



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:52 PM UTC

PDB ID : 2DXC / pdb_00002dxc
Title : Recombinant thiocyanate hydrolase, fully-matured form
Authors : Arakawa, T.; Kawano, Y.; Katayama, Y.; Yohda, M.; Odaka, M.
Deposited on : 2006-08-25
Resolution : 1.90 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

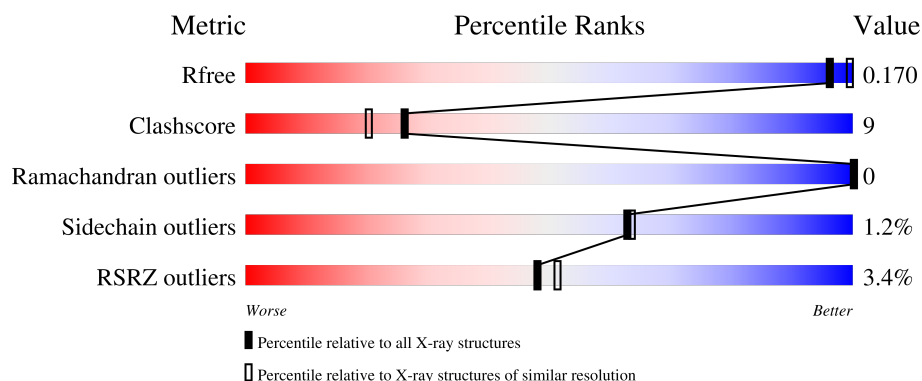
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	126	3% 82% 11% • 6%
1	D	126	3% 81% 13% 6%
1	G	126	4% 83% 13% 5%
1	J	126	3% 82% 13% • 5%
2	B	157	3% 80% 15% • •

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Mol	Chain	Length	Quality of chain
2	E	157	
2	H	157	
2	K	157	
3	C	243	
3	F	243	
3	I	243	
3	L	243	

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
5	TLA	E	3002	-	-	X	-
5	TLA	I	3003	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 18283 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 Thiocyanate hydrolase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	119	Total	C	N	O	S	0	0	0
			965	614	160	187	4			
1	D	119	Total	C	N	O	S	0	0	0
			965	614	160	187	4			
1	G	120	Total	C	N	O	S	0	0	0
			974	620	162	188	4			
1	J	120	Total	C	N	O	S	0	0	0
			974	620	162	188	4			

- Molecule 2 is a protein called Thiocyanate hydrolase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	152	Total	C	N	O	S	0	0	0
			1232	778	222	226	6			
2	E	151	Total	C	N	O	S	0	0	0
			1226	775	221	224	6			
2	H	156	Total	C	N	O	S	0	0	0
			1262	796	228	232	6			
2	K	152	Total	C	N	O	S	0	0	0
			1232	778	222	226	6			

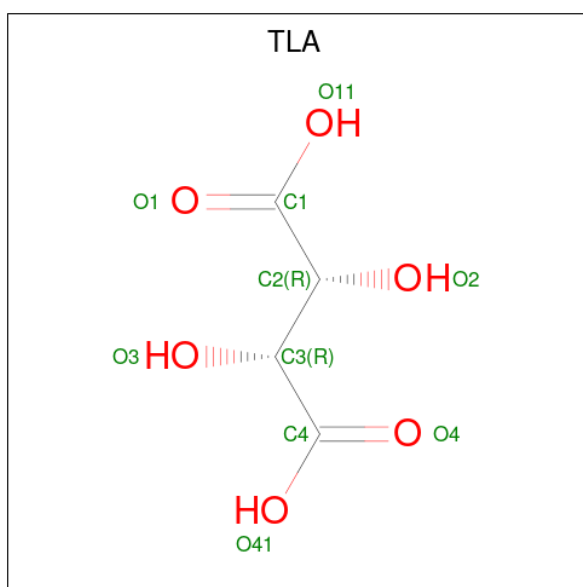
- Molecule 3 is a protein called Thiocyanate hydrolase subunit gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	217	Total	C	N	O	S	0	0	0
			1724	1098	304	314	8			
3	F	216	Total	C	N	O	S	0	0	0
			1715	1093	303	311	8			
3	I	217	Total	C	N	O	S	0	0	0
			1724	1098	304	314	8			
3	L	216	Total	C	N	O	S	0	0	0
			1715	1093	303	311	8			

- Molecule 4 is COBALT (III) ION (CCD ID: 3CO) (formula: Co).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total Co 1 1	0	0
4	F	1	Total Co 1 1	0	0
4	I	1	Total Co 1 1	0	0
4	L	1	Total Co 1 1	0	0

- Molecule 5 is L(+)-TARTARIC ACID (CCD ID: TLA) (formula: C₄H₆O₆).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total C O 10 4 6	0	0
5	E	1	Total C O 10 4 6	0	0
5	I	1	Total C O 10 4 6	0	0
5	L	1	Total C O 10 4 6	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	141	Total O 141 141	0	0

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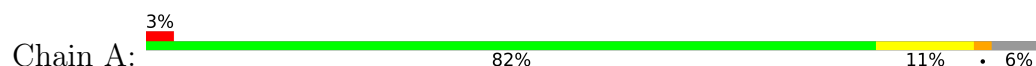
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	205	Total 205	O 205	0	0
6	C	300	Total 300	O 300	0	0
6	D	156	Total 156	O 156	0	0
6	E	190	Total 190	O 190	0	0
6	F	248	Total 248	O 248	0	0
6	G	150	Total 150	O 150	0	0
6	H	200	Total 200	O 200	0	0
6	I	302	Total 302	O 302	0	0
6	J	168	Total 168	O 168	0	0
6	K	196	Total 196	O 196	0	0
6	L	275	Total 275	O 275	0	0

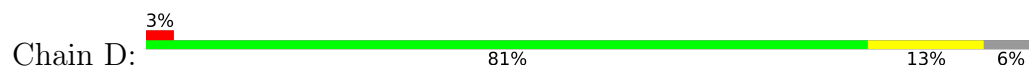
3 Residue-property plots [i](#)

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

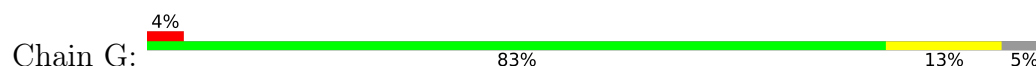
- Molecule 1: Thiocyanate hydrolase subunit alpha



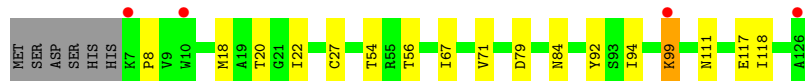
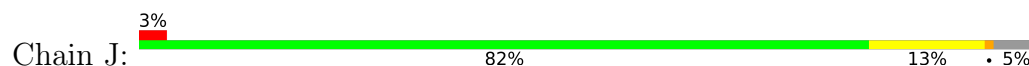
- Molecule 1: Thiocyanate hydrolase subunit alpha



- Molecule 1: Thiocyanate hydrolase subunit alpha



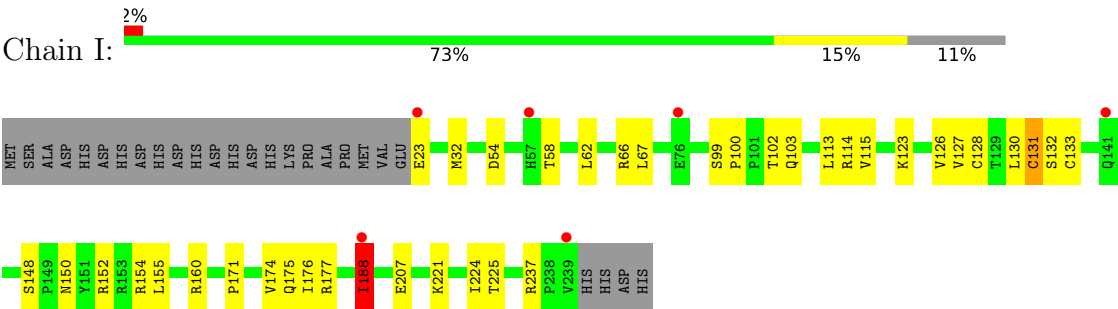
- Molecule 1: Thiocyanate hydrolase subunit alpha



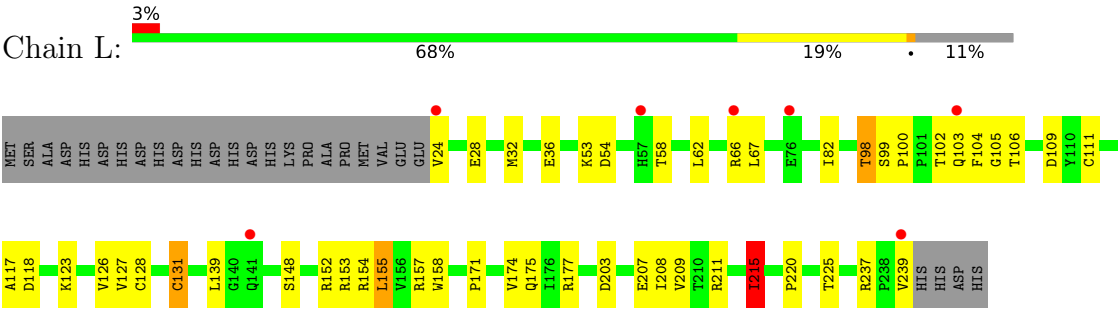
- Molecule 2: Thiocyanate hydrolase subunit beta



- Molecule 2: Thiocyanate hydrolase subunit beta



• Molecule 3: Thiocyanate hydrolase subunit gamma



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	114.87Å 170.53Å 175.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.85 – 1.90 41.85 – 1.90	Depositor EDS
% Data completeness (in resolution range)	96.8 (41.85-1.90) 97.6 (41.85-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	9.18 (at 1.89Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.171 , 0.193 0.170 , 0.170	Depositor DCC
R_{free} test set	13233 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	14.8	Xtriage
Anisotropy	0.481	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 52.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.013 for -h,l,k	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	18283	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.20% 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: 3CO, CSD, CSO, TLA

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	0.34	0/991	0.88	2/1342 (0.1%)
1	D	0.34	0/991	0.91	1/1342 (0.1%)
1	G	0.33	0/1000	0.86	1/1354 (0.1%)
1	J	0.34	0/1000	0.90	1/1354 (0.1%)
2	B	0.40	1/1264 (0.1%)	0.93	8/1720 (0.5%)
2	E	0.37	0/1258	0.89	2/1712 (0.1%)
2	H	0.36	0/1294	0.91	5/1757 (0.3%)
2	K	0.37	0/1264	0.87	5/1720 (0.3%)
3	C	0.36	0/1752	0.90	3/2391 (0.1%)
3	F	0.36	0/1743	0.91	5/2379 (0.2%)
3	I	0.36	0/1752	0.90	6/2391 (0.3%)
3	L	0.37	0/1743	0.92	8/2379 (0.3%)
All	All	0.36	1/16052 (0.0%)	0.90	47/21841 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	150	GLU	C-N	5.33	1.41	1.33

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	154	ARG	N-CA-C	9.39	123.25	111.69
3	L	154	ARG	N-CA-C	9.33	123.17	111.69
3	C	154	ARG	N-CA-C	9.30	123.13	111.69
3	F	154	ARG	N-CA-C	9.15	122.95	111.69
1	D	71	VAL	N-CA-C	8.52	119.32	110.72
1	G	71	VAL	N-CA-C	8.45	119.25	110.72
2	H	46	VAL	N-CA-C	-7.78	100.48	107.56
1	J	71	VAL	N-CA-C	7.56	118.35	110.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	71	VAL	N-CA-C	7.08	117.87	110.72
2	B	62	GLU	N-CA-C	-6.14	100.91	110.42
3	L	98	THR	N-CA-C	6.12	120.75	113.28
3	I	126	VAL	N-CA-C	5.92	117.89	108.89
2	K	62	GLU	N-CA-C	-5.83	101.39	110.42
3	I	237	ARG	CA-C-N	5.79	126.12	119.92
3	I	237	ARG	C-N-CA	5.79	126.12	119.92
2	H	83	GLY	N-CA-C	5.79	123.64	115.30
2	K	46	VAL	N-CA-C	-5.79	101.82	107.55
3	L	148	SER	N-CA-C	5.76	117.14	109.83
3	F	215	ILE	N-CA-C	-5.68	105.56	111.58
3	F	98	THR	N-CA-C	5.64	120.43	113.50
2	E	46	VAL	N-CA-C	-5.63	102.08	107.76
3	L	126	VAL	N-CA-C	5.59	117.38	108.89
2	B	150	GLU	CA-C-O	5.58	127.28	119.80
3	L	237	ARG	CA-C-N	5.56	125.47	119.85
3	L	237	ARG	C-N-CA	5.56	125.47	119.85
2	E	62	GLU	N-CA-C	-5.53	102.34	110.52
2	H	62	GLU	N-CA-C	-5.51	101.88	110.42
2	B	46	VAL	N-CA-C	-5.50	102.20	107.76
3	F	126	VAL	N-CA-C	5.46	117.19	108.89
2	K	83	GLY	N-CA-C	5.44	122.86	115.30
3	C	148	SER	N-CA-C	5.39	116.67	109.83
3	C	98	THR	N-CA-C	5.37	119.99	113.38
2	H	100	GLN	N-CA-C	5.37	117.56	111.11
2	H	125	PHE	N-CA-C	-5.36	106.24	112.89
2	B	149	GLY	CA-C-N	-5.35	113.93	122.66
2	B	149	GLY	C-N-CA	-5.35	113.93	122.66
2	B	83	GLY	N-CA-C	5.34	122.72	115.30
3	L	155	LEU	N-CA-C	5.26	117.42	111.11
2	B	100	GLN	N-CA-C	5.24	117.40	111.11
3	I	188	ILE	N-CA-C	-5.24	100.70	108.45
3	F	188	ILE	N-CA-C	-5.23	100.71	108.45
2	K	86	THR	N-CA-C	-5.20	102.36	110.42
2	K	100	GLN	N-CA-C	5.14	117.28	111.11
3	I	148	SER	N-CA-C	5.09	116.29	109.83
1	A	70	LEU	N-CA-C	-5.05	98.35	107.75
2	B	116	ALA	N-CA-C	-5.03	105.88	111.36
3	L	215	ILE	N-CA-C	-5.03	105.26	112.35

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	965	0	914	18	0
1	D	965	0	914	17	0
1	G	974	0	926	15	0
1	J	974	0	926	16	0
2	B	1232	0	1198	27	0
2	E	1226	0	1193	35	0
2	H	1262	0	1234	31	0
2	K	1232	0	1198	26	0
3	C	1724	0	1735	32	0
3	F	1715	0	1729	44	0
3	I	1724	0	1735	38	0
3	L	1715	0	1729	42	0
4	C	1	0	0	0	0
4	F	1	0	0	0	0
4	I	1	0	0	0	0
4	L	1	0	0	0	0
5	C	10	0	4	3	0
5	E	10	0	4	4	0
5	I	10	0	4	5	0
5	L	10	0	4	3	0
6	A	141	0	0	3	0
6	B	205	0	0	3	0
6	C	300	0	0	3	0
6	D	156	0	0	1	0
6	E	190	0	0	1	0
6	F	248	0	0	3	0
6	G	150	0	0	1	0
6	H	200	0	0	0	0
6	I	302	0	0	2	0
6	J	168	0	0	0	0
6	K	196	0	0	2	0
6	L	275	0	0	0	0
All	All	18283	0	15447	292	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 9.

All (292) 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)
3:I:113:LEU:HD11	3:I:188:ILE:HD12	1.26	1.13
3:I:115:VAL:HG22	3:I:188:ILE:HD11	1.41	1.03
1:A:26:GLN:H	1:A:26:GLN:HE21	1.03	0.95
2:K:134:LYS:HD2	2:K:138:MET:HE2	1.50	0.93
2:K:112:TRP:HZ2	5:L:3004:TLA:HB	0.94	0.91
1:D:45:ILE:HD12	1:D:63:ALA:O	1.72	0.90
3:L:211:ARG:O	3:L:215:ILE:HD13	1.71	0.90
2:E:70:LEU:HD22	3:F:53:LYS:HE3	1.55	0.87
3:L:208:ILE:HD13	3:L:220:PRO:HB2	1.59	0.85
1:D:45:ILE:HD11	1:D:96:PHE:CE1	2.12	0.84
2:H:58:ILE:HD11	2:H:60:TYR:CE1	2.13	0.84
1:J:67:ILE:HD13	1:J:94:ILE:HG13	1.60	0.83
3:F:170:LEU:HD13	3:F:176:ILE:HD11	1.60	0.83
2:E:67:ILE:HD11	3:F:239:VAL:HB	1.62	0.82
3:L:82:ILE:HD11	3:L:117:ALA:HB2	1.61	0.81
2:K:119:ILE:HD13	2:K:119:ILE:O	1.80	0.81
2:B:58:ILE:HD13	2:B:58:ILE:H	1.45	0.80
2:E:119:ILE:HD13	2:E:119:ILE:O	1.81	0.79
2:B:58:ILE:HD11	2:B:60:TYR:CE1	2.17	0.79
2:K:119:ILE:HD11	2:K:123:LYS:HD2	1.62	0.78
1:D:45:ILE:HD11	1:D:96:PHE:CZ	2.19	0.78
3:L:175:GLN:HE22	3:L:177:ARG:HH21	1.32	0.77
1:A:26:GLN:H	1:A:26:GLN:NE2	1.80	0.77
2:B:28:HIS:HD2	3:L:153:ARG:HH12	1.32	0.76
1:A:26:GLN:HE21	1:A:26:GLN:N	1.82	0.75
2:E:119:ILE:HD11	2:E:123:LYS:HD2	1.69	0.74
1:A:67:ILE:HG12	1:A:94:ILE:HD11	1.69	0.73
3:L:66:ARG:HH22	3:L:203:ASP:HA	1.54	0.73
2:E:67:ILE:HD11	3:F:239:VAL:CB	2.18	0.73
1:J:56:THR:HG23	1:J:118:ILE:HD12	1.72	0.72
1:A:67:ILE:HG12	1:A:94:ILE:CD1	2.19	0.72
3:I:175:GLN:HE22	3:I:177:ARG:HH21	1.36	0.72
3:F:175:GLN:HE22	3:F:177:ARG:HH11	1.35	0.71
2:E:24:HIS:ND1	2:K:24:HIS:HD2	1.87	0.71
2:K:134:LYS:HD2	2:K:138:MET:CE	2.21	0.70
3:L:82:ILE:CD1	3:L:117:ALA:HB2	2.21	0.70
1:A:67:ILE:HA	1:A:94:ILE:HD13	1.73	0.69
2:E:148:LEU:CD1	3:F:32:MET:HG3	2.23	0.69
3:F:102:THR:O	3:F:103:GLN:HB2	1.92	0.69
3:L:208:ILE:HD13	3:L:220:PRO:CB	2.23	0.68
2:H:112:TRP:HZ2	5:I:3003:TLA:HB	1.37	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:GLU:CD	1:A:86:GLU:H	2.02	0.67
3:I:188:ILE:H	3:I:188:ILE:HD13	1.61	0.66
2:H:148:LEU:HG	3:I:32:MET:HE2	1.77	0.66
2:B:28:HIS:CD2	3:L:153:ARG:HH12	2.13	0.65
2:B:66:GLU:HB2	2:B:69:GLU:HG3	1.78	0.65
2:K:66:GLU:HB2	2:K:69:GLU:HG3	1.79	0.65
3:C:221:LYS:HB2	3:C:224:ILE:HD13	1.77	0.65
1:G:45:ILE:HD11	1:G:118:ILE:HD13	1.79	0.65
3:I:62:LEU:HD23	6:I:3026:HOH:O	1.96	0.65
2:H:58:ILE:HD13	2:H:58:ILE:H	1.61	0.65
1:G:45:ILE:CD1	1:G:118:ILE:HD13	2.28	0.64
1:D:56:THR:HG23	1:D:118:ILE:HD12	1.80	0.64
2:H:35:ILE:HD12	2:H:35:ILE:N	2.12	0.64
2:E:66:GLU:HB2	2:E:69:GLU:HG3	1.78	0.64
2:H:66:GLU:HB2	2:H:69:GLU:HG3	1.78	0.64
3:I:115:VAL:CG2	3:I:188:ILE:HD11	2.23	0.64
1:J:67:ILE:HD12	1:J:92:TYR:HB3	1.79	0.64
2:K:5:ILE:HD12	2:K:5:ILE:H	1.61	0.63
1:J:20:THR:O	1:J:22:ILE:HD12	1.98	0.63
1:G:13:THR:HB	1:G:17:LYS:HE3	1.80	0.63
3:L:66:ARG:NH2	3:L:203:ASP:HA	2.14	0.63
3:F:115:VAL:HG13	3:F:188:ILE:HD11	1.81	0.63
3:F:142:SER:OG	3:F:147:ARG:HD3	1.98	0.63
3:F:170:LEU:CD1	3:F:176:ILE:HD11	2.29	0.63
1:D:45:ILE:HD13	1:D:60:THR:O	1.99	0.62
2:K:46:VAL:HG12	2:K:96:CYS:SG	2.39	0.62
2:E:148:LEU:HD11	3:F:32:MET:HG3	1.82	0.62
2:H:112:TRP:HZ2	5:I:3003:TLA:O3	1.82	0.62
3:C:134:TYR:CE1	3:C:215:ILE:HD11	2.34	0.62
2:K:84:VAL:CG1	2:K:119:ILE:HD12	2.30	0.61
2:H:58:ILE:HD12	3:I:150:ASN:CG	2.25	0.61
3:I:221:LYS:HB2	3:I:224:ILE:HD12	1.82	0.61
2:E:84:VAL:CG1	2:E:119:ILE:HD12	2.31	0.61
3:I:188:ILE:HD13	3:I:188:ILE:N	2.16	0.61
3:F:170:LEU:HD13	3:F:176:ILE:CD1	2.29	0.60
3:L:208:ILE:HD12	3:L:208:ILE:C	2.27	0.60
2:H:46:VAL:HG12	2:H:96:CYS:SG	2.41	0.60
6:B:302:HOH:O	3:C:29:ILE:HD11	2.02	0.59
1:D:45:ILE:HD11	1:D:96:PHE:HE1	1.67	0.59
3:C:175:GLN:HE22	3:C:177:ARG:HH11	1.49	0.59
2:K:3:SER:O	2:K:7:GLU:HG3	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:70:LEU:HD21	6:F:531:HOH:O	2.02	0.58
3:I:127:VAL:HG22	3:I:128:CYS:N	2.19	0.58
2:B:58:ILE:HD12	3:C:150:ASN:CG	2.28	0.58
2:E:134:LYS:HG2	3:F:37:LEU:HD13	1.86	0.58
2:E:112:TRP:CZ2	5:E:3002:TLA:H3	2.39	0.57
2:E:90:ARG:NH1	5:E:3002:TLA:O4	2.38	0.57
3:F:238:PRO:O	3:F:239:VAL:HB	2.04	0.57
2:H:90:ARG:HH12	5:I:3003:TLA:H3	1.70	0.57
1:D:43:VAL:CG1	1:D:67:ILE:HD11	2.35	0.56
2:B:71:ASN:HD21	3:C:53:LYS:NZ	2.02	0.56
2:E:119:ILE:HD13	2:E:119:ILE:C	2.30	0.56
3:L:139:LEU:HD21	3:L:215:ILE:HD11	1.86	0.56
3:I:102:THR:O	3:I:103:GLN:HB2	2.04	0.56
1:J:54:THR:HG22	2:K:46:VAL:HG21	1.88	0.56
3:L:127:VAL:HG22	3:L:128:CYS:N	2.19	0.56
1:A:26:GLN:HE22	3:C:111:CYS:HB2	1.70	0.56
2:H:32:PRO:HA	2:H:35:ILE:HD13	1.88	0.56
2:B:126:VAL:HG12	2:B:127:THR:O	2.06	0.55
2:B:58:ILE:H	2:B:58:ILE:CD1	2.18	0.55
3:C:221:LYS:CB	3:C:224:ILE:HD13	2.37	0.55
1:J:18:MET:HE3	1:J:27:CYS:SG	2.46	0.55
2:H:148:LEU:HG	3:I:32:MET:CE	2.37	0.55
2:K:5:ILE:HD12	2:K:5:ILE:N	2.21	0.54
3:C:224:ILE:HD12	3:C:224:ILE:N	2.21	0.54
2:B:112:TRP:HZ2	5:C:3001:TLA:O3	1.90	0.54
3:C:102:THR:O	3:C:103:GLN:HB2	2.07	0.54
3:I:131:CSD:HB3	5:I:3003:TLA:O41	2.08	0.54
1:D:53:TYR:HA	2:E:46:VAL:HG11	1.90	0.54
1:G:111:ASN:O	3:I:175:GLN:HG3	2.07	0.54
2:K:148:LEU:HG	3:L:32:MET:HG3	1.89	0.53
2:E:144:SER:OG	2:E:146:GLN:HG3	2.07	0.53
1:G:54:THR:HG22	2:H:46:VAL:HG21	1.89	0.53
3:F:131:CSD:O	3:F:152:ARG:HD3	2.09	0.53
2:E:148:LEU:HD13	3:F:32:MET:HG3	1.91	0.53
1:J:111:ASN:O	3:L:175:GLN:HG3	2.09	0.53
3:L:139:LEU:HD21	3:L:215:ILE:CD1	2.39	0.53
3:C:127:VAL:HG22	3:C:128:CYS:N	2.23	0.52
3:F:127:VAL:HG22	3:F:128:CYS:N	2.23	0.52
1:A:10:TRP:CZ3	1:J:8:PRO:HG2	2.44	0.52
3:I:171:PRO:HB2	3:I:174:VAL:HG23	1.92	0.52
3:F:171:PRO:HB2	3:F:174:VAL:HG23	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:41:ARG:HG2	2:K:12:HIS:CD2	2.45	0.52
3:L:207:GLU:HG2	3:L:225:THR:CG2	2.39	0.52
2:E:138:MET:HE1	2:E:141:ARG:NH2	2.25	0.52
3:F:67:LEU:C	3:F:67:LEU:HD23	2.34	0.52
1:G:94:ILE:HD12	1:G:118:ILE:HD12	1.92	0.52
2:B:58:ILE:HD13	2:B:58:ILE:N	2.15	0.52
3:I:221:LYS:HD2	3:I:224:ILE:HD12	1.92	0.52
3:I:23:GLU:O	3:I:23:GLU:HG2	2.10	0.52
3:F:129:THR:O	3:F:152:ARG:HD2	2.09	0.51
2:K:119:ILE:HD13	2:K:119:ILE:C	2.35	0.51
3:L:102:THR:O	3:L:103:GLN:HB2	2.08	0.51
2:B:58:ILE:HD11	2:B:60:TYR:CZ	2.45	0.51
2:B:58:ILE:CD1	2:B:58:ILE:N	2.72	0.51
1:G:117:GLU:C	1:G:118:ILE:HG13	2.35	0.51
1:D:20:THR:HA	3:F:104:PHE:HB3	1.93	0.51
2:E:141:ARG:HG2	2:E:147:GLY:O	2.11	0.51
2:B:46:VAL:O	2:B:46:VAL:HG23	2.10	0.51
2:K:136:VAL:O	2:K:140:GLU:HG3	2.11	0.51
3:L:131:CSD:O	3:L:152:ARG:HD2	2.09	0.51
3:L:208:ILE:HD12	3:L:209:VAL:N	2.26	0.51
2:H:91:ARG:HD3	3:I:131:CSD:OD2	2.10	0.51
1:D:111:ASN:O	3:F:175:GLN:HG3	2.10	0.51
3:F:207:GLU:HG2	3:F:225:THR:HG22	1.92	0.51
1:G:86:GLU:CD	1:G:86:GLU:H	2.18	0.51
3:C:127:VAL:HB	3:C:155:LEU:HD23	1.91	0.50
3:L:54:ASP:O	3:L:58:THR:HG23	2.11	0.50
2:H:58:ILE:HD13	2:H:58:ILE:N	2.26	0.50
3:C:131:CSD:O	3:C:152:ARG:HD2	2.12	0.50
1:D:43:VAL:CG2	1:D:67:ILE:HD11	2.42	0.49
1:D:117:GLU:O	1:D:118:ILE:HD13	2.12	0.49
3:F:62:LEU:HB3	3:F:63:PRO:HD3	1.94	0.49
3:F:103:GLN:HG3	6:F:319:HOH:O	2.11	0.49
3:F:115:VAL:HG13	3:F:188:ILE:CD1	2.41	0.49
3:I:62:LEU:H	3:I:62:LEU:HD22	1.76	0.49
6:B:357:HOH:O	3:C:29:ILE:HD12	2.12	0.49
3:F:188:ILE:HD12	3:F:188:ILE:C	2.37	0.49
3:C:123:LYS:HG3	3:C:170:LEU:HD21	1.93	0.49
1:A:119:PRO:HG2	1:A:122:TYR:HD2	1.78	0.48
2:B:126:VAL:HG13	2:B:130:GLU:HB2	1.95	0.48
2:E:90:ARG:HH22	5:E:3002:TLA:H2	1.78	0.48
2:E:107:PRO:HG3	2:H:35:ILE:HD11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:131:CSD:O	3:I:152:ARG:HD2	2.13	0.48
2:H:112:TRP:CZ2	5:I:3003:TLA:O3	2.57	0.48
2:E:107:PRO:HG3	2:H:35:ILE:CD1	2.44	0.48
3:I:62:LEU:HD22	3:I:62:LEU:N	2.29	0.48
3:I:113:LEU:CD1	3:I:188:ILE:HD12	2.19	0.48
1:J:117:GLU:O	1:J:118:ILE:HD13	2.14	0.48
1:D:43:VAL:HG13	1:D:67:ILE:HD11	1.95	0.47
3:F:207:GLU:HG2	3:F:225:THR:CG2	2.44	0.47
1:A:86:GLU:CD	1:A:86:GLU:N	2.71	0.47
2:E:91:ARG:HD3	3:F:131:CSD:OD2	2.15	0.47
3:I:160:ARG:NE	3:I:176:ILE:HD12	2.30	0.47
2:B:42:ALA:O	2:B:45:ARG:HG2	2.15	0.47
3:I:54:ASP:O	3:I:58:THR:HG23	2.14	0.47
1:A:84:ASN:ND2	2:K:124:GLN:HE21	2.12	0.47
3:I:67:LEU:HD23	3:I:67:LEU:C	2.39	0.47
2:K:46:VAL:CG1	2:K:96:CYS:SG	3.02	0.47
3:L:208:ILE:C	3:L:208:ILE:CD1	2.88	0.47
6:E:3118:HOH:O	3:F:49:HIS:HD2	1.98	0.47
3:L:207:GLU:HG2	3:L:225:THR:HG22	1.97	0.47
3:I:132:SER:O	3:I:133:CSO:C	2.63	0.46
1:D:114:LEU:C	1:D:114:LEU:HD23	2.40	0.46
2:E:118:ARG:HG3	2:E:122:ASP:OD2	2.15	0.46
2:H:56:VAL:HG12	2:K:55:ASP:C	2.41	0.46
3:C:132:SER:O	3:C:133:CSO:C	2.63	0.46
2:K:70:LEU:HG	3:L:53:LYS:HE3	1.97	0.46
2:B:112:TRP:CZ2	5:C:3001:TLA:H3	2.51	0.46
3:C:170:LEU:HD13	3:C:176:ILE:HD11	1.97	0.46
3:L:24:VAL:HG13	3:L:28:GLU:HB2	1.97	0.46
2:B:37:HIS:HE1	2:E:8:GLU:OE2	1.99	0.46
2:H:48:HIS:HB2	3:I:130:LEU:O	2.16	0.46
3:I:99:SER:HB2	3:I:100:PRO:HD3	1.98	0.46
2:B:65:GLU:OE1	2:B:70:LEU:HB2	2.16	0.46
1:D:67:ILE:N	1:D:67:ILE:HD12	2.31	0.46
3:L:62:LEU:O	3:L:66:ARG:HG2	2.15	0.45
1:J:94:ILE:HD12	1:J:94:ILE:N	2.31	0.45
2:H:31:ALA:O	2:H:35:ILE:CD1	2.64	0.45
3:F:154:ARG:NH2	3:F:165:GLU:OE2	2.40	0.45
6:K:341:HOH:O	3:L:239:VAL:HB	2.16	0.45
1:A:79:ASP:HA	6:A:313:HOH:O	2.17	0.45
3:F:201:THR:OG1	3:F:204:GLN:HG3	2.16	0.45
3:I:113:LEU:HD11	3:I:188:ILE:CD1	2.19	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:207:GLU:HG2	3:I:225:THR:CG2	2.46	0.45
2:E:90:ARG:HH12	5:E:3002:TLA:C4	2.30	0.44
1:A:71:VAL:HG11	1:A:117:GLU:OE2	2.17	0.44
2:K:138:MET:HE1	3:L:36:GLU:CD	2.42	0.44
3:L:171:PRO:HB2	3:L:174:VAL:HG23	1.98	0.44
2:B:71:ASN:HD21	3:C:53:LYS:HZ1	1.66	0.44
3:L:67:LEU:C	3:L:67:LEU:HD23	2.43	0.44
3:L:131:CSD:HB3	5:L:3004:TLA:O41	2.18	0.44
1:G:31:MET:HE1	6:G:2088:HOH:O	2.17	0.44
6:D:246:HOH:O	1:G:7:LYS:HB2	2.17	0.43
3:F:127:VAL:HB	3:F:155:LEU:HD23	2.00	0.43
2:H:45:ARG:HH11	2:H:100:GLN:HE22	1.64	0.43
2:H:58:ILE:HD12	3:I:150:ASN:ND2	2.33	0.43
3:L:127:VAL:HB	3:L:155:LEU:HD23	1.99	0.43
3:C:171:PRO:HB2	3:C:174:VAL:HG23	1.99	0.43
1:A:20:THR:HA	3:C:104:PHE:HB3	2.00	0.43
1:A:34:LYS:HD3	6:A:2521:HOH:O	2.17	0.43
3:C:161:GLN:HG2	6:F:426:HOH:O	2.19	0.43
2:H:28:HIS:ND1	2:H:28:HIS:N	2.66	0.43
2:E:116:ALA:O	2:E:119:ILE:HG22	2.18	0.43
1:G:41:ASP:HB2	1:G:67:ILE:HD12	1.99	0.43
1:J:99:LYS:HB2	1:J:99:LYS:NZ	2.34	0.43
3:L:175:GLN:NE2	3:L:177:ARG:HH21	2.09	0.43
1:G:13:THR:CB	1:G:17:LYS:HE3	2.45	0.43
2:H:46:VAL:CG1	2:H:96:CYS:SG	3.07	0.43
3:L:106:THR:OG1	3:L:109:ASP:HB2	2.19	0.43
3:F:126:VAL:HG12	3:F:127:VAL:N	2.33	0.43
2:K:90:ARG:HH12	5:L:3004:TLA:H3	1.83	0.43
3:L:98:THR:HA	3:L:103:GLN:OE1	2.19	0.43
2:B:67:ILE:HG12	3:C:239:VAL:HA	2.01	0.43
1:D:121:ARG:HG3	1:D:122:TYR:CD1	2.54	0.43
1:J:79:ASP:HB3	1:J:84:ASN:O	2.18	0.43
2:K:80:ALA:HA	2:K:85:TRP:O	2.19	0.43
2:B:142:VAL:HG21	3:C:24:VAL:HG21	2.01	0.42
2:E:80:ALA:HA	2:E:85:TRP:O	2.19	0.42
3:F:132:SER:O	3:F:133:CSO:C	2.67	0.42
3:I:123:LYS:HD3	3:I:123:LYS:C	2.44	0.42
3:F:171:PRO:HD2	3:F:174:VAL:HG21	2.01	0.42
3:F:238:PRO:O	3:F:239:VAL:CB	2.67	0.42
3:I:175:GLN:NE2	3:I:177:ARG:HH21	2.12	0.42
2:B:112:TRP:CZ2	5:C:3001:TLA:C3	3.03	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:36:GLU:O	3:C:40:GLU:HB2	2.19	0.42
2:B:48:HIS:HB2	3:C:130:LEU:O	2.18	0.42
3:F:157:ARG:HD3	3:F:158:TRP:CH2	2.54	0.42
2:E:127:THR:OG1	2:E:130:GLU:HG3	2.20	0.42
2:H:11:ARG:HD3	6:K:320:HOH:O	2.20	0.42
2:H:80:ALA:HA	2:H:85:TRP:O	2.20	0.42
3:I:175:GLN:HE22	3:I:177:ARG:NH2	2.12	0.42
2:B:124:GLN:HE21	1:J:84:ASN:ND2	2.18	0.42
3:L:215:ILE:CD1	3:L:215:ILE:N	2.82	0.42
3:I:114:ARG:O	3:I:188:ILE:HD13	2.20	0.41
3:C:106:THR:OG1	3:C:109:ASP:HB2	2.20	0.41
3:F:175:GLN:NE2	3:F:177:ARG:HH11	2.10	0.41
2:H:39:LEU:HD12	2:H:39:LEU:HA	1.92	0.41
3:L:118:ASP:OD2	3:L:123:LYS:HD2	2.20	0.41
1:G:7:LYS:HB2	1:G:8:PRO:HD3	2.01	0.41
1:J:20:THR:HA	3:L:104:PHE:HB3	2.01	0.41
3:C:113:LEU:HD11	3:C:188:ILE:HG12	2.03	0.41
2:E:119:ILE:C	2:E:119:ILE:CD1	2.93	0.41
1:J:67:ILE:HD12	1:J:92:TYR:CB	2.48	0.41
2:E:67:ILE:HD11	3:F:239:VAL:CA	2.51	0.41
2:E:136:VAL:O	2:E:140:GLU:HG3	2.20	0.41
2:K:69:GLU:HB3	2:K:109:TYR:CD1	2.56	0.41
2:H:45:ARG:NH1	2:H:100:GLN:HE22	2.19	0.41
1:A:79:ASP:HB3	1:A:84:ASN:O	2.19	0.41
2:B:137:GLU:HB3	6:B:228:HOH:O	2.21	0.41
6:C:3155:HOH:O	3:F:161:GLN:HG2	2.20	0.41
3:C:67:LEU:HD23	3:C:67:LEU:C	2.45	0.41
2:H:116:ALA:O	2:H:119:ILE:HG22	2.21	0.41
3:I:127:VAL:HB	3:I:155:LEU:HD23	2.03	0.41
2:K:138:MET:HE1	3:L:36:GLU:OE1	2.21	0.41
3:L:99:SER:N	3:L:100:PRO:CD	2.84	0.41
3:L:157:ARG:HD3	3:L:158:TRP:CH2	2.56	0.41
2:B:58:ILE:HD12	3:C:150:ASN:ND2	2.36	0.41
3:C:54:ASP:O	3:C:58:THR:HG23	2.21	0.40
3:C:221:LYS:HE2	6:C:3214:HOH:O	2.21	0.40
1:D:43:VAL:HG22	1:D:67:ILE:HD11	2.03	0.40
2:E:108:TYR:CZ	3:F:147:ARG:HD2	2.56	0.40
1:A:110:ALA:HA	6:A:1016:HOH:O	2.21	0.40
1:G:12:ARG:HD2	6:I:3086:HOH:O	2.20	0.40
3:L:105:GLY:HA3	3:L:111:CYS:SG	2.60	0.40
3:C:66:ARG:HD2	6:C:3116:HOH:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:102:THR:HB	3:F:104:PHE:CE2	2.56	0.40
1:G:7:LYS:N	1:G:8:PRO:CD	2.84	0.40
3:I:160:ARG:CD	3:I:176:ILE:HD12	2.52	0.40
2:E:48:HIS:HB2	3:F:130:LEU:O	2.22	0.40
1:J:92:TYR:O	1:J:94:ILE:HD12	2.21	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	117/126 (93%)	111 (95%)	6 (5%)	0	100	100
1	D	117/126 (93%)	111 (95%)	6 (5%)	0	100	100
1	G	118/126 (94%)	113 (96%)	5 (4%)	0	100	100
1	J	118/126 (94%)	113 (96%)	5 (4%)	0	100	100
2	B	150/157 (96%)	146 (97%)	4 (3%)	0	100	100
2	E	149/157 (95%)	146 (98%)	3 (2%)	0	100	100
2	H	154/157 (98%)	150 (97%)	4 (3%)	0	100	100
2	K	150/157 (96%)	147 (98%)	3 (2%)	0	100	100
3	C	213/243 (88%)	206 (97%)	7 (3%)	0	100	100
3	F	212/243 (87%)	201 (95%)	11 (5%)	0	100	100
3	I	213/243 (88%)	206 (97%)	7 (3%)	0	100	100
3	L	212/243 (87%)	204 (96%)	8 (4%)	0	100	100
All	All	1923/2104 (91%)	1854 (96%)	69 (4%)	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	101/108 (94%)	99 (98%)	2 (2%)	48	46
1	D	101/108 (94%)	100 (99%)	1 (1%)	68	70
1	G	102/108 (94%)	102 (100%)	0	100	100
1	J	102/108 (94%)	101 (99%)	1 (1%)	68	70
2	B	130/134 (97%)	128 (98%)	2 (2%)	57	56
2	E	129/134 (96%)	127 (98%)	2 (2%)	55	54
2	H	133/134 (99%)	129 (97%)	4 (3%)	36	30
2	K	130/134 (97%)	129 (99%)	1 (1%)	73	75
3	C	188/212 (89%)	187 (100%)	1 (0%)	81	84
3	F	187/212 (88%)	184 (98%)	3 (2%)	55	54
3	I	188/212 (89%)	186 (99%)	2 (1%)	65	67
3	L	187/212 (88%)	186 (100%)	1 (0%)	81	84
All	All	1678/1816 (92%)	1658 (99%)	20 (1%)	63	63

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	MET
1	A	26	GLN
2	B	58	ILE
2	B	150	GLU
3	C	198	ASP
1	D	25	PRO
2	E	46	VAL
2	E	119	ILE
3	F	37	LEU
3	F	173	GLU
3	F	239	VAL
2	H	28	HIS
2	H	35	ILE
2	H	39	LEU

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Mol	Chain	Res	Type
2	H	58	ILE
3	I	66	ARG
3	I	188	ILE
1	J	99	LYS
2	K	119	ILE
3	L	215	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	87	ASN
1	A	111	ASN
2	B	26	GLN
2	B	28	HIS
2	B	37	HIS
2	B	71	ASN
2	B	124	GLN
3	C	57	HIS
3	C	141	GLN
3	C	169	GLN
3	C	175	GLN
1	D	38	ASN
1	D	87	ASN
2	E	94	GLN
2	E	100	GLN
2	E	146	GLN
3	F	49	HIS
3	F	169	GLN
3	F	175	GLN
1	G	14	HIS
1	G	38	ASN
1	G	84	ASN
2	H	25	GLN
2	H	100	GLN
2	H	124	GLN
3	I	112	ASN
3	I	124	HIS
3	I	141	GLN
3	I	175	GLN
1	J	38	ASN
2	K	12	HIS

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Mol	Chain	Res	Type
2	K	24	HIS
2	K	100	GLN
2	K	124	GLN
2	K	146	GLN
3	L	175	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues are modelled in this entry.

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	CSO	I	133	4	3,6,7	0.73	0	1,6,8	1.59	0
3	CSO	L	133	4	3,6,7	0.70	0	1,6,8	1.49	0
3	CSD	I	131	4	4,7,8	3.01	1 (25%)	1,8,10	2.16	1 (100%)
3	CSD	C	131	4	4,7,8	2.53	1 (25%)	1,8,10	2.16	1 (100%)
3	CSO	F	133	4	3,6,7	0.74	0	1,6,8	1.20	0
3	CSD	L	131	4	4,7,8	2.72	1 (25%)	1,8,10	2.18	1 (100%)
3	CSD	F	131	4	4,7,8	2.84	1 (25%)	1,8,10	2.23	1 (100%)
3	CSO	C	133	4	3,6,7	0.76	0	1,6,8	1.20	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	CSO	I	133	4	-	0/1/5/7	-
3	CSO	L	133	4	-	0/1/5/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CSD	I	131	4	-	0/2/6/8	-
3	CSD	C	131	4	-	0/2/6/8	-
3	CSO	F	133	4	-	0/1/5/7	-
3	CSD	L	131	4	-	0/2/6/8	-
3	CSD	F	131	4	-	0/2/6/8	-
3	CSO	C	133	4	-	0/1/5/7	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	131	CSD	OD1-SG	-5.84	1.42	1.47
3	F	131	CSD	OD1-SG	-5.49	1.42	1.47
3	L	131	CSD	OD1-SG	-5.25	1.42	1.47
3	C	131	CSD	OD1-SG	-4.85	1.43	1.47

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	131	CSD	OD1-SG-CB	2.23	109.71	105.60
3	L	131	CSD	OD1-SG-CB	2.18	109.61	105.60
3	C	131	CSD	OD1-SG-CB	2.16	109.58	105.60
3	I	131	CSD	OD1-SG-CB	2.16	109.58	105.60

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	133	CSO	1	0
3	I	131	CSD	3	0
3	C	131	CSD	1	0
3	F	133	CSO	1	0
3	L	131	CSD	2	0
3	F	131	CSD	2	0
3	C	133	CSO	1	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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
5	TLA	L	3004	-	9,9,9	2.07	4 (44%)	12,12,12	0.89	0
5	TLA	E	3002	-	9,9,9	1.97	3 (33%)	12,12,12	0.89	0
5	TLA	I	3003	-	9,9,9	2.16	5 (55%)	12,12,12	0.99	1 (8%)
5	TLA	C	3001	-	9,9,9	2.04	4 (44%)	12,12,12	0.88	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
5	TLA	L	3004	-	-	4/12/12/12	-
5	TLA	E	3002	-	-	4/12/12/12	-
5	TLA	I	3003	-	-	4/12/12/12	-
5	TLA	C	3001	-	-	4/12/12/12	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	I	3003	TLA	O2-C2	3.65	1.49	1.42
5	L	3004	TLA	O2-C2	3.47	1.49	1.42
5	C	3001	TLA	O2-C2	3.24	1.48	1.42
5	E	3002	TLA	O1-C1	3.05	1.31	1.22
5	I	3003	TLA	O1-C1	2.84	1.30	1.22
5	L	3004	TLA	O1-C1	2.83	1.30	1.22
5	C	3001	TLA	O1-C1	2.72	1.30	1.22
5	C	3001	TLA	O11-C1	-2.63	1.22	1.30
5	E	3002	TLA	O2-C2	2.62	1.47	1.42
5	E	3002	TLA	O11-C1	-2.45	1.22	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	3004	TLA	O11-C1	-2.29	1.23	1.30
5	I	3003	TLA	O11-C1	-2.26	1.23	1.30
5	I	3003	TLA	O4-C4	2.20	1.28	1.22
5	C	3001	TLA	O4-C4	2.18	1.28	1.22
5	L	3004	TLA	O4-C4	2.14	1.28	1.22
5	I	3003	TLA	C2-C1	2.02	1.55	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	3003	TLA	O41-C4-C3	2.17	119.34	113.31

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	3001	TLA	O11-C1-C2-C3
5	E	3002	TLA	O11-C1-C2-C3
5	L	3004	TLA	O11-C1-C2-C3
5	C	3001	TLA	O1-C1-C2-C3
5	L	3004	TLA	O1-C1-C2-C3
5	E	3002	TLA	O1-C1-C2-C3
5	I	3003	TLA	O11-C1-C2-C3
5	C	3001	TLA	O11-C1-C2-O2
5	L	3004	TLA	O11-C1-C2-O2
5	I	3003	TLA	O1-C1-C2-C3
5	C	3001	TLA	O1-C1-C2-O2
5	E	3002	TLA	O11-C1-C2-O2
5	L	3004	TLA	O1-C1-C2-O2
5	I	3003	TLA	O11-C1-C2-O2
5	E	3002	TLA	O1-C1-C2-O2
5	I	3003	TLA	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	L	3004	TLA	3	0
5	E	3002	TLA	4	0
5	I	3003	TLA	5	0
5	C	3001	TLA	3	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

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	119/126 (94%)	-0.03	4 (3%)	48	51	9, 15, 30, 36	0
1	D	119/126 (94%)	-0.12	4 (3%)	48	51	9, 13, 29, 31	0
1	G	120/126 (95%)	-0.10	5 (4%)	40	43	9, 15, 29, 41	0
1	J	120/126 (95%)	-0.24	4 (3%)	49	52	9, 12, 27, 42	0
2	B	152/157 (96%)	-0.27	5 (3%)	49	52	8, 12, 26, 31	0
2	E	151/157 (96%)	-0.19	7 (4%)	37	40	8, 13, 31, 40	0
2	H	156/157 (99%)	-0.18	8 (5%)	33	36	8, 12, 26, 56	0
2	K	152/157 (96%)	-0.27	4 (2%)	57	61	8, 12, 28, 39	0
3	C	215/243 (88%)	-0.17	6 (2%)	55	59	8, 13, 25, 44	0
3	F	214/243 (88%)	0.11	7 (3%)	49	52	9, 16, 30, 39	0
3	I	215/243 (88%)	-0.24	6 (2%)	55	59	8, 13, 23, 42	0
3	L	214/243 (88%)	-0.19	7 (3%)	49	52	8, 13, 26, 40	0
All	All	1947/2104 (92%)	-0.16	67 (3%)	48	51	8, 13, 27, 56	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	239	VAL	8.3
3	I	239	VAL	8.3
3	F	239	VAL	8.3
3	L	239	VAL	8.1
2	H	28	HIS	6.4
2	H	156	ALA	6.1
2	H	2	SER	5.6
1	A	50	ASP	5.4
3	F	103	GLN	5.3
3	L	103	GLN	5.2
1	D	50	ASP	5.1

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Mol	Chain	Res	Type	RSRZ
2	H	155	LYS	4.8
2	H	157	LYS	4.8
2	B	150	GLU	4.6
2	K	3	SER	4.4
2	H	3	SER	4.3
3	L	57	HIS	4.3
3	F	76	GLU	4.1
3	F	141	GLN	3.9
1	G	126	ALA	3.9
3	C	198	ASP	3.8
3	I	57	HIS	3.7
3	I	76	GLU	3.6
1	J	7	LYS	3.6
3	I	23	GLU	3.5
2	B	154	PRO	3.5
1	A	126	ALA	3.4
1	G	7	LYS	3.4
1	A	8	PRO	3.4
3	C	23	GLU	3.3
2	E	70	LEU	3.3
1	A	125	LYS	3.2
1	D	86	GLU	3.2
3	L	66	ARG	3.0
3	C	76	GLU	2.9
2	E	145	GLY	2.9
2	E	65	GLU	2.8
2	K	154	PRO	2.7
1	G	125	LYS	2.7
3	C	141	GLN	2.6
2	K	65	GLU	2.6
3	I	188	ILE	2.6
3	I	141	GLN	2.6
3	L	24	VAL	2.6
2	B	65	GLU	2.5
1	D	126	ALA	2.5
3	F	188	ILE	2.5
3	F	198	ASP	2.5
2	H	146	GLN	2.4
2	K	5	ILE	2.4
2	E	152	LEU	2.4
3	C	50	ARG	2.4
1	G	8	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
2	E	146	GLN	2.4
1	J	10	TRP	2.4
2	B	70	LEU	2.3
2	H	65	GLU	2.3
1	D	10	TRP	2.3
2	E	148	LEU	2.3
3	F	199	GLY	2.3
2	E	137	GLU	2.2
3	L	76	GLU	2.2
2	B	137	GLU	2.2
1	J	126	ALA	2.2
1	J	99	LYS	2.2
3	L	141	GLN	2.1
1	G	10	TRP	2.1

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	CSO	C	133	7/8	0.96	0.07	10,11,14,17	1
3	CSD	F	131	8/9	0.96	0.08	11,13,14,15	2
3	CSD	C	131	8/9	0.97	0.07	9,11,13,13	2
3	CSO	F	133	7/8	0.97	0.07	11,13,16,17	1
3	CSO	I	133	7/8	0.97	0.06	11,11,13,17	1
3	CSD	L	131	8/9	0.97	0.09	9,11,14,15	2
3	CSO	L	133	7/8	0.97	0.07	9,10,14,14	1
3	CSD	I	131	8/9	0.98	0.07	10,12,13,14	1

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	TLA	I	3003	10/10	0.58	0.37	44,46,50,51	0
5	TLA	E	3002	10/10	0.70	0.26	34,41,46,46	0
5	TLA	L	3004	10/10	0.70	0.27	32,36,39,41	0
5	TLA	C	3001	10/10	0.75	0.22	27,31,31,35	0
4	3CO	F	301	1/1	0.98	0.03	14,14,14,14	1
4	3CO	I	301	1/1	0.99	0.04	7,7,7,7	1
4	3CO	L	301	1/1	0.99	0.03	9,9,9,9	1
4	3CO	C	301	1/1	0.99	0.08	6,6,6,6	1

6.5 Other polymers [i](#)

There are no such residues in this entry.