



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:16 AM UTC

PDB ID : 2IV1 / pdb_00002iv1
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 : 2006-06-08
Resolution : 1.88 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

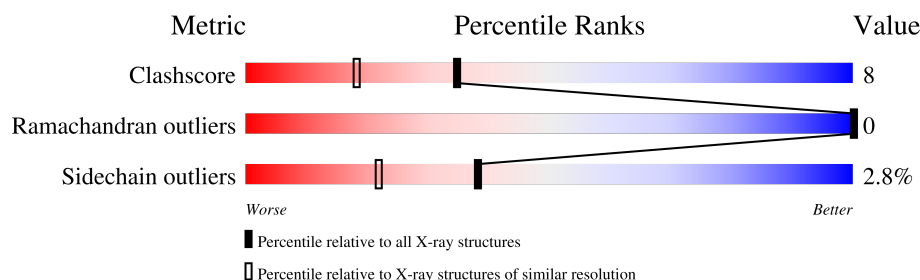
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.88 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	190562	1234 (1.88-1.88)
Ramachandran outliers	187476	1222 (1.88-1.88)
Sidechain outliers	187428	1222 (1.88-1.88)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	156	87% 13% .
1	B	156	88% 11% .
1	C	156	88% 12% .
1	D	156	89% 10% .
1	E	156	87% 12% ..
1	F	156	88% 11% .
1	G	156	86% 13% .
1	H	156	88% 12%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	I	156	 90%9%•
1	J	156	 85%14%•

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14604 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	766	197	228	5			
1	B	156	Total	C	N	O	S	0	1	0
			1201	771	197	228	5			
1	C	156	Total	C	N	O	S	0	2	0
			1206	776	197	228	5			
1	D	156	Total	C	N	O	S	0	0	0
			1196	766	197	228	5			
1	E	156	Total	C	N	O	S	0	1	0
			1201	771	197	228	5			
1	F	156	Total	C	N	O	S	0	2	0
			1206	776	197	228	5			
1	G	156	Total	C	N	O	S	0	1	0
			1201	771	197	228	5			
1	H	156	Total	C	N	O	S	0	2	0
			1206	776	197	228	5			
1	I	156	Total	C	N	O	S	0	1	0
			1201	771	197	228	5			
1	J	156	Total	C	N	O	S	0	1	0
			1201	771	197	228	5			

There are 10 discrepancies between the modelled and reference sequences:

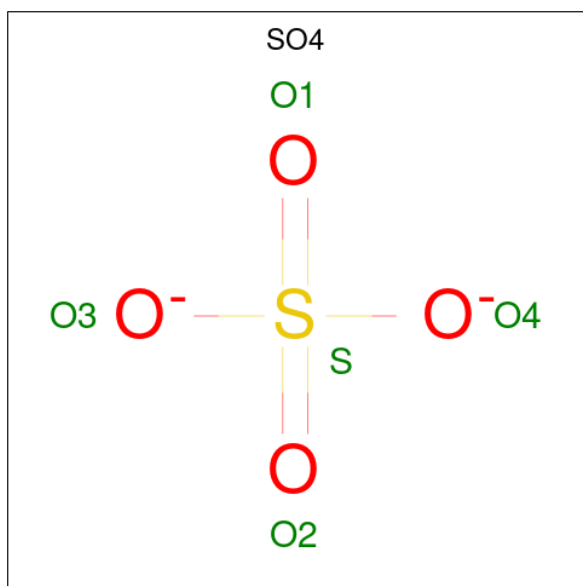
Chain	Residue	Modelled	Actual	Comment	Reference
A	96	GLN	ARG	engineered mutation	UNP P00816
B	96	GLN	ARG	engineered mutation	UNP P00816
C	96	GLN	ARG	engineered mutation	UNP P00816
D	96	GLN	ARG	engineered mutation	UNP P00816
E	96	GLN	ARG	engineered mutation	UNP P00816
F	96	GLN	ARG	engineered mutation	UNP P00816
G	96	GLN	ARG	engineered mutation	UNP P00816
H	96	GLN	ARG	engineered mutation	UNP P00816
I	96	GLN	ARG	engineered mutation	UNP P00816

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
J	96	GLN	ARG	engineered mutation	UNP P00816

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

Continued on next page...

Continued from previous page...

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

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	213	Total 213	O 213	0	0
4	B	241	Total 241	O 241	0	0
4	C	229	Total 229	O 229	0	0
4	D	241	Total 241	O 241	0	0
4	E	234	Total 234	O 234	0	0
4	F	252	Total 252	O 252	0	0
4	G	262	Total 262	O 262	0	0
4	H	259	Total 259	O 259	0	0
4	I	272	Total 272	O 272	0	0
4	J	266	Total 266	O 266	0	0

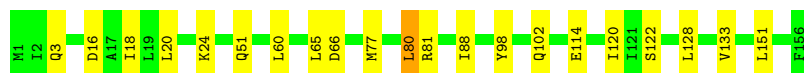
3 Residue-property plots [i](#)

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. 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. 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

Chain A:  87% 13% .



• Molecule 1: CYANATE HYDRATASE

Chain B:  88% 11% .



• Molecule 1: CYANATE HYDRATASE

Chain C:  88% 12% .



• Molecule 1: CYANATE HYDRATASE

Chain D:  89% 10% .



• Molecule 1: CYANATE HYDRATASE

Chain E:  87% 12% ..



• Molecule 1: CYANATE HYDRATASE

Chain F:  88% 11% .



- Molecule 1: CYANATE HYDRATASE

Chain G: 86% 13%



- Molecule 1: CYANATE HYDRATASE

Chain H: 88% 12%



- Molecule 1: CYANATE HYDRATASE

Chain I: 90% 9%



- Molecule 1: CYANATE HYDRATASE

Chain J: 85% 14%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	82.24Å 82.60Å 84.30Å 61.90° 72.35° 69.56°	Depositor
Resolution (Å)	76.70 – 1.88	Depositor
% Data completeness (in resolution range)	96.9 (76.70-1.88)	Depositor
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.138 , 0.184	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	14604	wwPDB-VP
Average B, all atoms (Å ²)	19.0	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	0.97	0/1213	0.91	1/1639 (0.1%)
1	B	0.98	0/1221	0.92	0/1650
1	C	1.00	0/1229	0.93	0/1662
1	D	0.99	0/1213	0.92	0/1639
1	E	1.01	0/1221	0.93	2/1651 (0.1%)
1	F	1.03	0/1229	0.91	0/1662
1	G	1.00	0/1221	0.93	0/1650
1	H	1.01	0/1229	0.89	0/1662
1	I	0.99	0/1221	0.92	0/1651
1	J	1.02	0/1221	1.00	1/1651 (0.1%)
All	All	1.00	0/12218	0.93	4/16517 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	36	THR	N-CA-C	-7.39	104.41	113.50
1	A	122	SER	N-CA-C	5.58	118.34	109.96
1	E	36	THR	N-CA-C	-5.49	106.42	113.23
1	E	36	THR	N-CA-CB	-5.00	102.64	110.44

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	1238	18	0
1	B	1201	0	1249	14	0
1	C	1206	0	1260	16	0
1	D	1196	0	1238	17	0
1	E	1201	0	1249	19	0
1	F	1206	0	1260	23	0
1	G	1201	0	1249	29	0
1	H	1206	0	1260	21	0
1	I	1201	0	1249	13	0
1	J	1201	0	1249	31	0
2	A	15	0	0	0	0
2	B	10	0	0	0	0
2	C	20	0	0	1	0
2	D	10	0	0	0	0
2	E	10	0	0	0	0
2	F	10	0	0	1	0
2	G	10	0	0	1	0
2	H	10	0	0	0	0
2	I	5	0	0	0	0
2	J	10	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	1	0
3	C	1	0	0	0	0
3	F	1	0	0	0	0
3	G	2	0	0	0	0
3	H	1	0	0	0	0
3	I	2	0	0	1	0
3	J	1	0	0	0	0
4	A	213	0	0	3	0
4	B	241	0	0	6	0
4	C	229	0	0	5	0
4	D	241	0	0	11	0
4	E	234	0	0	6	0
4	F	252	0	0	2	0
4	G	262	0	0	7	0
4	H	259	0	0	5	1
4	I	272	0	0	2	0
4	J	266	0	0	9	1
All	All	14604	0	12501	185	1

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 8.

All (185) 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:F:1:MET:CE	1:F:2:ILE:HG22	1.58	1.32
1:G:60:LEU:HD22	4:G:2107:HOH:O	1.13	1.27
1:I:2:ILE:HD11	1:I:78[A]:ILE:HD11	1.25	1.13
1:H:2:ILE:HD11	1:H:78[A]:ILE:HD11	1.14	1.12
1:E:2:ILE:HD11	1:E:78[A]:ILE:HD11	1.20	1.11
1:J:1:MET:HE3	1:J:2:ILE:HG22	1.24	1.10
1:H:1:MET:HE3	1:H:2:ILE:HG22	1.22	1.10
1:C:2:ILE:HD11	1:C:78[A]:ILE:HD11	1.29	1.10
1:J:2:ILE:HD11	1:J:78[B]:ILE:HD11	1.07	1.07
1:F:2:ILE:HD11	1:F:78[A]:ILE:HD11	1.09	1.05
1:F:1:MET:HE3	1:F:2:ILE:HG22	1.12	1.04
1:J:1:MET:CE	1:J:2:ILE:HG22	1.90	1.02
1:H:66:ASP:HB3	4:H:2151:HOH:O	1.63	0.99
1:J:25:LYS:HE2	4:J:2080:HOH:O	1.62	0.98
4:C:2036:HOH:O	1:G:1:MET:SD	2.20	0.98
1:E:140:GLU:HG2	4:E:2212:HOH:O	1.64	0.96
4:E:2035:HOH:O	1:H:1:MET:SD	2.22	0.96
1:H:1:MET:CE	1:H:2:ILE:HG22	1.95	0.95
1:J:1:MET:HE3	1:J:2:ILE:CG2	1.97	0.95
1:F:1:MET:CE	1:F:2:ILE:CG2	2.45	0.94
1:J:2:ILE:HD11	1:J:78[B]:ILE:CD1	1.97	0.94
1:F:1:MET:HE3	1:F:2:ILE:CG2	1.97	0.94
1:D:25:LYS:HE2	4:D:2074:HOH:O	1.66	0.93
1:H:1:MET:HE3	1:H:2:ILE:CG2	1.97	0.93
1:J:2:ILE:CD1	1:J:78[B]:ILE:HD11	1.99	0.93
1:F:2:ILE:HD11	1:F:78[A]:ILE:CD1	1.99	0.92
1:A:60:LEU:HD22	4:A:2082:HOH:O	1.69	0.92
1:G:1:MET:HE2	1:G:2:ILE:H	1.36	0.90
1:G:1:MET:CE	4:G:2006:HOH:O	2.20	0.88
1:H:2:ILE:HD11	1:H:78[A]:ILE:CD1	2.02	0.87
1:B:25:LYS:HE2	4:B:2060:HOH:O	1.74	0.86
4:D:2037:HOH:O	1:J:1:MET:SD	2.32	0.86
1:E:140:GLU:HG2	4:E:2211:HOH:O	1.76	0.84
1:E:2:ILE:HD11	1:E:78[A]:ILE:CD1	2.05	0.83
1:G:25:LYS:HE2	4:G:2087:HOH:O	1.79	0.81
1:C:2:ILE:HD11	1:C:78[A]:ILE:CD1	2.10	0.81
1:I:66:ASP:HB2	4:I:2160:HOH:O	1.78	0.81
1:F:2:ILE:CD1	1:F:78[A]:ILE:HD11	2.03	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:140:GLU:HG2	4:D:2217:HOH:O	1.79	0.80
1:H:2:ILE:CD1	1:H:78[A]:ILE:HD11	2.05	0.80
1:I:2:ILE:HD11	1:I:78[A]:ILE:CD1	2.08	0.79
1:D:132:LYS:HE2	4:D:2201:HOH:O	1.84	0.77
1:G:1:MET:CE	1:G:1:MET:HA	2.14	0.77
1:F:87:ARG:HD2	2:F:1158:SO4:O1	1.85	0.77
1:F:1:MET:HE1	1:F:2:ILE:HG22	1.66	0.75
1:G:1:MET:HA	1:G:1:MET:HE3	1.68	0.74
1:G:1:MET:HE1	4:H:2201:HOH:O	1.87	0.74
1:D:132:LYS:CE	4:D:2201:HOH:O	2.36	0.74
1:J:60:LEU:HD22	4:J:2097:HOH:O	1.89	0.72
1:G:1:MET:HE2	4:G:2006:HOH:O	1.88	0.71
1:J:127:LYS:HD2	4:J:2111:HOH:O	1.89	0.71
1:G:1:MET:HE2	1:G:2:ILE:N	2.07	0.70
1:C:140:GLU:HG2	4:C:2205:HOH:O	1.90	0.69
1:G:36:THR:CG2	1:G:38:LEU:H	2.06	0.69
1:B:132:LYS:HG3	1:F:116:PHE:CE1	2.28	0.69
1:J:140:GLU:HG2	4:J:2232:HOH:O	1.93	0.67
1:G:114:GLU:HG3	1:H:1:MET:HE1	1.75	0.67
1:C:36:THR:CG2	1:C:38:LEU:H	2.08	0.66
1:C:25:LYS:HE2	4:C:2068:HOH:O	1.96	0.66
1:E:36:THR:HG21	1:E:43:VAL:HG21	1.77	0.65
1:J:137:GLU:HG2	4:J:2237:HOH:O	1.96	0.64
4:B:2222:HOH:O	1:F:133:VAL:HG21	1.98	0.63
1:F:1:MET:HE3	1:F:2:ILE:N	2.14	0.62
1:G:87:ARG:HD2	2:G:1158:SO4:O4	1.98	0.62
1:H:60:LEU:HD22	4:H:2095:HOH:O	1.99	0.62
1:D:140:GLU:OE1	4:D:2219:HOH:O	2.16	0.61
1:J:36:THR:HG21	1:J:43:VAL:HG21	1.83	0.61
1:G:36:THR:HG23	1:G:38:LEU:H	1.64	0.61
1:C:36:THR:HG21	1:C:43:VAL:HG21	1.83	0.60
1:E:40:GLU:OE1	4:E:2093:HOH:O	2.16	0.60
1:J:40:GLU:OE1	4:J:2102:HOH:O	2.16	0.59
1:G:114:GLU:HG3	1:H:1:MET:CE	2.31	0.59
1:A:133:VAL:HG21	4:D:2224:HOH:O	2.03	0.59
1:A:66:ASP:HB2	4:A:2115:HOH:O	2.02	0.59
1:C:36:THR:HG22	1:C:38:LEU:H	1.67	0.59
1:F:1:MET:HE3	1:F:2:ILE:H	1.67	0.59
1:G:33:ALA:O	1:G:36:THR:HB	2.03	0.58
1:D:25:LYS:CE	4:D:2074:HOH:O	2.39	0.58
1:J:1:MET:CE	1:J:2:ILE:CG2	2.70	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:120:ILE:HD11	1:I:151:LEU:HD12	1.86	0.57
1:A:16:ASP:HB3	1:B:10:ILE:HD11	1.86	0.57
1:A:16:ASP:CG	1:B:10:ILE:HD11	2.30	0.57
1:D:51:GLN:NE2	1:D:81:ARG:HH21	2.04	0.56
1:G:36:THR:HG21	1:G:43:VAL:HG21	1.87	0.56
1:A:114:GLU:HG3	1:J:1:MET:HE1	1.89	0.55
1:F:120:ILE:HD11	1:F:151:LEU:HD12	1.89	0.55
1:A:24:LYS:NZ	4:A:2063:HOH:O	2.40	0.55
1:D:56:ASP:OD1	1:D:59:ARG:NH2	2.39	0.55
1:G:120:ILE:HD11	1:G:151:LEU:HD12	1.88	0.55
1:G:1:MET:HE1	4:G:2006:HOH:O	1.97	0.54
1:A:120:ILE:HD11	1:A:151:LEU:HD12	1.89	0.54
3:B:1159:CL:CL	4:B:2094:HOH:O	2.55	0.54
1:C:51:GLN:NE2	1:C:81:ARG:HH21	2.06	0.53
1:J:127:LYS:NZ	1:J:127:LYS:HB3	2.24	0.53
1:J:36:THR:CG2	1:J:38:LEU:H	2.21	0.53
1:B:56:ASP:OD1	1:B:59:ARG:NH2	2.40	0.53
1:B:18:ILE:HG23	1:B:65:LEU:HD13	1.91	0.53
1:D:137:GLU:HG3	4:D:2212:HOH:O	2.08	0.53
1:E:36:THR:HG22	1:E:38:LEU:H	1.74	0.53
1:E:51:GLN:NE2	1:E:81:ARG:HH21	2.08	0.52
1:B:34:ASP:HB2	4:B:2086:HOH:O	2.08	0.52
2:C:1158:SO4:O4	1:I:87:ARG:NH1	2.42	0.52
1:G:36:THR:HG22	1:G:38:LEU:H	1.75	0.52
1:E:36:THR:CG2	1:E:38:LEU:H	2.22	0.51
1:E:33:ALA:O	1:E:36:THR:HB	2.10	0.51
1:F:6:ILE:HD13	1:G:48:LEU:HD22	1.93	0.51
1:A:20:LEU:HG	1:A:24:LYS:HE3	1.92	0.51
1:A:114:GLU:HG3	1:J:1:MET:CE	2.41	0.51
1:I:51:GLN:NE2	1:I:81:ARG:HH21	2.09	0.50
1:E:87:ARG:HB3	1:G:88:ILE:HD11	1.92	0.50
1:E:2:ILE:CD1	1:E:78[A]:ILE:HD11	2.14	0.50
1:F:3:GLN:HB3	1:F:77:MET:HE3	1.93	0.50
1:J:36:THR:HG23	1:J:38:LEU:H	1.77	0.49
1:D:25:LYS:NZ	4:D:2074:HOH:O	2.45	0.49
1:D:88:ILE:HD12	1:D:98:TYR:CZ	2.48	0.49
1:I:140:GLU:HG2	4:I:2242:HOH:O	2.10	0.49
1:J:33:ALA:O	1:J:36:THR:HB	2.13	0.49
1:J:1:MET:HE1	1:J:2:ILE:HG22	1.89	0.49
1:D:25:LYS:CB	1:D:27:LEU:HD13	2.42	0.49
1:J:127:LYS:CD	4:J:2111:HOH:O	2.54	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:127:LYS:HD2	4:F:2119:HOH:O	2.13	0.49
1:F:25:LYS:HB2	1:F:27:LEU:HD22	1.94	0.48
1:H:127:LYS:NZ	4:H:2216:HOH:O	2.45	0.48
1:C:36:THR:HG23	1:C:38:LEU:H	1.76	0.48
1:G:140:GLU:HG2	4:G:2241:HOH:O	2.14	0.48
1:A:88:ILE:HD12	1:A:98:TYR:CZ	2.49	0.47
1:C:33:ALA:O	1:C:36:THR:HB	2.15	0.47
1:D:25:LYS:HB3	1:D:27:LEU:HD13	1.96	0.47
1:I:87:ARG:C	1:I:88:ILE:HD13	2.39	0.47
1:A:16:ASP:CB	1:B:10:ILE:HD11	2.44	0.47
1:A:51:GLN:NE2	1:A:81:ARG:HH21	2.13	0.47
1:H:88:ILE:HD12	1:H:98:TYR:CZ	2.49	0.47
1:A:3:GLN:HB3	1:A:77:MET:HE3	1.97	0.47
1:J:25:LYS:CE	4:J:2080:HOH:O	2.41	0.47
1:D:132:LYS:CD	4:D:2201:HOH:O	2.62	0.47
4:B:2094:HOH:O	1:F:115:LYS:NZ	2.47	0.46
1:C:87:ARG:HB3	1:H:88:ILE:HD11	1.97	0.46
1:J:77:MET:HE2	1:J:77:MET:HB3	1.84	0.46
1:G:1:MET:CE	1:G:1:MET:CA	2.89	0.46
1:I:87:ARG:HB3	1:J:88:ILE:HD11	1.97	0.46
1:C:88:ILE:HD12	1:C:98:TYR:CZ	2.51	0.45
1:E:77:MET:HB3	1:E:77:MET:HE2	1.73	0.45
1:G:51:GLN:NE2	1:G:81:ARG:HH21	2.14	0.45
1:G:77:MET:HE2	1:G:77:MET:HB3	1.85	0.45
1:C:77:MET:HG2	4:C:2137:HOH:O	2.16	0.45
1:H:1:MET:CE	1:H:2:ILE:CG2	2.77	0.45
1:H:51:GLN:NE2	1:H:81:ARG:HH21	2.14	0.45
1:I:80:LEU:N	3:I:1159:CL:CL	2.82	0.45
1:B:5:GLN:HE22	1:B:10:ILE:HD12	1.81	0.45
1:G:1:MET:HE2	1:G:1:MET:HA	1.96	0.45
1:F:66:ASP:HB3	4:F:2141:HOH:O	2.16	0.44
1:I:74:LEU:HA	1:I:77:MET:HG3	1.99	0.44
1:B:77:MET:HG2	4:B:2145:HOH:O	2.17	0.44
1:B:88:ILE:HD12	1:B:98:TYR:CZ	2.53	0.44
1:J:3:GLN:HB3	1:J:77:MET:HE3	2.00	0.44
1:H:77:MET:HE2	1:H:77:MET:HB3	1.74	0.44
1:C:34:ASP:HB2	4:C:2080:HOH:O	2.18	0.44
1:C:113:HIS:HB3	1:I:78[A]:ILE:HD12	2.01	0.43
1:A:77:MET:HE2	1:A:77:MET:HB3	1.77	0.43
1:H:74:LEU:HA	1:H:77:MET:HG3	1.99	0.43
1:G:25:LYS:CE	4:G:2087:HOH:O	2.52	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:120:ILE:HD11	1:D:151:LEU:HD12	2.01	0.43
1:A:18:ILE:HG23	1:A:65:LEU:HD13	2.01	0.42
1:H:151:LEU:HD23	4:H:2243:HOH:O	2.19	0.42
1:D:6:ILE:HD13	1:F:48:LEU:HD22	2.00	0.42
1:F:74:LEU:HA	1:F:77:MET:HG3	2.01	0.42
1:J:51:GLN:NE2	1:J:81:ARG:HH21	2.17	0.42
1:E:25:LYS:HB3	1:E:27:LEU:HD13	2.02	0.42
1:H:2:ILE:CD1	1:H:78[A]:ILE:CD1	2.83	0.42
1:I:77:MET:HB3	1:I:77:MET:HE2	1.57	0.42
1:G:74:LEU:HA	1:G:77:MET:HG3	2.01	0.42
1:B:86:ASP:O	1:E:87:ARG:NH2	2.53	0.41
1:A:88:ILE:HD11	1:D:87:ARG:HB3	2.01	0.41
1:C:3:GLN:HB3	1:C:77:MET:HE3	2.02	0.41
1:E:80:LEU:C	1:E:80:LEU:HD13	2.44	0.41
1:F:77:MET:HE2	1:F:77:MET:HB3	1.78	0.41
1:H:46:ALA:HB1	1:H:53:LEU:HG	2.03	0.41
1:E:140:GLU:OE1	4:E:2213:HOH:O	2.20	0.41
1:A:80:LEU:C	1:A:80:LEU:HD13	2.46	0.40
1:E:127:LYS:NZ	4:E:2187:HOH:O	2.50	0.40
1:J:120:ILE:HD11	1:J:151:LEU:HD12	2.03	0.40
1:E:114:GLU:HG3	1:F:1:MET:CE	2.51	0.40
1:J:2:ILE:CD1	1:J:78[B]:ILE:CD1	2.78	0.40
1:J:127:LYS:HE2	4:J:2129:HOH:O	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:2156:HOH:O	4:J:2143:HOH:O[1_546]	2.13	0.07

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	154/156 (99%)	151 (98%)	3 (2%)	0	100	100
1	B	155/156 (99%)	152 (98%)	3 (2%)	0	100	100
1	C	156/156 (100%)	153 (98%)	3 (2%)	0	100	100
1	D	154/156 (99%)	151 (98%)	3 (2%)	0	100	100
1	E	155/156 (99%)	152 (98%)	3 (2%)	0	100	100
1	F	156/156 (100%)	153 (98%)	3 (2%)	0	100	100
1	G	155/156 (99%)	152 (98%)	3 (2%)	0	100	100
1	H	156/156 (100%)	153 (98%)	3 (2%)	0	100	100
1	I	155/156 (99%)	152 (98%)	3 (2%)	0	100	100
1	J	155/156 (99%)	151 (97%)	4 (3%)	0	100	100
All	All	1551/1560 (99%)	1520 (98%)	31 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	127/127 (100%)	124 (98%)	3 (2%)	43	27
1	B	128/127 (101%)	123 (96%)	5 (4%)	28	12
1	C	129/127 (102%)	126 (98%)	3 (2%)	44	29
1	D	127/127 (100%)	123 (97%)	4 (3%)	35	18
1	E	128/127 (101%)	123 (96%)	5 (4%)	28	12
1	F	129/127 (102%)	127 (98%)	2 (2%)	55	43
1	G	128/127 (101%)	122 (95%)	6 (5%)	23	8
1	H	129/127 (102%)	126 (98%)	3 (2%)	44	29
1	I	128/127 (101%)	125 (98%)	3 (2%)	44	29
1	J	128/127 (101%)	124 (97%)	4 (3%)	35	18
All	All	1281/1270 (101%)	1243 (97%)	38 (3%)	38	19

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	80	LEU
1	A	102	GLN
1	A	128	LEU
1	B	80	LEU
1	B	102	GLN
1	B	128[A]	LEU
1	B	128[B]	LEU
1	B	133	VAL
1	C	27	LEU
1	C	36	THR
1	C	102	GLN
1	D	27	LEU
1	D	102	GLN
1	D	127	LYS
1	D	137	GLU
1	E	27	LEU
1	E	31	GLU
1	E	34	ASP
1	E	36	THR
1	E	102	GLN
1	F	27	LEU
1	F	102	GLN
1	G	1	MET
1	G	27	LEU
1	G	36	THR
1	G	102	GLN
1	G	128[A]	LEU
1	G	128[B]	LEU
1	H	27	LEU
1	H	80	LEU
1	H	102	GLN
1	I	77	MET
1	I	102	GLN
1	I	128	LEU
1	J	27	LEU
1	J	36	THR
1	J	102	GLN
1	J	133	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 32 ligands modelled in this entry, 10 are monoatomic - leaving 22 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
2	SO4	J	1158	-	4,4,4	0.22	0	6,6,6	0.22	0
2	SO4	A	1158	-	4,4,4	0.35	0	6,6,6	1.31	1 (16%)
2	SO4	D	1157	-	4,4,4	0.25	0	6,6,6	0.31	0
2	SO4	I	1157	-	4,4,4	0.37	0	6,6,6	0.58	0
2	SO4	J	1157	-	4,4,4	0.28	0	6,6,6	0.19	0
2	SO4	C	1159	-	4,4,4	0.25	0	6,6,6	1.28	0
2	SO4	A	1159	-	4,4,4	0.27	0	6,6,6	0.10	0
2	SO4	E	1157	-	4,4,4	0.26	0	6,6,6	0.33	0
2	SO4	D	1158	-	4,4,4	0.33	0	6,6,6	0.21	0
2	SO4	H	1158	-	4,4,4	0.25	0	6,6,6	0.30	0
2	SO4	G	1157	-	4,4,4	0.20	0	6,6,6	0.34	0
2	SO4	G	1158	-	4,4,4	0.24	0	6,6,6	1.57	1 (16%)
2	SO4	C	1160	-	4,4,4	0.22	0	6,6,6	0.14	0
2	SO4	B	1157	-	4,4,4	0.24	0	6,6,6	0.53	0
2	SO4	E	1158	-	4,4,4	0.24	0	6,6,6	0.26	0
2	SO4	F	1158	-	4,4,4	0.26	0	6,6,6	0.95	0
2	SO4	C	1157	-	4,4,4	0.28	0	6,6,6	0.63	0
2	SO4	A	1157	-	4,4,4	0.24	0	6,6,6	0.25	0
2	SO4	H	1157	-	4,4,4	0.22	0	6,6,6	0.29	0
2	SO4	C	1158	-	4,4,4	1.26	1 (25%)	6,6,6	1.03	0
2	SO4	B	1158	-	4,4,4	0.19	0	6,6,6	0.44	0
2	SO4	F	1157	-	4,4,4	0.26	0	6,6,6	0.29	0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1158	SO4	O1-S	-2.44	1.30	1.44

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	1158	SO4	O4-S-O2	-2.87	94.57	109.56
2	A	1158	SO4	O4-S-O2	-2.13	98.41	109.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	1158	SO4	1	0
2	F	1158	SO4	1	0
2	C	1158	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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.