



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:50 AM GMT

PDB ID : 2IVQ
Title : SITE DIRECTED MUTAGENESIS OF KEY RESIDUES INVOLVED IN
THE CATALYTIC MECHANISM OF CYANASE
Authors : Guilloton, M.; Walsh, M.A.; Joachimiak, A.; Anderson, P.M.
Deposited on : 2006-06-14
Resolution : 2.10 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

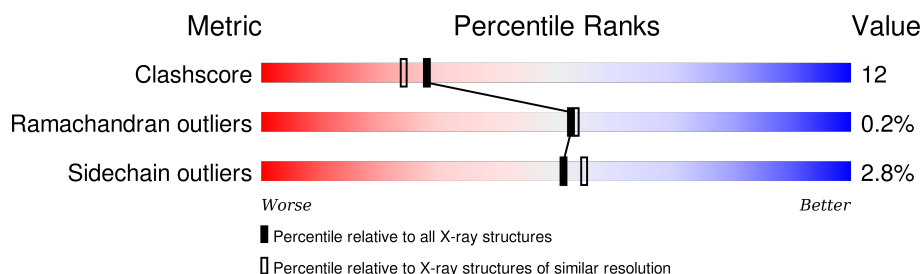
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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))
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)




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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	156	 81% 17% •
1	B	156	 83% 17% •
1	C	156	 77% 21% •
1	D	156	 85% 15% •
1	E	156	 80% 19% •
1	F	156	 85% 15% •
1	G	156	 81% 18% •

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

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CL	C	1159	-	-	X	-
2	CL	I	1160	-	-	X	-
2	CL	J	1160	-	-	X	-
3	SO4	F	1158	-	-	X	-
3	SO4	I	1158	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13229 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called CYANATE HYDRATASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	156	Total	C	N	O	S	0	0	0
			1196	767	197	227	5			
1	B	156	Total	C	N	O	S	0	0	0
			1196	767	197	227	5			
1	C	156	Total	C	N	O	S	0	1	0
			1202	772	198	227	5			
1	D	156	Total	C	N	O	S	0	0	0
			1196	767	197	227	5			
1	E	156	Total	C	N	O	S	0	0	0
			1196	767	197	227	5			
1	F	156	Total	C	N	O	S	0	0	0
			1196	767	197	227	5			
1	G	156	Total	C	N	O	S	0	0	0
			1196	767	197	227	5			
1	H	156	Total	C	N	O	S	0	0	0
			1196	767	197	227	5			
1	I	156	Total	C	N	O	S	0	0	0
			1196	767	197	227	5			
1	J	156	Total	C	N	O	S	0	1	0
			1202	772	198	227	5			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	96	LYS	ARG	ENGINEERED MUTATION	UNP P00816
B	96	LYS	ARG	ENGINEERED MUTATION	UNP P00816
C	96	LYS	ARG	ENGINEERED MUTATION	UNP P00816
D	96	LYS	ARG	ENGINEERED MUTATION	UNP P00816
E	96	LYS	ARG	ENGINEERED MUTATION	UNP P00816
F	96	LYS	ARG	ENGINEERED MUTATION	UNP P00816
G	96	LYS	ARG	ENGINEERED MUTATION	UNP P00816
H	96	LYS	ARG	ENGINEERED MUTATION	UNP P00816
I	96	LYS	ARG	ENGINEERED MUTATION	UNP P00816

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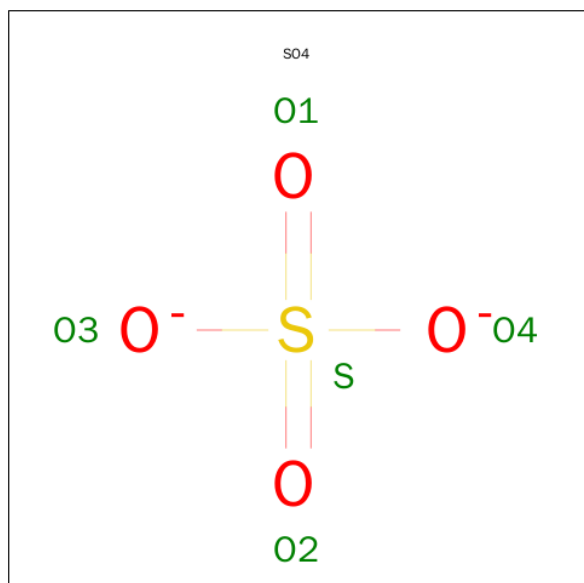
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Chain	Residue	Modelled	Actual	Comment	Reference
J	96	LYS	ARG	ENGINEERED MUTATION	UNP P00816

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

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

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	J	1	Total	O	S	0	0
			5	4	1		
3	J	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is water.

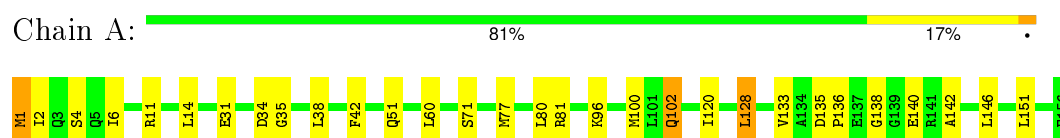
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	112	Total	O		0	0
			112	112			
4	B	130	Total	O		0	0
			130	130			
4	C	107	Total	O		0	0
			107	107			
4	D	114	Total	O		0	0
			114	114			
4	E	131	Total	O		0	0
			131	131			
4	F	116	Total	O		0	0
			116	116			
4	G	98	Total	O		0	0
			98	98			
4	H	108	Total	O		0	0
			108	108			
4	I	91	Total	O		0	0
			91	91			
4	J	117	Total	O		0	0
			117	117			

3 Residue-property plots [i](#)

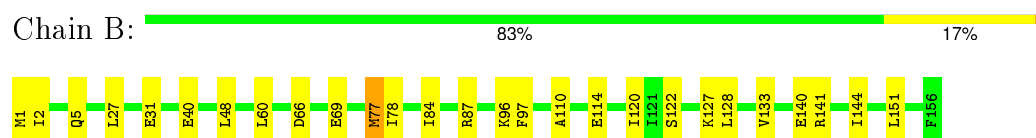
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

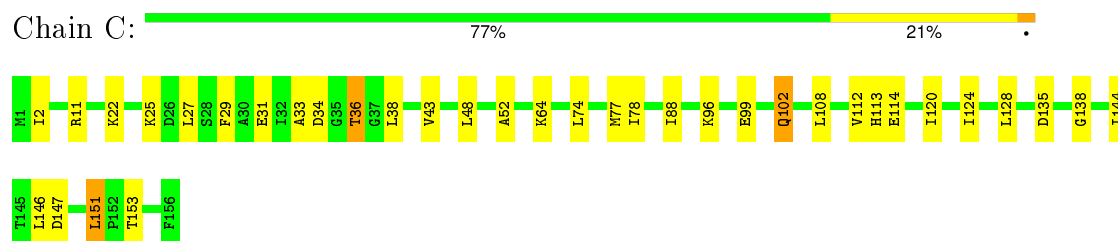
• Molecule 1: CYANATE HYDRATASE



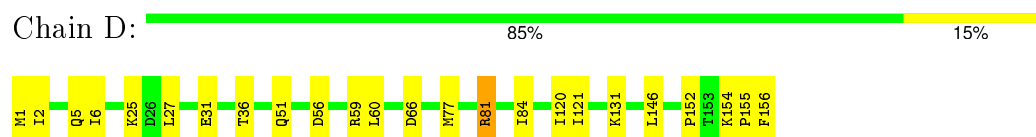
• Molecule 1: CYANATE HYDRATASE



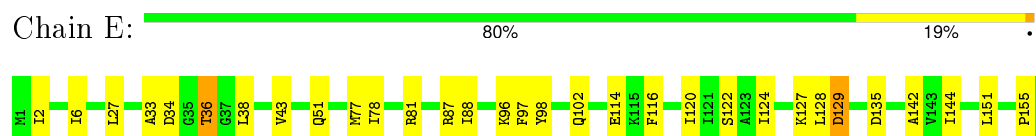
• Molecule 1: CYANATE HYDRATASE




• Molecule 1: CYANATE HYDRATASE



• Molecule 1: CYANATE HYDRATASE




• Molecule 1: CYANATE HYDRATASE

Chain F:  85% 15%




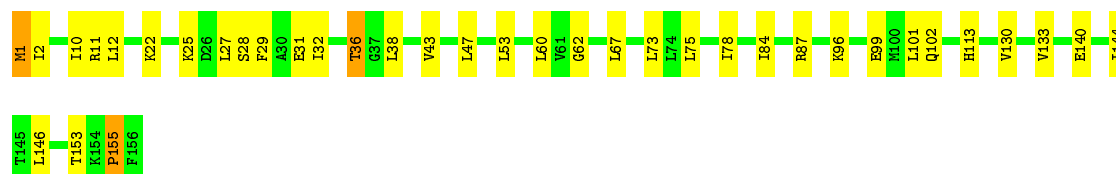
- Molecule 1: CYANATE HYDRATASE

Chain G:  81% 18% •




- Molecule 1: CYANATE HYDRATASE

Chain H:  76% 22% •




- Molecule 1: CYANATE HYDRATASE

Chain I:  81% 19%



- Molecule 1: CYANATE HYDRATASE

Chain J:  79% 19% •



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	76.88 Å 80.84 Å 82.65 Å 69.99° 71.98° 66.17°	Depositor
Resolution (Å)	76.03 – 2.10	Depositor
% Data completeness (in resolution range)	95.7 (76.03-2.10)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.180 , 0.243	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13229	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.94	0/1213	0.94	3/1638 (0.2%)
1	B	0.99	2/1213 (0.2%)	0.90	0/1638
1	C	0.92	0/1222	0.93	3/1649 (0.2%)
1	D	0.99	1/1213 (0.1%)	0.94	2/1638 (0.1%)
1	E	0.93	0/1213	0.90	0/1638
1	F	0.90	0/1213	0.87	2/1638 (0.1%)
1	G	0.89	0/1213	0.87	2/1638 (0.1%)
1	H	0.94	0/1213	0.95	3/1638 (0.2%)
1	I	0.86	0/1213	0.85	0/1638
1	J	0.97	0/1222	0.91	1/1649 (0.1%)
All	All	0.93	3/12148 (0.0%)	0.90	16/16402 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	69	GLU	CG-CD	5.35	1.59	1.51
1	B	69	GLU	CB-CG	5.32	1.62	1.52
1	D	31	GLU	CG-CD	5.30	1.59	1.51

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	11	ARG	NE-CZ-NH2	8.33	124.46	120.30
1	A	11	ARG	NE-CZ-NH1	-7.14	116.73	120.30
1	D	66	ASP	CB-CG-OD1	6.38	124.05	118.30
1	A	1	MET	CG-SD-CE	6.27	110.23	100.20
1	C	11	ARG	NE-CZ-NH2	6.03	123.31	120.30
1	H	11	ARG	NE-CZ-NH1	-5.90	117.35	120.30
1	A	11	ARG	NE-CZ-NH2	5.78	123.19	120.30
1	C	11	ARG	NE-CZ-NH1	-5.77	117.42	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	1	MET	CG-SD-CE	5.77	109.43	100.20
1	H	1	MET	CG-SD-CE	5.76	109.41	100.20
1	G	11	ARG	NE-CZ-NH2	5.67	123.14	120.30
1	C	147	ASP	CB-CG-OD2	5.59	123.33	118.30
1	D	81	ARG	NE-CZ-NH2	-5.47	117.56	120.30
1	F	11	ARG	NE-CZ-NH1	-5.34	117.63	120.30
1	G	11	ARG	NE-CZ-NH1	-5.33	117.63	120.30
1	F	100	MET	CG-SD-CE	5.08	108.33	100.20

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	1196	0	1243	27	0
1	B	1196	0	1243	31	0
1	C	1202	0	1256	51	0
1	D	1196	0	1243	22	0
1	E	1196	0	1243	37	0
1	F	1196	0	1243	26	0
1	G	1196	0	1243	35	0
1	H	1196	0	1243	44	0
1	I	1196	0	1243	32	0
1	J	1202	0	1256	48	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	2	0	0	3	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	2	0	0	0	0
2	G	1	0	0	1	0
2	H	1	0	0	0	0
2	I	1	0	0	2	0
2	J	2	0	0	4	0
3	A	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	10	0	0	1	0
3	C	5	0	0	0	0
3	D	15	0	0	0	0
3	E	10	0	0	0	0
3	F	15	0	0	2	0
3	G	15	0	0	1	0
3	H	15	0	0	0	0
3	I	15	0	0	2	0
3	J	10	0	0	1	0
4	A	112	0	0	4	0
4	B	130	0	0	7	0
4	C	107	0	0	6	0
4	D	114	0	0	2	0
4	E	131	0	0	5	0
4	F	116	0	0	4	0
4	G	98	0	0	3	0
4	H	108	0	0	4	0
4	I	91	0	0	4	0
4	J	117	0	0	4	0
All	All	13229	0	12456	287	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 12.

All (287) 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:J:1:MET:CE	1:J:2:ILE:HG22	1.62	1.29
1:D:1:MET:CE	1:D:2:ILE:HG22	1.62	1.29
2:I:1160:CL:CL	2:J:1160:CL:CL	1.29	1.28
1:A:1:MET:CE	1:A:2:ILE:HG22	1.64	1.26
1:J:2:ILE:HD11	1:J:78:ILE:HD11	1.29	1.13
1:B:1:MET:HE2	1:B:2:ILE:HG22	1.20	1.11
1:B:1:MET:CE	1:B:2:ILE:HG22	1.81	1.10
1:C:27:LEU:HD12	1:C:31:GLU:OE1	1.52	1.09
1:D:1:MET:HE3	1:D:2:ILE:HG22	1.29	1.08
1:I:2:ILE:HD11	1:I:78:ILE:HD11	1.33	1.08
1:H:2:ILE:HD11	1:H:78:ILE:CD1	1.84	1.08
1:H:2:ILE:HD11	1:H:78:ILE:HD11	1.11	1.07
1:G:2:ILE:HD11	1:G:78:ILE:HD11	1.32	1.06
1:F:2:ILE:HD11	1:F:78:ILE:HD11	1.11	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:LEU:HD13	4:B:2047:HOH:O	1.55	1.05
1:B:2:ILE:HD11	1:B:78:ILE:HD11	1.39	1.04
1:J:1:MET:HE3	1:J:2:ILE:HG22	1.39	1.02
1:A:1:MET:HE2	1:A:2:ILE:HG22	1.40	1.01
1:F:2:ILE:HD11	1:F:78:ILE:CD1	1.90	1.01
1:J:1:MET:HE2	1:J:2:ILE:HG22	1.40	1.00
1:H:1:MET:HE3	1:H:2:ILE:HG22	1.43	1.00
1:E:2:ILE:HD11	1:E:78:ILE:HD11	1.41	0.99
1:C:2:ILE:HD11	1:C:78:ILE:HD11	1.45	0.97
1:D:1:MET:HE2	1:D:2:ILE:HG22	1.46	0.95
1:J:96[A]:LYS:NZ	1:J:99:GLU:OE2	2.02	0.90
1:I:101:LEU:HD21	4:J:2020:HOH:O	1.72	0.89
1:C:114:GLU:HG3	1:I:1:MET:CE	2.03	0.89
1:F:2:ILE:CD1	1:F:78:ILE:HD11	2.01	0.89
1:A:1:MET:HE2	1:A:2:ILE:CG2	2.03	0.88
1:A:1:MET:CE	1:A:2:ILE:CG2	2.52	0.88
1:B:1:MET:HE3	1:B:2:ILE:H	1.39	0.86
1:B:1:MET:HE3	4:B:2004:HOH:O	1.76	0.86
4:A:2091:HOH:O	1:J:153:THR:HG23	1.75	0.85
1:G:114:GLU:HG3	1:H:1:MET:HE1	1.58	0.85
1:C:36:THR:HG22	1:C:38:LEU:H	1.44	0.83
1:G:2:ILE:HD11	1:G:78:ILE:CD1	2.09	0.82
1:B:1:MET:HE2	1:B:2:ILE:CG2	2.08	0.82
1:C:96[B]:LYS:HE3	2:C:1159:CL:CL	2.19	0.80
1:C:48:LEU:HD22	1:G:6:ILE:HD13	1.63	0.80
1:B:2:ILE:HD11	1:B:78:ILE:CD1	2.09	0.80
1:G:36:THR:HG21	1:G:43:VAL:HG21	1.64	0.79
1:D:6:ILE:HD13	1:F:48:LEU:HD22	1.63	0.79
1:C:114:GLU:HG3	1:I:1:MET:HE3	1.66	0.78
1:E:114:GLU:HG3	1:F:1:MET:CE	2.16	0.76
1:I:96:LYS:HG3	1:J:120:ILE:HD12	1.66	0.76
1:H:1:MET:CE	1:H:2:ILE:HG22	2.15	0.75
1:H:2:ILE:CD1	1:H:78:ILE:HD11	2.06	0.75
1:G:114:GLU:HG3	1:H:1:MET:CE	2.17	0.74
1:H:36:THR:HG21	1:H:43:VAL:HG21	1.70	0.73
1:I:2:ILE:CD1	1:I:78:ILE:HD11	2.16	0.72
1:F:140:GLU:HG2	4:F:2105:HOH:O	1.88	0.72
1:J:36:THR:HG21	1:J:43:VAL:HG21	1.71	0.72
1:J:36:THR:HG22	1:J:38:LEU:H	1.55	0.72
1:A:96:LYS:HG3	1:D:120:ILE:HD12	1.71	0.72
1:E:114:GLU:HG3	1:F:1:MET:HE1	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:2:ILE:HG21	1:H:113:HIS:O	1.90	0.71
1:A:1:MET:HE3	1:A:2:ILE:HG22	1.66	0.71
1:A:100:MET:HB3	4:A:2080:HOH:O	1.91	0.70
1:E:36:THR:HG21	1:E:43:VAL:HG21	1.72	0.70
1:J:2:ILE:HD11	1:J:78:ILE:CD1	2.16	0.70
1:H:96:LYS:HE3	1:J:96[B]:LYS:HZ1	1.56	0.70
1:B:48:LEU:HD22	1:E:6:ILE:HD13	1.74	0.69
1:H:73:LEU:HD12	4:H:2059:HOH:O	1.93	0.69
1:D:1:MET:HE2	1:D:2:ILE:CG2	2.23	0.68
1:G:36:THR:HG22	1:G:38:LEU:H	1.57	0.68
1:A:6:ILE:HD13	1:I:48:LEU:HD22	1.74	0.68
1:C:52:ALA:O	4:C:2040:HOH:O	2.10	0.68
1:C:124:ILE:HD12	4:I:2088:HOH:O	1.93	0.67
1:H:96:LYS:NZ	1:H:99:GLU:OE2	2.28	0.67
1:J:36:THR:CG2	1:J:38:LEU:H	2.08	0.66
1:E:2:ILE:CD1	1:E:78:ILE:HD11	2.20	0.66
4:E:2060:HOH:O	1:G:127:LYS:HD2	1.95	0.65
1:E:120:ILE:HD12	1:G:96:LYS:HG3	1.77	0.65
1:C:124:ILE:CD1	4:I:2088:HOH:O	2.44	0.65
1:H:133:VAL:O	1:H:133:VAL:HG23	1.97	0.64
1:C:36:THR:CG2	1:C:38:LEU:HB2	2.27	0.64
2:C:1158:CL:CL	2:J:1160:CL:CL	2.89	0.64
1:H:96:LYS:HZ1	1:J:96[B]:LYS:HE2	1.62	0.64
1:C:2:ILE:HD11	1:C:78:ILE:CD1	2.23	0.63
1:B:1:MET:HE3	1:B:2:ILE:N	2.11	0.63
1:H:96:LYS:CE	1:J:96[B]:LYS:NZ	2.62	0.63
1:B:2:ILE:CD1	1:B:78:ILE:HD11	2.20	0.63
1:F:18:ILE:HG23	1:F:65:LEU:HD13	1.81	0.63
1:E:88:ILE:HD12	1:E:98:TYR:CZ	2.35	0.61
1:H:96:LYS:CE	1:J:96[B]:LYS:HZ1	2.13	0.61
1:E:36:THR:HG23	1:E:38:LEU:HB2	1.83	0.60
1:E:114:GLU:HG3	1:F:1:MET:HE2	1.84	0.60
1:A:1:MET:HE3	4:A:2001:HOH:O	2.00	0.60
1:B:1:MET:CE	4:B:2004:HOH:O	2.41	0.60
1:C:27:LEU:CD1	1:C:31:GLU:OE1	2.41	0.60
1:D:1:MET:CE	1:D:2:ILE:CG2	2.57	0.59
1:F:108:LEU:O	1:F:112:VAL:HG23	2.01	0.59
1:J:1:MET:HE3	1:J:2:ILE:CG2	2.25	0.59
1:G:33:ALA:O	1:G:36:THR:HB	2.02	0.59
1:H:96:LYS:HE2	1:J:96[B]:LYS:NZ	2.18	0.59
1:J:1:MET:HE3	1:J:2:ILE:N	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:120:ILE:HD11	2:J:1160:CL:CL	2.40	0.58
1:C:96[B]:LYS:NZ	4:C:2082:HOH:O	1.89	0.58
1:G:124:ILE:HG23	1:H:153:THR:OG1	2.04	0.57
1:I:122:SER:HB2	1:I:151:LEU:HD11	1.85	0.57
1:G:51:GLN:NE2	1:G:81:ARG:HH21	2.02	0.57
1:C:113:HIS:HB3	1:I:78:ILE:HD12	1.86	0.57
1:E:36:THR:HG22	1:E:38:LEU:H	1.69	0.57
1:I:132:LYS:HE2	1:J:115:LYS:O	2.05	0.57
1:F:2:ILE:CD1	1:F:78:ILE:CD1	2.74	0.57
1:D:5:GLN:HG2	1:D:77:MET:HE2	1.87	0.57
1:H:133:VAL:O	1:H:133:VAL:CG2	2.53	0.56
1:E:78:ILE:HD12	1:F:113:HIS:HB3	1.87	0.56
1:G:80:LEU:HD13	1:G:80:LEU:C	2.24	0.56
1:B:114:GLU:HG3	1:D:1:MET:HE1	1.87	0.56
1:J:2:ILE:CD1	1:J:78:ILE:HD11	2.19	0.56
1:A:1:MET:HE1	1:A:2:ILE:HG22	1.75	0.56
1:C:33:ALA:O	1:C:36:THR:HB	2.05	0.56
3:I:1158:SO4:O3	1:J:87:ARG:HD2	2.05	0.56
1:I:101:LEU:CD2	4:J:2020:HOH:O	2.42	0.55
1:J:36:THR:HG23	1:J:38:LEU:HB2	1.87	0.55
1:A:51:GLN:NE2	1:A:81:ARG:HH21	2.04	0.55
1:B:40:GLU:N	3:B:1157:SO4:O2	2.35	0.55
4:C:2032:HOH:O	1:H:101:LEU:HB3	2.06	0.55
1:G:36:THR:HG21	1:G:43:VAL:CG2	2.35	0.55
1:D:51:GLN:NE2	1:D:81:ARG:HH21	2.04	0.55
1:A:146:LEU:HD11	1:D:146:LEU:HD11	1.89	0.55
1:C:25:LYS:CB	1:C:27:LEU:HD22	2.37	0.55
1:C:96[A]:LYS:NZ	1:C:99:GLU:OE2	2.30	0.54
1:C:113:HIS:O	1:I:2:ILE:HG21	2.08	0.54
1:C:120:ILE:HG13	1:C:151:LEU:HD12	1.88	0.54
1:B:27:LEU:HA	1:B:31:GLU:OE2	2.08	0.54
1:D:56:ASP:OD1	1:D:59:ARG:NH2	2.41	0.53
1:B:1:MET:CE	1:B:2:ILE:H	2.15	0.53
1:E:88:ILE:HG13	4:G:2059:HOH:O	2.08	0.53
1:G:60:LEU:HD22	4:G:2030:HOH:O	2.08	0.53
1:C:34:ASP:O	1:C:64:LYS:NZ	2.42	0.53
1:H:36:THR:HG23	1:H:38:LEU:HB2	1.91	0.52
1:F:6:ILE:HD13	1:G:48:LEU:HD22	1.89	0.52
1:D:154:LYS:HB2	4:D:2114:HOH:O	2.08	0.52
1:C:25:LYS:HB2	1:C:27:LEU:HD22	1.91	0.52
1:H:2:ILE:CD1	1:H:78:ILE:CD1	2.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:146:LEU:HD11	1:H:146:LEU:HD11	1.92	0.52
1:A:142:ALA:CB	1:D:121:ILE:HD12	2.40	0.52
1:H:96:LYS:NZ	1:J:96[B]:LYS:HE2	2.24	0.52
1:E:36:THR:CG2	1:E:38:LEU:H	2.23	0.51
1:A:31:GLU:O	1:A:34:ASP:HB2	2.10	0.51
1:F:1:MET:CE	1:F:2:ILE:HG22	2.39	0.51
1:F:51:GLN:NE2	1:F:81:ARG:HH21	2.08	0.51
1:E:124:ILE:CD1	4:E:2044:HOH:O	2.58	0.51
1:G:38:LEU:HD22	1:H:155:PRO:HB3	1.91	0.51
1:G:2:ILE:CD1	1:G:78:ILE:CD1	2.88	0.51
1:B:96:LYS:HG3	1:F:120:ILE:HD12	1.93	0.51
1:E:128:LEU:HD23	1:E:128:LEU:C	2.31	0.51
1:G:36:THR:CG2	1:G:38:LEU:H	2.22	0.51
2:I:1160:CL:CL	1:J:96[A]:LYS:HE2	2.48	0.50
1:H:28:SER:OG	1:H:31:GLU:HG3	2.10	0.50
1:J:1:MET:HE2	1:J:2:ILE:CG2	2.25	0.50
1:E:135:ASP:OD1	1:G:149:LYS:CD	2.59	0.50
1:H:10:ILE:HD13	4:H:2025:HOH:O	2.12	0.50
1:B:1:MET:CE	1:B:2:ILE:N	2.73	0.50
1:B:97:PHE:HE2	1:B:144:ILE:HD12	1.76	0.50
1:H:96:LYS:HE2	1:J:96[B]:LYS:HZ3	1.76	0.50
1:C:96[B]:LYS:HE2	4:E:2107:HOH:O	2.12	0.49
1:A:4:SER:C	1:A:77:MET:HE2	2.32	0.49
1:F:34:ASP:HB2	4:F:2037:HOH:O	2.12	0.49
1:J:34:ASP:O	1:J:64:LYS:NZ	2.45	0.49
1:C:135:ASP:HB3	1:C:138:GLY:O	2.13	0.49
1:A:38:LEU:HD22	1:J:155:PRO:CB	2.42	0.49
1:C:108:LEU:O	1:C:112:VAL:HG23	2.11	0.49
1:D:152:PRO:HG2	1:D:154:LYS:HE2	1.94	0.49
1:C:2:ILE:HG22	4:C:2002:HOH:O	2.11	0.49
1:B:122:SER:HB2	1:B:151:LEU:HD11	1.93	0.49
4:A:2079:HOH:O	1:F:96:LYS:HG2	2.13	0.49
1:A:14:LEU:HD11	1:A:71:SER:HB3	1.94	0.49
1:C:96[B]:LYS:NZ	1:E:96:LYS:HZ2	2.11	0.49
1:E:97:PHE:HE2	1:E:144:ILE:HD13	1.78	0.49
1:H:53:LEU:HD12	1:H:75:LEU:HD13	1.95	0.49
1:C:36:THR:HG21	1:C:43:VAL:HG21	1.94	0.48
1:D:25:LYS:CB	1:D:27:LEU:HD13	2.43	0.48
1:G:2:ILE:CD1	1:G:78:ILE:HD11	2.23	0.48
1:A:35:GLY:O	1:A:60:LEU:HD22	2.13	0.48
1:E:77:MET:HG2	4:E:2086:HOH:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:LEU:HD22	1:J:155:PRO:HB3	1.94	0.48
1:B:141:ARG:HD3	4:B:2120:HOH:O	2.13	0.48
1:E:102:GLN:HE22	1:G:84:ILE:H	1.61	0.48
1:E:87:ARG:HD3	3:G:1158:SO4:O1	2.13	0.48
1:I:123:ALA:HB3	1:J:96[A]:LYS:HE3	1.96	0.48
1:J:80:LEU:HD13	1:J:80:LEU:C	2.35	0.47
1:F:149:LYS:NZ	4:F:2112:HOH:O	2.46	0.47
1:D:77:MET:HG2	4:D:2057:HOH:O	2.15	0.47
1:E:36:THR:CG2	1:E:38:LEU:HB2	2.45	0.47
1:G:42:PHE:CE1	1:H:155:PRO:HA	2.50	0.47
1:E:128:LEU:HD23	1:E:129:ASP:N	2.29	0.47
1:C:2:ILE:CD1	1:C:78:ILE:HD11	2.31	0.47
4:C:2032:HOH:O	1:H:101:LEU:CD1	2.63	0.47
1:E:122:SER:HB2	1:E:151:LEU:HD11	1.97	0.47
1:J:60:LEU:HD22	4:J:2043:HOH:O	2.14	0.47
1:H:140:GLU:HG2	4:H:2099:HOH:O	2.15	0.47
1:B:5:GLN:HG2	1:B:77:MET:HE2	1.97	0.47
1:C:74:LEU:HA	1:C:77:MET:HG3	1.97	0.47
1:G:36:THR:CG2	1:G:38:LEU:HB2	2.45	0.46
1:D:36:THR:HG22	1:D:60:LEU:HD23	1.96	0.46
1:C:22:LYS:HE3	1:C:29:PHE:CE1	2.50	0.46
1:H:36:THR:HG22	1:H:38:LEU:H	1.80	0.46
1:J:96[B]:LYS:HE3	2:J:1160:CL:CL	2.52	0.46
1:C:114:GLU:HA	1:I:2:ILE:CG2	2.45	0.46
1:C:36:THR:CG2	1:C:38:LEU:H	2.21	0.46
1:C:153:THR:OG1	1:I:124:ILE:HG23	2.14	0.46
1:E:135:ASP:OD1	1:G:149:LYS:HD3	2.16	0.46
1:B:133:VAL:C	4:B:2119:HOH:O	2.53	0.46
3:I:1158:SO4:O3	1:J:87:ARG:CD	2.63	0.46
1:J:51:GLN:NE2	1:J:81:ARG:HH21	2.13	0.46
1:E:88:ILE:HD12	1:E:98:TYR:CE1	2.51	0.45
1:E:142:ALA:HB2	1:G:121:ILE:HD12	1.98	0.45
1:C:96[B]:LYS:NZ	1:E:96:LYS:NZ	2.65	0.45
1:J:25:LYS:CB	1:J:27:LEU:HD13	2.46	0.45
1:C:22:LYS:HE3	1:C:29:PHE:CD1	2.51	0.45
1:J:36:THR:CG2	1:J:38:LEU:HB2	2.46	0.45
1:G:18:ILE:HG23	1:G:65:LEU:HD13	1.98	0.45
1:A:128:LEU:HD12	1:A:128:LEU:C	2.37	0.45
1:H:32:ILE:HG21	1:H:47:LEU:HD11	1.99	0.45
1:A:102:GLN:NE2	1:D:84:ILE:H	2.15	0.44
1:B:120:ILE:HD12	1:F:96:LYS:HG3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:ILE:HD11	1:A:151:LEU:HD12	2.00	0.44
1:I:88:ILE:HD11	1:J:87:ARG:HB3	2.00	0.44
1:H:25:LYS:O	1:H:27:LEU:HD13	2.16	0.44
1:H:25:LYS:O	1:H:27:LEU:CD1	2.66	0.44
1:G:25:LYS:HB3	1:G:27:LEU:HD13	1.99	0.44
1:J:40:GLU:N	3:J:1157:SO4:O3	2.46	0.44
1:I:22:LYS:HE3	1:I:29:PHE:CE1	2.53	0.44
1:C:96[B]:LYS:NZ	1:E:96:LYS:HD3	2.32	0.44
1:I:122:SER:OG	1:I:125:ASN:N	2.50	0.44
1:C:2:ILE:HD13	1:I:113:HIS:O	2.18	0.44
1:C:96[B]:LYS:HZ1	1:E:96:LYS:HD3	1.83	0.44
1:F:1:MET:HE3	1:F:2:ILE:HG22	1.99	0.44
1:J:1:MET:HE3	1:J:2:ILE:H	1.82	0.43
1:E:51:GLN:NE2	1:E:81:ARG:HH21	2.15	0.43
1:C:36:THR:HG23	1:C:38:LEU:HB2	2.00	0.43
1:A:135:ASP:O	1:A:138:GLY:N	2.43	0.43
2:C:1159:CL:CL	2:G:1160:CL:CL	3.11	0.43
1:F:34:ASP:CB	4:F:2037:HOH:O	2.67	0.43
1:I:51:GLN:NE2	1:I:81:ARG:HH21	2.17	0.43
1:I:143:VAL:HG13	1:J:145:THR:CG2	2.49	0.43
1:C:78:ILE:HD12	1:I:113:HIS:HB3	2.01	0.43
1:I:122:SER:HG	1:I:125:ASN:H	1.66	0.43
1:C:77:MET:HG2	4:C:2056:HOH:O	2.19	0.43
1:A:142:ALA:HB2	1:D:121:ILE:HD12	2.00	0.43
1:B:97:PHE:CE2	1:B:144:ILE:HD12	2.54	0.42
1:G:77:MET:HG2	4:G:2044:HOH:O	2.19	0.42
1:H:22:LYS:HE3	1:H:29:PHE:CE1	2.54	0.42
1:D:154:LYS:HA	1:D:155:PRO:HD3	1.93	0.42
1:G:80:LEU:C	1:G:80:LEU:CD1	2.87	0.42
1:C:144:ILE:N	1:C:144:ILE:HD12	2.34	0.42
1:B:110:ALA:HB1	1:F:29:PHE:CE1	2.54	0.42
1:I:135:ASP:OD1	4:I:2083:HOH:O	2.22	0.42
1:I:121:ILE:HD12	1:J:142:ALA:CB	2.50	0.42
1:G:36:THR:HG23	1:G:38:LEU:HB2	2.02	0.42
1:E:33:ALA:O	1:E:36:THR:HB	2.20	0.42
1:H:22:LYS:NZ	1:I:3:GLN:OE1	2.46	0.42
1:F:87:ARG:NH1	3:F:1158:SO4:O4	2.53	0.42
1:C:25:LYS:HB2	1:C:27:LEU:CD2	2.49	0.41
1:A:142:ALA:HB3	1:D:121:ILE:HD12	2.01	0.41
1:C:25:LYS:HB3	1:C:27:LEU:HD22	2.02	0.41
1:A:42:PHE:CE1	1:J:155:PRO:HA	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:102:GLN:NE2	1:G:84:ILE:H	2.18	0.41
1:H:12:LEU:HA	1:H:12:LEU:HD23	1.93	0.41
1:B:84:ILE:H	1:F:102:GLN:HE22	1.67	0.41
1:B:87:ARG:HD2	3:F:1158:SO4:O2	2.20	0.41
1:I:130:VAL:HG22	1:I:144:ILE:HG12	2.02	0.41
1:H:62:GLY:HA2	1:H:67:LEU:HD12	2.02	0.41
1:J:5:GLN:NE2	4:J:2010:HOH:O	2.52	0.41
1:J:28:SER:OG	1:J:31:GLU:HG3	2.20	0.41
1:E:124:ILE:HD13	4:E:2044:HOH:O	2.21	0.41
1:H:130:VAL:HG22	1:H:144:ILE:HG12	2.02	0.41
1:J:88:ILE:HD12	1:J:98:TYR:CZ	2.56	0.41
1:I:121:ILE:HD12	1:J:142:ALA:HB2	2.02	0.41
1:C:88:ILE:HD11	1:H:87:ARG:HB3	2.02	0.41
1:E:116:PHE:CE1	1:G:132:LYS:HG3	2.56	0.41
1:C:102:GLN:NE2	1:H:84:ILE:H	2.19	0.41
1:G:154:LYS:HD2	4:H:2042:HOH:O	2.20	0.41
1:B:1:MET:HE1	1:B:2:ILE:HG22	1.91	0.41
1:I:97:PHE:HB3	1:J:101:LEU:HD21	2.03	0.41
1:B:140:GLU:HG2	4:B:2119:HOH:O	2.20	0.40
1:A:80:LEU:HD22	1:A:80:LEU:HA	1.91	0.40
1:C:102:GLN:HE22	1:H:84:ILE:H	1.69	0.40
1:C:114:GLU:HA	1:I:2:ILE:HG21	2.03	0.40
1:F:1:MET:HE3	1:F:2:ILE:O	2.21	0.40
1:E:78:ILE:HD13	1:E:78:ILE:HG21	1.80	0.40
1:C:2:ILE:HD13	1:C:2:ILE:HG21	1.85	0.40
1:I:51:GLN:NE2	4:I:2042:HOH:O	2.48	0.40
1:B:66:ASP:HB2	4:B:2043:HOH:O	2.22	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	154/156 (99%)	148 (96%)	5 (3%)	1 (1%)	30	24
1	B	154/156 (99%)	148 (96%)	6 (4%)	0	100	100
1	C	155/156 (99%)	151 (97%)	4 (3%)	0	100	100
1	D	154/156 (99%)	148 (96%)	6 (4%)	0	100	100
1	E	154/156 (99%)	149 (97%)	4 (3%)	1 (1%)	30	24
1	F	154/156 (99%)	151 (98%)	3 (2%)	0	100	100
1	G	154/156 (99%)	149 (97%)	5 (3%)	0	100	100
1	H	154/156 (99%)	149 (97%)	4 (3%)	1 (1%)	30	24
1	I	154/156 (99%)	150 (97%)	4 (3%)	0	100	100
1	J	155/156 (99%)	150 (97%)	5 (3%)	0	100	100
All	All	1542/1560 (99%)	1493 (97%)	46 (3%)	3 (0%)	52	53

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	155	PRO
1	A	136	PRO
1	E	155	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	127/127 (100%)	123 (97%)	4 (3%)	47	50
1	B	127/127 (100%)	124 (98%)	3 (2%)	57	61
1	C	128/127 (101%)	124 (97%)	4 (3%)	47	50
1	D	127/127 (100%)	125 (98%)	2 (2%)	70	76
1	E	127/127 (100%)	122 (96%)	5 (4%)	39	39
1	F	127/127 (100%)	125 (98%)	2 (2%)	70	76
1	G	127/127 (100%)	123 (97%)	4 (3%)	47	50
1	H	127/127 (100%)	124 (98%)	3 (2%)	57	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	127/127 (100%)	124 (98%)	3 (2%)	57	61
1	J	128/127 (101%)	123 (96%)	5 (4%)	39	39
All	All	1272/1270 (100%)	1237 (97%)	35 (3%)	51	55

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	102	GLN
1	A	128	LEU
1	A	133	VAL
1	A	140	GLU
1	B	77	MET
1	B	127	LYS
1	B	128	LEU
1	C	36	THR
1	C	102	GLN
1	C	128	LEU
1	C	151	LEU
1	D	131	LYS
1	D	156	PHE
1	E	27	LEU
1	E	34	ASP
1	E	36	THR
1	E	127	LYS
1	E	129	ASP
1	F	27	LEU
1	F	128	LEU
1	G	34	ASP
1	G	36	THR
1	G	77	MET
1	G	128	LEU
1	H	36	THR
1	H	60	LEU
1	H	102	GLN
1	I	60	LEU
1	I	66	ASP
1	I	128	LEU
1	J	27	LEU
1	J	36	THR
1	J	102	GLN
1	J	127	LYS

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Mol	Chain	Res	Type
1	J	129	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	51	GLN
1	A	102	GLN
1	B	51	GLN
1	B	102	GLN
1	C	51	GLN
1	C	102	GLN
1	D	51	GLN
1	D	76	GLN
1	D	102	GLN
1	E	51	GLN
1	E	102	GLN
1	F	5	GLN
1	F	51	GLN
1	F	76	GLN
1	F	102	GLN
1	G	5	GLN
1	G	51	GLN
1	G	102	GLN
1	H	5	GLN
1	H	51	GLN
1	H	76	GLN
1	H	102	GLN
1	I	51	GLN
1	I	102	GLN
1	J	5	GLN
1	J	51	GLN
1	J	102	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 37 ligands modelled in this entry, 13 are monoatomic - leaving 24 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	SO4	A	1157	-	4,4,4	0.36	0	6,6,6	0.79	0
3	SO4	A	1158	-	4,4,4	0.15	0	6,6,6	0.17	0
3	SO4	B	1157	-	4,4,4	0.29	0	6,6,6	0.44	0
3	SO4	B	1158	-	4,4,4	0.23	0	6,6,6	0.27	0
3	SO4	C	1157	-	4,4,4	0.24	0	6,6,6	0.68	0
3	SO4	D	1157	-	4,4,4	0.28	0	6,6,6	0.34	0
3	SO4	D	1158	-	4,4,4	1.01	0	6,6,6	1.08	1 (16%)
3	SO4	D	1159	-	4,4,4	0.22	0	6,6,6	0.43	0
3	SO4	E	1157	-	4,4,4	0.24	0	6,6,6	0.38	0
3	SO4	E	1158	-	4,4,4	0.15	0	6,6,6	0.26	0
3	SO4	F	1157	-	4,4,4	0.29	0	6,6,6	0.44	0
3	SO4	F	1158	-	4,4,4	1.31	1 (25%)	6,6,6	1.42	1 (16%)
3	SO4	F	1159	-	4,4,4	0.26	0	6,6,6	0.23	0
3	SO4	G	1157	-	4,4,4	0.11	0	6,6,6	0.78	0
3	SO4	G	1158	-	4,4,4	1.30	1 (25%)	6,6,6	2.18	2 (33%)
3	SO4	G	1159	-	4,4,4	0.15	0	6,6,6	0.19	0
3	SO4	H	1157	-	4,4,4	0.21	0	6,6,6	0.43	0
3	SO4	H	1158	-	4,4,4	0.86	0	6,6,6	0.98	0
3	SO4	H	1159	-	4,4,4	0.23	0	6,6,6	0.46	0
3	SO4	I	1157	-	4,4,4	0.16	0	6,6,6	0.32	0
3	SO4	I	1158	-	4,4,4	0.83	0	6,6,6	1.33	0
3	SO4	I	1159	-	4,4,4	0.24	0	6,6,6	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	J	1157	-	4,4,4	0.53	0	6,6,6	0.45	0
3	SO4	J	1158	-	4,4,4	0.37	0	6,6,6	0.61	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SO4	A	1157	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1158	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1157	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1158	-	-	0/0/0/0	0/0/0/0
3	SO4	C	1157	-	-	0/0/0/0	0/0/0/0
3	SO4	D	1157	-	-	0/0/0/0	0/0/0/0
3	SO4	D	1158	-	-	0/0/0/0	0/0/0/0
3	SO4	D	1159	-	-	0/0/0/0	0/0/0/0
3	SO4	E	1157	-	-	0/0/0/0	0/0/0/0
3	SO4	E	1158	-	-	0/0/0/0	0/0/0/0
3	SO4	F	1157	-	-	0/0/0/0	0/0/0/0
3	SO4	F	1158	-	-	0/0/0/0	0/0/0/0
3	SO4	F	1159	-	-	0/0/0/0	0/0/0/0
3	SO4	G	1157	-	-	0/0/0/0	0/0/0/0
3	SO4	G	1158	-	-	0/0/0/0	0/0/0/0
3	SO4	G	1159	-	-	0/0/0/0	0/0/0/0
3	SO4	H	1157	-	-	0/0/0/0	0/0/0/0
3	SO4	H	1158	-	-	0/0/0/0	0/0/0/0
3	SO4	H	1159	-	-	0/0/0/0	0/0/0/0
3	SO4	I	1157	-	-	0/0/0/0	0/0/0/0
3	SO4	I	1158	-	-	0/0/0/0	0/0/0/0
3	SO4	I	1159	-	-	0/0/0/0	0/0/0/0
3	SO4	J	1157	-	-	0/0/0/0	0/0/0/0
3	SO4	J	1158	-	-	0/0/0/0	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	1158	SO4	O3-S	-2.20	1.39	1.47
3	G	1158	SO4	O1-S	-2.19	1.39	1.47

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1158	SO4	O4-S-O3	2.26	118.15	108.98
3	F	1158	SO4	O4-S-O3	2.45	118.93	108.98
3	G	1158	SO4	O4-S-O3	2.84	120.52	108.98
3	G	1158	SO4	O2-S-O1	4.19	122.79	109.50

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1157	SO4	1	0
3	F	1158	SO4	2	0
3	G	1158	SO4	1	0
3	I	1158	SO4	2	0
3	J	1157	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](#)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.