	2.01	0.43
1:L:53:TRP:CD1	1:L:53:TRP:C	2.97	0.43
1:A:45:VAL:HG23	1:A:62:PRO:HG2	2.01	0.43
1:G:71:TRP:NE1	1:G:73:ALA:HB2	2.34	0.42
1:H:50:ARG:HG2	1:H:54:GLU:OE2	2.18	0.42
1:K:149:THR:O	1:K:150:LYS:O	2.37	0.42
1:L:140:MET:HB2	1:L:140:MET:HE3	1.79	0.42
1:D:140:MET:HE2	1:E:65:PHE:CE2	2.54	0.42
1:A:72:ILE:O	1:A:73:ALA:CB	2.64	0.42
1:F:43:THR:HG23	1:F:45:VAL:H	1.84	0.42
1:G:55:GLU:OE2	3:G:158:SO4:S	2.77	0.42
3:B:156:SO4:O1	3:B:157:SO4:S	2.77	0.42
1:C:43:THR:HG22	1:C:45:VAL:H	1.85	0.42
1:D:19:LEU:HD13	1:D:106:TRP:NE1	2.35	0.42
1:F:56:THR:OG1	1:F:58:ILE:HG12	2.20	0.42
1:I:146:TRP:HA	1:I:147:PRO:HD3	1.93	0.42
1:J:75:ASP:OD1	1:J:77:THR:HB	2.19	0.42
1:A:19:LEU:HD21	1:A:56:THR:HG21	2.02	0.42
1:G:108:SER:OG	1:G:111:GLU:HB2	2.19	0.42
1:J:56:THR:OG1	1:J:58:ILE:CG1	2.67	0.42
1:A:19:LEU:HD11	1:A:104:CYS:HB3	2.01	0.42
1:B:61:GLN:O	1:B:62:PRO:C	2.61	0.42
1:C:25:ILE:CG2	1:C:26:ASN:N	2.82	0.42
1:I:68:MET:HG3	1:I:82:PHE:CD2	2.55	0.42
1:K:5:HIS:CD2	1:K:77:THR:HG22	2.55	0.42
1:A:1:MET:HE1	1:I:5:HIS:HE1	1.83	0.42
1:G:146:TRP:HA	1:G:147:PRO:HD3	1.86	0.42
1:A:1:MET:HB2	1:A:1:MET:HE2	1.67	0.42
1:F:72:ILE:O	1:F:73:ALA:HB3	2.19	0.42
1:F:140:MET:HE2	1:K:136:TYR:CE2	2.54	0.42
1:G:122:LEU:HD23	1:G:122:LEU:HA	1.92	0.42
1:I:136:TYR:CG	1:I:140:MET:HE1	2.54	0.42
1:L:37:HIS:HD2	3:L:156:SO4:S	2.43	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:19:LEU:CD2	1:D:56:THR:HG21	2.49	0.42
1:F:95:GLN:O	1:F:97:HIS:HD2	2.03	0.42
1:G:51:GLU:HA	1:G:54:GLU:HB2	2.02	0.42
1:G:66:ILE:O	1:G:67:ARG:HB3	2.19	0.42
1:H:43:THR:HB	1:H:46:GLU:HB2	2.02	0.42
1:J:43:THR:HG22	1:J:44:LEU:H	1.83	0.42
1:J:54:GLU:O	1:J:98:ASP:HB2	2.19	0.42
1:D:26:ASN:C	1:D:28:LYS:H	2.28	0.42
1:D:91:ILE:HG23	1:D:106:TRP:CE2	2.54	0.42
1:F:15:GLU:HB2	1:F:91:ILE:HD12	2.01	0.42
1:F:43:THR:HG22	1:F:46:GLU:N	2.11	0.42
1:H:11:VAL:HG23	1:H:83:LEU:HD11	2.01	0.42
1:K:63:GLN:HG3	1:K:86:ILE:HA	2.01	0.42
1:A:66:ILE:HD11	1:A:85:ALA:HB2	2.03	0.41
1:G:112:ILE:O	1:G:118:LEU:HD11	2.19	0.41
1:I:41:ASP:HB3	1:I:148:PHE:HE1	1.81	0.41
1:B:20:VAL:HG12	1:B:105:ARG:HG2	2.01	0.41
1:F:81:ARG:HH12	1:F:83:LEU:HD13	1.84	0.41
1:F:140:MET:O	1:F:140:MET:HG2	2.20	0.41
1:G:89:GLU:CD	1:G:89:GLU:H	2.28	0.41
1:C:142:GLY:O	1:G:67:ARG:NH2	2.53	0.41
1:F:110:GLU:CD	1:F:110:GLU:H	2.28	0.41
1:G:22:GLU:OE2	1:G:105:ARG:NH2	2.53	0.41
1:H:13:HIS:CD2	1:H:130:TYR:OH	2.74	0.41
1:A:34:PRO:HA	1:A:55:GLU:OE1	2.20	0.41
1:A:141:ILE:C	1:A:141:ILE:HD12	2.46	0.41
1:D:44:LEU:HD23	1:D:44:LEU:HA	1.88	0.41
1:E:81:ARG:HD2	1:E:122:LEU:HD13	2.02	0.41
1:F:11:VAL:HG11	1:F:130:TYR:CD1	2.56	0.41
1:F:148:PHE:HA	1:G:148:PHE:HA	2.02	0.41
1:J:61:GLN:O	1:J:86:ILE:HG12	2.21	0.41
1:K:107:VAL:CG2	1:K:111:GLU:HB3	2.51	0.41
1:A:39:GLU:C	1:I:2:PHE:CD2	2.99	0.41
1:H:68:MET:HA	1:H:81:ARG:O	2.21	0.41
1:H:122:LEU:HA	1:H:125:GLU:HB2	2.03	0.41
1:J:120:SER:OG	1:J:122:LEU:HB2	2.21	0.41
1:C:29:ALA:C	1:C:30:LEU:HD13	2.46	0.41
1:D:8:VAL:HG12	1:D:84:PHE:HE1	1.86	0.41
1:D:77:THR:HA	1:D:78:PRO:HD3	1.97	0.41
1:G:91:ILE:HG22	1:G:92:CYS:N	2.26	0.41
1:D:19:LEU:HD11	1:D:104:CYS:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:125:GLU:O	1:F:126:SER:C	2.63	0.41
1:H:107:VAL:HG12	1:H:112:ILE:HG13	2.02	0.41
1:D:4:PRO:CG	1:D:80:LEU:HD22	2.51	0.41
1:D:19:LEU:HD21	1:D:56:THR:CG2	2.49	0.41
1:E:44:LEU:HD23	1:E:44:LEU:HA	1.82	0.41
1:F:140:MET:HE2	1:K:136:TYR:CD2	2.56	0.41
1:H:63:GLN:NE2	1:H:87:GLU:H	2.18	0.41
1:I:43:THR:HB	1:I:46:GLU:H	1.85	0.41
1:I:63:GLN:NE2	1:I:87:GLU:H	2.19	0.41
1:J:22:GLU:HB3	1:J:102:ASP:HB2	2.01	0.41
1:J:107:VAL:CG1	1:J:112:ILE:CG1	2.99	0.41
1:K:107:VAL:HG23	1:K:111:GLU:CD	2.46	0.41
1:B:23:GLU:HG3	1:B:100:ASP:O	2.21	0.41
1:E:14:ALA:HB2	1:E:88:LEU:HB2	2.03	0.41
1:F:72:ILE:O	1:F:77:THR:O	2.39	0.41
1:H:32:ASN:ND2	1:H:35:ALA:HB3	2.36	0.41
1:J:61:GLN:CA	1:J:61:GLN:HE21	2.34	0.41
1:C:1:MET:SD	1:G:5:HIS:CE1	3.14	0.40
1:C:138:LEU:C	1:C:140:MET:N	2.78	0.40
1:K:55:GLU:OE2	3:K:157:SO4:S	2.78	0.40
1:L:17:LYS:HB3	1:L:106:TRP:HB3	2.03	0.40
1:A:16:GLY:C	1:A:17:LYS:HG2	2.46	0.40
3:B:156:SO4:S	3:B:157:SO4:O4	2.76	0.40
1:D:14:ALA:HB3	1:D:106:TRP:HZ3	1.86	0.40
1:D:67:ARG:HG2	1:D:68:MET:H	1.86	0.40
1:D:122:LEU:HA	1:D:122:LEU:HD23	1.84	0.40
1:I:37:HIS:HB2	3:I:156:SO4:O3	2.22	0.40
1:D:36:GLY:HA3	1:D:51:GLU:CD	2.47	0.40
1:C:66:ILE:HD11	1:C:85:ALA:HB2	2.03	0.40
1:F:19:LEU:HB2	1:F:106:TRP:CH2	2.56	0.40
1:F:63:GLN:HE21	1:F:63:GLN:HB2	1.66	0.40
1:F:98:ASP:O	1:F:99:SER:C	2.64	0.40
1:J:140:MET:HE3	1:J:140:MET:HB2	1.89	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	148/153 (97%)	137 (93%)	8 (5%)	3 (2%)	6	10
1	B	148/153 (97%)	134 (90%)	11 (7%)	3 (2%)	6	10
1	C	148/153 (97%)	136 (92%)	12 (8%)	0	100	100
1	D	148/153 (97%)	126 (85%)	17 (12%)	5 (3%)	3	4
1	E	148/153 (97%)	134 (90%)	13 (9%)	1 (1%)	18	34
1	F	148/153 (97%)	130 (88%)	14 (10%)	4 (3%)	4	6
1	G	148/153 (97%)	128 (86%)	14 (10%)	6 (4%)	2	3
1	H	148/153 (97%)	137 (93%)	8 (5%)	3 (2%)	6	10
1	I	148/153 (97%)	117 (79%)	24 (16%)	7 (5%)	2	2
1	J	148/153 (97%)	133 (90%)	13 (9%)	2 (1%)	9	17
1	K	148/153 (97%)	134 (90%)	11 (7%)	3 (2%)	6	10
1	L	148/153 (97%)	121 (82%)	20 (14%)	7 (5%)	2	2
All	All	1776/1836 (97%)	1567 (88%)	165 (9%)	44 (2%)	4	7

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	25	ILE
1	G	93	PRO
1	G	94	THR
1	G	96	PRO
1	H	26	ASN
1	H	73	ALA
1	I	125	GLU
1	K	73	ALA
1	L	73	ALA
1	A	26	ASN
1	D	27	GLY
1	D	95	GLN

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Mol	Chain	Res	Type
1	E	26	ASN
1	F	4	PRO
1	G	54	GLU
1	I	25	ILE
1	I	93	PRO
1	I	111	GLU
1	I	124	ALA
1	K	72	ILE
1	L	26	ASN
1	L	72	ILE
1	L	74	PRO
1	B	73	ALA
1	D	93	PRO
1	F	99	SER
1	J	75	ASP
1	L	24	THR
1	L	39	GLU
1	L	93	PRO
1	A	139	GLU
1	B	67	ARG
1	G	95	GLN
1	I	39	GLU
1	B	75	ASP
1	D	73	ALA
1	D	74	PRO
1	F	73	ALA
1	K	25	ILE
1	H	96	PRO
1	J	67	ARG
1	I	34	PRO
1	A	73	ALA
1	G	73	ALA

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	130/132 (98%)	107 (82%)	23 (18%)	2	3
1	B	130/132 (98%)	113 (87%)	17 (13%)	4	8
1	C	130/132 (98%)	110 (85%)	20 (15%)	2	5
1	D	130/132 (98%)	109 (84%)	21 (16%)	2	4
1	E	130/132 (98%)	117 (90%)	13 (10%)	7	15
1	F	130/132 (98%)	113 (87%)	17 (13%)	4	8
1	G	130/132 (98%)	106 (82%)	24 (18%)	1	3
1	H	130/132 (98%)	108 (83%)	22 (17%)	2	4
1	I	130/132 (98%)	110 (85%)	20 (15%)	2	5
1	J	130/132 (98%)	110 (85%)	20 (15%)	2	5
1	K	130/132 (98%)	115 (88%)	15 (12%)	5	11
1	L	130/132 (98%)	106 (82%)	24 (18%)	1	3
All	All	1560/1584 (98%)	1324 (85%)	236 (15%)	3	5

All (236) 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	25	ILE
1	A	26	ASN
1	A	28	LYS
1	A	30	LEU
1	A	45	VAL
1	A	52	LEU
1	A	59	SER
1	A	61	GLN
1	A	67	ARG
1	A	71	TRP
1	A	72	ILE
1	A	75	ASP
1	A	80	LEU
1	A	89	GLU
1	A	107	VAL
1	A	110	GLU
1	A	113	LEU
1	A	127	ILE
1	A	143	ASP

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Mol	Chain	Res	Type
1	A	149	THR
1	B	1	MET
1	B	20	VAL
1	B	24	THR
1	B	28	LYS
1	B	30	LEU
1	B	45	VAL
1	B	50	ARG
1	B	52	LEU
1	B	67	ARG
1	B	89	GLU
1	B	99	SER
1	B	107	VAL
1	B	110	GLU
1	B	113	LEU
1	B	114	GLN
1	B	139	GLU
1	B	140	MET
1	C	1	MET
1	C	20	VAL
1	C	25	ILE
1	C	26	ASN
1	C	30	LEU
1	C	43	THR
1	C	45	VAL
1	C	52	LEU
1	C	62	PRO
1	C	67	ARG
1	C	80	LEU
1	C	89	GLU
1	C	94	THR
1	C	107	VAL
1	C	110	GLU
1	C	113	LEU
1	C	127	ILE
1	C	132	SER
1	C	139	GLU
1	C	141	ILE
1	D	1	MET
1	D	20	VAL
1	D	28	LYS
1	D	43	THR

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Mol	Chain	Res	Type
1	D	45	VAL
1	D	52	LEU
1	D	61	GLN
1	D	63	GLN
1	D	67	ARG
1	D	75	ASP
1	D	76	LYS
1	D	80	LEU
1	D	94	THR
1	D	99	SER
1	D	105	ARG
1	D	107	VAL
1	D	112	ILE
1	D	113	LEU
1	D	116	SER
1	D	119	ARG
1	D	139	GLU
1	E	1	MET
1	E	20	VAL
1	E	39	GLU
1	E	43	THR
1	E	45	VAL
1	E	52	LEU
1	E	67	ARG
1	E	76	LYS
1	E	80	LEU
1	E	94	THR
1	E	105	ARG
1	E	110	GLU
1	E	113	LEU
1	F	1	MET
1	F	26	ASN
1	F	39	GLU
1	F	43	THR
1	F	52	LEU
1	F	61	GLN
1	F	72	ILE
1	F	80	LEU
1	F	90	GLN
1	F	94	THR
1	F	95	GLN
1	F	100	ASP

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Mol	Chain	Res	Type
1	F	105	ARG
1	F	110	GLU
1	F	113	LEU
1	F	127	ILE
1	F	134	GLN
1	G	1	MET
1	G	20	VAL
1	G	28	LYS
1	G	30	LEU
1	G	39	GLU
1	G	43	THR
1	G	45	VAL
1	G	56	THR
1	G	58	ILE
1	G	61	GLN
1	G	63	GLN
1	G	71	TRP
1	G	75	ASP
1	G	76	LYS
1	G	80	LEU
1	G	91	ILE
1	G	95	GLN
1	G	105	ARG
1	G	111	GLU
1	G	112	ILE
1	G	113	LEU
1	G	143	ASP
1	G	149	THR
1	G	150	LYS
1	H	1	MET
1	H	17	LYS
1	H	20	VAL
1	H	24	THR
1	H	26	ASN
1	H	28	LYS
1	H	30	LEU
1	H	52	LEU
1	H	58	ILE
1	H	61	GLN
1	H	67	ARG
1	H	72	ILE
1	H	80	LEU

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Mol	Chain	Res	Type
1	H	89	GLU
1	H	94	THR
1	H	107	VAL
1	H	110	GLU
1	H	113	LEU
1	H	127	ILE
1	H	134	GLN
1	H	139	GLU
1	H	150	LYS
1	I	20	VAL
1	I	22	GLU
1	I	25	ILE
1	I	30	LEU
1	I	39	GLU
1	I	42	GLU
1	I	52	LEU
1	I	67	ARG
1	I	90	GLN
1	I	94	THR
1	I	95	GLN
1	I	102	ASP
1	I	105	ARG
1	I	110	GLU
1	I	113	LEU
1	I	118	LEU
1	I	125	GLU
1	I	139	GLU
1	I	149	THR
1	I	150	LYS
1	J	1	MET
1	J	30	LEU
1	J	39	GLU
1	J	45	VAL
1	J	50	ARG
1	J	52	LEU
1	J	58	ILE
1	J	61	GLN
1	J	67	ARG
1	J	80	LEU
1	J	100	ASP
1	J	105	ARG
1	J	107	VAL

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Mol	Chain	Res	Type
1	J	110	GLU
1	J	113	LEU
1	J	114	GLN
1	J	125	GLU
1	J	135	ARG
1	J	149	THR
1	J	150	LYS
1	K	1	MET
1	K	20	VAL
1	K	24	THR
1	K	30	LEU
1	K	52	LEU
1	K	61	GLN
1	K	63	GLN
1	K	80	LEU
1	K	89	GLU
1	K	90	GLN
1	K	113	LEU
1	K	114	GLN
1	K	119	ARG
1	K	135	ARG
1	K	139	GLU
1	L	8	VAL
1	L	17	LYS
1	L	22	GLU
1	L	25	ILE
1	L	30	LEU
1	L	43	THR
1	L	52	LEU
1	L	59	SER
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
1	L	102	ASP
1	L	103	CYS
1	L	108	SER
1	L	110	GLU
1	L	113	LEU

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Mol	Chain	Res	Type
1	L	119	ARG
1	L	123	VAL
1	L	149	THR
1	L	150	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	HIS
1	A	63	GLN
1	A	134	GLN
1	B	13	HIS
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	61	GLN
1	C	63	GLN
1	C	95	GLN
1	D	13	HIS
1	D	69	HIS
1	D	114	GLN
1	D	134	GLN
1	E	13	HIS
1	E	26	ASN
1	E	61	GLN
1	E	63	GLN
1	E	95	GLN
1	E	134	GLN
1	F	13	HIS
1	F	63	GLN
1	F	64	HIS
1	F	69	HIS
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	G	131	GLN

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Mol	Chain	Res	Type
1	H	13	HIS
1	H	63	GLN
1	H	95	GLN
1	H	134	GLN
1	I	63	GLN
1	I	114	GLN
1	J	13	HIS
1	J	61	GLN
1	J	63	GLN
1	J	90	GLN
1	K	13	HIS
1	K	63	GLN
1	L	5	HIS
1	L	13	HIS
1	L	32	ASN
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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 60 ligands modelled in this entry, 24 are monoatomic - leaving 36 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	J	156	2	4,4,4	0.30	0	6,6,6	0.79	0
3	SO4	B	158	-	4,4,4	0.38	0	6,6,6	0.69	0
3	SO4	J	158	-	4,4,4	0.32	0	6,6,6	0.25	0
3	SO4	E	157	2	4,4,4	0.26	0	6,6,6	0.45	0
3	SO4	A	156	2	4,4,4	0.39	0	6,6,6	0.87	0
3	SO4	A	158	-	4,4,4	0.27	0	6,6,6	0.72	0
3	SO4	I	156	2	4,4,4	0.29	0	6,6,6	0.22	0
3	SO4	H	157	2	4,4,4	0.40	0	6,6,6	0.50	0
3	SO4	K	157	2	4,4,4	0.23	0	6,6,6	0.51	0
3	SO4	H	156	2	4,4,4	0.18	0	6,6,6	0.59	0
3	SO4	L	157	-	4,4,4	0.25	0	6,6,6	0.48	0
3	SO4	D	157	2	4,4,4	0.31	0	6,6,6	0.64	0
3	SO4	C	158	-	4,4,4	0.39	0	6,6,6	0.22	0
3	SO4	D	158	-	4,4,4	0.34	0	6,6,6	0.55	0
3	SO4	K	156	2	4,4,4	0.28	0	6,6,6	0.48	0
3	SO4	F	156	2	4,4,4	0.21	0	6,6,6	0.47	0
3	SO4	G	158	2	4,4,4	0.24	0	6,6,6	0.43	0
3	SO4	C	157	2	4,4,4	0.30	0	6,6,6	0.60	0
3	SO4	G	156	2	4,4,4	0.31	0	6,6,6	0.26	0
3	SO4	J	157	2	4,4,4	0.23	0	6,6,6	0.26	0
3	SO4	G	157	-	4,4,4	0.26	0	6,6,6	0.77	0
3	SO4	E	158	-	4,4,4	0.23	0	6,6,6	0.50	0
3	SO4	I	158	-	4,4,4	0.32	0	6,6,6	0.36	0
3	SO4	E	156	2	4,4,4	0.34	0	6,6,6	0.66	0
3	SO4	F	158	-	4,4,4	0.37	0	6,6,6	0.57	0
3	SO4	I	157	-	4,4,4	0.19	0	6,6,6	0.28	0
3	SO4	B	157	2	4,4,4	0.52	0	6,6,6	0.85	0
3	SO4	H	158	-	4,4,4	0.35	0	6,6,6	0.83	0
3	SO4	F	157	2	4,4,4	0.31	0	6,6,6	0.41	0
3	SO4	L	158	-	4,4,4	0.23	0	6,6,6	0.19	0
3	SO4	A	157	2	4,4,4	0.29	0	6,6,6	0.89	0
3	SO4	C	156	2	4,4,4	0.21	0	6,6,6	0.51	0
3	SO4	D	156	2	4,4,4	0.25	0	6,6,6	0.28	0
3	SO4	K	158	-	4,4,4	0.38	0	6,6,6	0.46	0
3	SO4	L	156	2	4,4,4	0.21	0	6,6,6	0.39	0
3	SO4	B	156	2	4,4,4	0.17	0	6,6,6	1.00	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.

19 monomers are involved in 44 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	J	156	SO4	1	0
3	E	157	SO4	4	0
3	I	156	SO4	1	0
3	H	157	SO4	6	0
3	K	157	SO4	1	0
3	H	156	SO4	1	0
3	L	157	SO4	2	0
3	D	157	SO4	3	0
3	K	156	SO4	1	0
3	G	158	SO4	7	0
3	C	157	SO4	4	0
3	G	156	SO4	2	0
3	J	157	SO4	1	0
3	B	157	SO4	6	0
3	F	157	SO4	1	0
3	A	157	SO4	6	0
3	D	156	SO4	2	0
3	L	156	SO4	1	0
3	B	156	SO4	2	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%)	-1.39	0 100 100	9, 26, 45, 62	2 (1%)
1	B	150/153 (98%)	-1.42	0 100 100	10, 26, 41, 51	2 (1%)
1	C	150/153 (98%)	-1.37	0 100 100	13, 30, 57, 60	2 (1%)
1	D	150/153 (98%)	-1.09	0 100 100	18, 39, 70, 75	2 (1%)
1	E	150/153 (98%)	-1.32	0 100 100	13, 31, 58, 60	2 (1%)
1	F	150/153 (98%)	-1.22	0 100 100	10, 34, 64, 69	2 (1%)
1	G	150/153 (98%)	-1.15	0 100 100	19, 39, 69, 72	2 (1%)
1	H	150/153 (98%)	-1.27	0 100 100	10, 37, 58, 63	2 (1%)
1	I	150/153 (98%)	-0.94	0 100 100	13, 50, 89, 93	2 (1%)
1	J	150/153 (98%)	-1.26	0 100 100	11, 34, 66, 69	2 (1%)
1	K	150/153 (98%)	-1.25	0 100 100	10, 38, 56, 62	2 (1%)
1	L	150/153 (98%)	-0.97	0 100 100	14, 50, 85, 92	2 (1%)
All	All	1800/1836 (98%)	-1.22	0 100 100	9, 36, 67, 93	24 (1%)

There are no RSRZ outliers to report.

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 ⓘ

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	L	155	1/1	0.97	0.05	123,123,123,123	0
2	MN	I	155	1/1	0.98	0.04	86,86,86,86	0
3	SO4	I	156	5/5	0.98	0.04	88,89,89,90	0
3	SO4	I	157	5/5	0.98	0.05	98,99,99,100	0
3	SO4	I	158	5/5	0.98	0.11	81,82,82,83	0
3	SO4	K	156	5/5	0.98	0.04	56,58,60,60	0
3	SO4	L	156	5/5	0.98	0.04	94,94,95,95	0
3	SO4	L	158	5/5	0.98	0.07	94,95,95,95	0
2	MN	L	154	1/1	0.99	0.03	87,87,87,87	0
2	MN	E	154	1/1	0.99	0.03	43,43,43,43	0
3	SO4	A	156	5/5	0.99	0.03	34,34,35,35	0
3	SO4	B	156	5/5	0.99	0.04	33,34,34,35	0
3	SO4	C	156	5/5	0.99	0.03	52,54,55,55	0
3	SO4	C	158	5/5	0.99	0.03	44,46,48,49	0
3	SO4	D	156	5/5	0.99	0.04	64,65,67,67	0
3	SO4	D	157	5/5	0.99	0.03	42,43,47,47	0
3	SO4	D	158	5/5	0.99	0.04	56,57,59,59	0
3	SO4	E	156	5/5	0.99	0.03	46,47,49,49	0
3	SO4	E	158	5/5	0.99	0.04	44,48,48,49	0
3	SO4	F	156	5/5	0.99	0.03	59,60,61,62	0
3	SO4	F	157	5/5	0.99	0.03	52,53,54,56	0
3	SO4	F	158	5/5	0.99	0.03	51,51,53,54	0
3	SO4	G	156	5/5	0.99	0.02	62,62,65,65	0
3	SO4	G	157	5/5	0.99	0.04	52,52,55,55	0
3	SO4	H	156	5/5	0.99	0.04	60,61,62,63	0
3	SO4	H	157	5/5	0.99	0.03	42,43,46,47	0
3	SO4	H	158	5/5	0.99	0.03	34,35,37,39	0
2	MN	G	154	1/1	0.99	0.03	54,54,54,54	0
2	MN	G	155	1/1	0.99	0.04	54,54,54,54	0
2	MN	I	154	1/1	0.99	0.03	96,96,96,96	0
3	SO4	J	157	5/5	0.99	0.03	54,55,57,57	0
3	SO4	J	158	5/5	0.99	0.03	60,60,61,62	0
2	MN	B	154	1/1	0.99	0.03	37,37,37,37	0
3	SO4	K	158	5/5	0.99	0.04	38,39,41,42	0
2	MN	J	154	1/1	0.99	0.02	52,52,52,52	0
3	SO4	L	157	5/5	0.99	0.04	72,73,75,75	0
2	MN	K	155	1/1	0.99	0.03	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	E	157	5/5	1.00	0.02	41,43,45,45	0
2	MN	D	154	1/1	1.00	0.04	54,54,54,54	0
2	MN	J	155	1/1	1.00	0.01	53,53,53,53	0
2	MN	K	154	1/1	1.00	0.01	52,52,52,52	0
2	MN	D	155	1/1	1.00	0.01	57,57,57,57	0
2	MN	A	155	1/1	1.00	0.01	40,40,40,40	0
2	MN	E	155	1/1	1.00	0.02	55,55,55,55	0
3	SO4	G	158	5/5	1.00	0.03	44,46,48,50	0
2	MN	F	154	1/1	1.00	0.02	58,58,58,58	0
3	SO4	A	157	5/5	1.00	0.02	24,25,28,33	0
3	SO4	A	158	5/5	1.00	0.04	30,30,31,31	0
2	MN	F	155	1/1	1.00	0.01	53,53,53,53	0
3	SO4	B	157	5/5	1.00	0.03	22,22,27,29	0
3	SO4	B	158	5/5	1.00	0.03	29,30,33,35	0
3	SO4	J	156	5/5	1.00	0.02	57,57,57,58	0
2	MN	A	154	1/1	1.00	0.02	33,33,33,33	0
3	SO4	C	157	5/5	1.00	0.03	35,36,37,39	0
2	MN	B	155	1/1	1.00	0.03	42,42,42,42	0
3	SO4	K	157	5/5	1.00	0.03	43,43,45,45	0
2	MN	H	154	1/1	1.00	0.02	56,56,56,56	0
2	MN	H	155	1/1	1.00	0.03	51,51,51,51	0
2	MN	C	154	1/1	1.00	0.02	51,51,51,51	0
2	MN	C	155	1/1	1.00	0.02	46,46,46,46	0

6.5 Other polymers [i](#)

There are no such residues in this entry.