



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 03:06 PM GMT

PDB ID : 2DXC
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 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/ValidationPDFNotes.html>

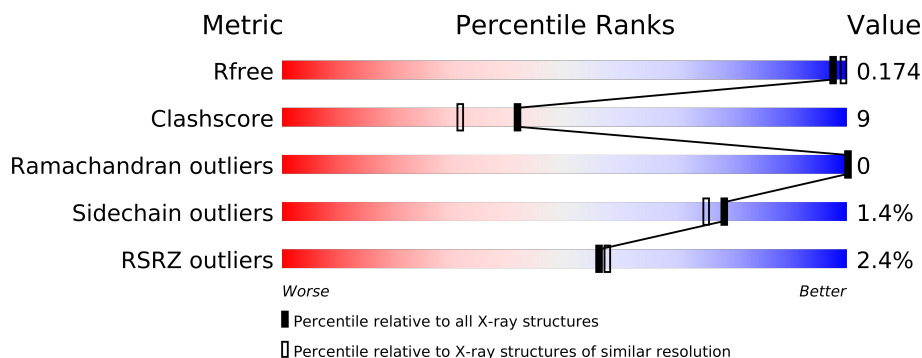
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	3684 (1.90-1.90)
Clashscore	79885	4465 (1.90-1.90)
Ramachandran outliers	78287	4413 (1.90-1.90)
Sidechain outliers	78261	4414 (1.90-1.90)
RSRZ outliers	66119	3686 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	126	
1	D	126	
1	G	126	
1	J	126	
2	B	157	
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 that are outliers for geometric or electron-

density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
5	TLA	C	3001	-	X
5	TLA	E	3002	-	X
5	TLA	I	3003	-	X
5	TLA	L	3004	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 18283 atoms, of which 0 are hydrogen and 0 are deuterium.

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			

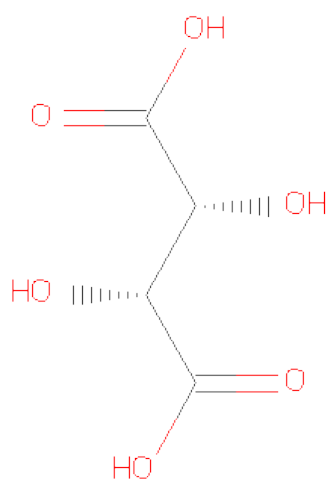
- Molecule 3 is a protein called Thiocyanate hydrolase subunit gamma.

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 (three-letter code: 3CO) (formula: Co).

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

- Molecule 5 is L(+)-TARTARIC ACID (three-letter code: TLA) (formula: C₄H₆O₆).



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

- Molecule 6 is water.

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

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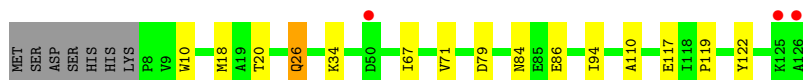
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	205	Total 205	O 205	0	0
6	C	300	Total 300	O 300	0	0
6	D	156	Total 156	O 156	0	0
6	E	190	Total 190	O 190	0	0
6	F	248	Total 248	O 248	0	0
6	G	150	Total 150	O 150	0	0
6	H	200	Total 200	O 200	0	0
6	I	302	Total 302	O 302	0	0
6	J	168	Total 168	O 168	0	0
6	K	196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

3 Residue-property plots

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.

- Molecule 1: Thiocyanate hydrolase subunit alpha

Chain A: 



- Molecule 1: Thiocyanate hydrolase subunit alpha

Chain D: 



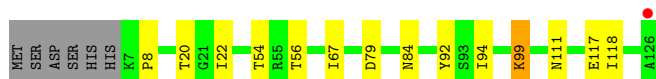
- Molecule 1: Thiocyanate hydrolase subunit alpha

Chain G: 



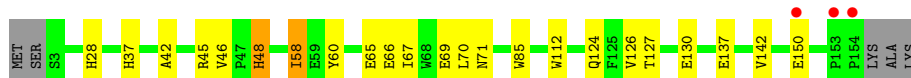
- Molecule 1: Thiocyanate hydrolase subunit alpha

Chain J: 



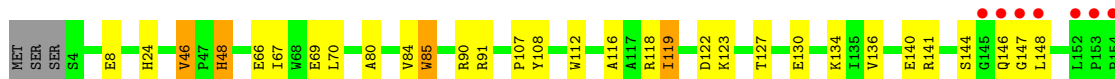
- Molecule 2: Thiocyanate hydrolase subunit beta

Chain B: 



- Molecule 2: Thiocyanate hydrolase subunit beta

Chain E: 



LYS
ALA
LYS

- Molecule 2: Thiocyanate hydrolase subunit beta

Chain H:

MET S2 S3 R11 H28 A31 P32 I35 L39 F40 R41 R45 V46 V47 H48 V56 P57 I58 E59 Y60 E66 E69 A80 W85 R90 R91 C96 Q100 W112 A116 I119 L148 K155 A156 K157

- Molecule 2: Thiocyanate hydrolase subunit beta

Chain K:

MET SER S3 I5 R6 E7 H12 H24 V46 F47 H48 D55 E66 E69 L70 A80 V84 W85 R90 C96 Y109 W112 I119 K123 Q124 K134 I135 V136 E137 M138 E140 S144 G145 Q146 G147 L148 L152 P153 P154 LYS ALA

LYS

- Molecule 3: Thiocyanate hydrolase subunit gamma

Chain C:

MET SER ALA ASP HIS HIS ASP HIS HIS ASP HIS HIS ASP ASP PRO ALA PRO MET VAL E23 V24 I29 E36 E40 K53 D54 T58 R66 T102 Q103 F104 G105 T106 D109 Y110 C111 N112 L113 K123 V127 C128 L129 C131 S132 C133 Y134 M150 Y151 R152 L155 Q161 P171 V174 Q175 I176 R177 I188 D198 I215 K221 I224 V239 HIS HIS ASP HIS

- Molecule 3: Thiocyanate hydrolase subunit gamma

Chain F:

MET SER ALA ASP HIS HIS ASP HIS HIS ASP HIS HIS ASP ASP PRO ALA PRO MET VAL GLU V24 K32 L37 H49 K53 L62 P63 L67 T102 Q103 F104 V115 V126 V127 C128 T129 L130 C131 S132 C133 S142 R147 R152 R153 R154 L155 V156 R157 W158 Q161 E165 L170 P171 V174 Q175 I176 R177 I188 E195 D198 G199 W200 T201 Q204 E207 T225 P238 V239 HIS HIS ASP HIS

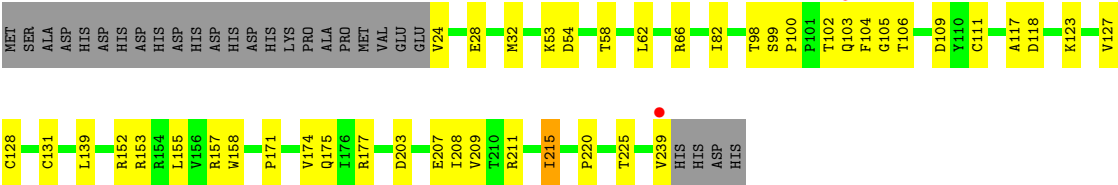
- Molecule 3: Thiocyanate hydrolase subunit gamma

Chain I:

MET SER ALA ASP HIS HIS ASP HIS HIS ASP HIS HIS ASP ASP PRO ALA PRO MET VAL GLU E23 M32 D54 H57 T58 L62 R66 L67 S99 P100 P101 T102 Q103 L113 R114 V115 V127 C128 T129 L130 C131 S132 C133 N150 Y151 R152 L155 R160 P171 V174 Q175 I176 R177 I188 E207 K221 I224 T225 V239 HIS HIS ASP HIS

- Molecule 3: Thiocyanate hydrolase subunit gamma

Chain L:



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 0.174 , 0.174	Depositor DCC
R_{free} test set	13233 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	14.8	Xtriage
Anisotropy	0.481	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 39.9	EDS
Estimated twinning fraction	0.013 for -h,l,k	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 263388 reflections	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.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CSO, CSD, 3CO, 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	0.33	0/991	0.62	0/1342
1	D	0.33	0/991	0.62	0/1342
1	G	0.33	0/1000	0.59	0/1354
1	J	0.34	0/1000	0.61	0/1354
2	B	0.32	0/1264	0.60	0/1720
2	E	0.30	0/1258	0.58	0/1712
2	H	0.30	0/1294	0.58	0/1757
2	K	0.31	0/1264	0.57	0/1720
3	C	0.29	0/1752	0.60	0/2391
3	F	0.29	0/1743	0.59	0/2379
3	I	0.29	0/1752	0.59	0/2391
3	L	0.29	0/1743	0.61	0/2379
All	All	0.31	0/16052	0.60	0/21841

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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	14	0
1	J	974	0	926	15	0
2	B	1232	0	1198	26	0
2	E	1226	0	1193	33	0
2	H	1262	0	1234	31	0
2	K	1232	0	1198	24	0
3	C	1724	0	1735	31	0
3	F	1715	0	1729	45	0
3	I	1724	0	1735	37	0
3	L	1715	0	1729	39	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	5	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	0	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	284	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 9.

All (284) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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:HE21	1:A:26:GLN:H	1.03	0.95
2:K:112:TRP:HZ2	5:L:3004:TLA:HB	0.94	0.91

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:K:134:LYS:HD2	2:K:138:MET:HE2	1.62	0.82
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:O	2:E:119:ILE:HD13	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:NE2	1:A:26:GLN:H	1.80	0.77
2:B:28:HIS:HD2	3:L:153:ARG:HH12	1.32	0.76
1:A:26:GLN:N	1:A:26:GLN:HE21	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
5:E:3002:TLA:HA	3:F:131:CSD:HD2	1.39	0.70
2:H:148:LEU:HG	3:I:32:MET:HE2	1.73	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
3:I:188:ILE:HD13	3:I:188:ILE:H	1.61	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:221:LYS:HB2	3:C:224:ILE:HD13	1.77	0.65
3:I:62:LEU:HD23	6:I:3026:HOH:O	1.96	0.65
1:G:45:ILE:HD11	1:G:118:ILE:HD13	1.79	0.65
2:H:58:ILE:H	2:H:58:ILE:HD13	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:N	2:H:35:ILE:HD12	2.12	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: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
2:K:5:ILE:H	2:K:5:ILE:HD12	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:170:LEU:CD1	3:F:176:ILE:HD11	2.29	0.63
1:A:86:GLU:H	1:A:86:GLU:CD	2.02	0.63
3:F:142:SER:OG	3:F:147:ARG:HD3	1.98	0.63
3:F:115:VAL:HG13	3:F:188:ILE:HD11	1.81	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
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:N	3:I:188:ILE:HD13	2.16	0.61
3:F:170:LEU:HD13	3:F:176:ILE:CD1	2.29	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
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: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:H:112:TRP:CZ2	5:I:3003:TLA:O3	2.57	0.57
3:F:238:PRO:O	3:F:239:VAL:HB	2.04	0.57
2:E:90:ARG:NH1	5:E:3002:TLA:O4	2.38	0.57
2:H:90:ARG:HH12	5:I:3003:TLA:H3	1.70	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:58:ILE:HD12	3:I:150:ASN:CG	2.25	0.56
1:D:43:VAL:CG1	1:D:67:ILE:HD11	2.35	0.56
3:L:139:LEU:HD21	3:L:215:ILE:HD11	1.86	0.56
2:B:71:ASN:HD21	3:C:53:LYS:NZ	2.02	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
3:L:208:ILE:HD12	3:L:208:ILE:C	2.27	0.56
2:B:126:VAL:HG12	2:B:127:THR:O	2.06	0.55
2:B:58:ILE:CD1	2:B:58:ILE:H	2.18	0.55
3:C:221:LYS:CB	3:C:224:ILE:HD13	2.37	0.55
2:H:148:LEU:HG	3:I:32:MET:CE	2.37	0.55
2:K:5:ILE:N	2:K:5:ILE:HD12	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:G:111:ASN:O	3:I:175:GLN:HG3	2.07	0.54
1:D:53:TYR:HA	2:E:46:VAL:HG11	1.90	0.54
2:K:148:LEU:HG	3:L:32:MET:HG3	1.89	0.53
2:B:58:ILE:HD12	3:C:150:ASN:CG	2.28	0.53
1:G:54:THR:HG22	2:H:46:VAL:HG21	1.89	0.53
2:E:144:SER:OG	2:E:146:GLN:HG3	2.07	0.53
3:F:131:CSD:O	3:F:152:ARG:HD3	2.09	0.53
3:C:127:VAL:HG22	3:C:128:CYS:N	2.23	0.53
1:J:111:ASN:O	3:L:175:GLN:HG3	2.09	0.53
2:E:148:LEU:HD13	3:F:32:MET:HG3	1.91	0.53
3:L:139:LEU:HD21	3:L:215:ILE:CD1	2.39	0.53
3:F:127:VAL:HG22	3:F:128:CYS:N	2.23	0.52
3:I:171:PRO:HB2	3:I:174:VAL:HG23	1.92	0.52
1:A:10:TRP:CZ3	1:J:8:PRO:HG2	2.44	0.52
3:L:207:GLU:HG2	3:L:225:THR:CG2	2.39	0.52
3:F:171:PRO:HB2	3:F:174:VAL:HG23	1.90	0.52
2:H:41:ARG:HG2	2:K:12:HIS:CD2	2.45	0.52
2:H:112:TRP:HZ2	5:I:3003:TLA:HB	1.52	0.52
1:G:94:ILE:HD12	1:G:118:ILE:HD12	1.92	0.52
2:B:58:ILE:N	2:B:58:ILE:HD13	2.15	0.52
3:I:221:LYS:HD2	3:I:224:ILE:HD12	1.92	0.52
2:E:119:ILE:C	2:E:119:ILE:HD13	2.30	0.52
3:I:23:GLU:HG2	3:I:23:GLU:O	2.10	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:F:129:THR:O	3:F:152:ARG:HD2	2.09	0.51
3:L:102:THR:O	3:L:103:GLN:HB2	2.08	0.51
2:B:58:ILE:CD1	2:B:58:ILE:N	2.72	0.51
2:B:58:ILE:HD11	2:B:60:TYR:CZ	2.45	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
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:K:136:VAL:O	2:K:140:GLU:HG3	2.11	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
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:N	2:H:58:ILE:HD13	2.26	0.50
3:C:131:CSD:O	3:C:152:ARG:HD2	2.12	0.50
3:F:103:GLN:HG3	6:F:319:HOH:O	2.11	0.49
1:D:117:GLU:O	1:D:118:ILE:HD13	2.12	0.49
3:F:115:VAL:HG13	3:F:188:ILE:CD1	2.41	0.49
1:D:43:VAL:CG2	1:D:67:ILE:HD11	2.42	0.49
3:F:62:LEU:HB3	3:F:63:PRO:HD3	1.94	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:C:123:LYS:HG3	3:C:170:LEU:HD21	1.93	0.49
2:E:90:ARG:HH22	5:E:3002:TLA:H2	1.78	0.48
2:B:126:VAL:HG13	2:B:130:GLU:HB2	1.95	0.48
1:A:119:PRO:HG2	1:A:122:TYR:HD2	1.78	0.48
2:E:107:PRO:HG3	2:H:35:ILE:HD11	1.95	0.48
3:I:131:CSD:O	3:I:152:ARG:HD2	2.13	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
3:I:62:LEU:N	3:I:62:LEU:HD22	2.29	0.48
2:E:107:PRO:HG3	2:H:35:ILE:CD1	2.44	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
2:E:91:ARG:HD3	3:F:131:CSD:OD2	2.15	0.47
3:F:67:LEU:C	3:F:67:LEU:HD23	2.34	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
2:K:119:ILE:HD13	2:K:119:ILE:C	2.35	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:K:46:VAL:CG1	2:K:96:CYS:SG	3.02	0.47
1:A:84:ASN:ND2	2:K:124:GLN:HE21	2.12	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
2:E:118:ARG:HG3	2:E:122:ASP:OD2	2.15	0.46
1:G:117:GLU:C	1:G:118:ILE:HG13	2.35	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
1:G:86:GLU:CD	1:G:86:GLU:H	2.18	0.46
3:I:99:SER:HB2	3:I:100:PRO:HD3	1.98	0.46
2:H:48:HIS:HB2	3:I:130:LEU:O	2.16	0.46
2:B:65:GLU:OE1	2:B:70:LEU:HB2	2.16	0.46
1:D:67:ILE:HD12	1:D:67:ILE:N	2.31	0.46
3:L:62:LEU:O	3:L:66:ARG:HG2	2.15	0.45
1:J:94:ILE:N	1:J:94:ILE:HD12	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
3:I:113:LEU:HD11	3:I:188:ILE:CD1	2.19	0.45
1:A:79:ASP:HA	6:A:313:HOH:O	2.17	0.45
3:I:207:GLU:HG2	3:I:225:THR:CG2	2.46	0.45
3:F:201:THR:OG1	3:F:204:GLN:HG3	2.16	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
3:F:188:ILE:HD12	3:F:188:ILE:C	2.37	0.44
3:L:171:PRO:HB2	3:L:174:VAL:HG23	1.98	0.44
3:L:131:CSD:HB3	5:L:3004:TLA:O41	2.18	0.44
3:F:127:VAL:HB	3:F:155:LEU:HD23	2.00	0.43
6:D:246:HOH:O	1:G:7:LYS:HB2	2.17	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
2:H:28:HIS:N	2:H:28:HIS:ND1	2.66	0.43
3:C:161:GLN:HG2	6:F:426:HOH:O	2.19	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:E:116:ALA:O	2:E:119:ILE:HG22	2.18	0.43
3:L:175:GLN:NE2	3:L:177:ARG:HH21	2.09	0.43
1:G:41:ASP:HB2	1:G:67:ILE:HD12	1.99	0.43
1:J:99:LYS:NZ	1:J:99:LYS:HB2	2.34	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
2:K:90:ARG:HH12	5:L:3004:TLA:H3	1.83	0.43
3:F:126:VAL:HG12	3:F:127:VAL:N	2.33	0.43
3:L:98:THR:HA	3:L:103:GLN:OE1	2.19	0.43
1:A:86:GLU:N	1:A:86:GLU:CD	2.71	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
3:F:132:SER:O	3:F:133:CSO:C	2.67	0.42
2:E:80:ALA:HA	2:E:85:TRP:O	2.19	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
3:F:171:PRO:HD2	3:F:174:VAL:HG21	2.01	0.42
2:B:112:TRP:CZ2	5:C:3001:TLA:C3	3.03	0.42
3:C:36:GLU:O	3:C:40:GLU:HB2	2.19	0.42
3:F:157:ARG:HD3	3:F:158:TRP:CH2	2.54	0.42
2:B:48:HIS:HB2	3:C:130:LEU:O	2.18	0.42
2:E:127:THR:OG1	2:E:130:GLU:HG3	2.20	0.42
3:I:67:LEU:HD23	3:I:67:LEU:C	2.39	0.42
1:D:114:LEU:HD23	1:D:114:LEU:C	2.40	0.42
3:I:175:GLN:HE22	3:I:177:ARG:NH2	2.12	0.42
2:H:80:ALA:HA	2:H:85:TRP:O	2.20	0.42
2:H:11:ARG:HD3	6:K:320:HOH:O	2.20	0.42
3:L:215:ILE:CD1	3:L:215:ILE:N	2.82	0.42
2:B:124:GLN:HE21	1:J:84:ASN:ND2	2.18	0.42
3:I:114:ARG:O	3:I:188:ILE:HD13	2.20	0.41
3:F:175:GLN:NE2	3:F:177:ARG:HH11	2.10	0.41
2:H:56:VAL:HG12	2:K:55:ASP:C	2.41	0.41
2:H:39:LEU:HD12	2:H:39:LEU:HA	1.92	0.41
3:C:106:THR:OG1	3:C:109:ASP:HB2	2.20	0.41
3:L:118:ASP:OD2	3:L:123:LYS:HD2	2.20	0.41
1:J:20:THR:HA	3:L:104:PHE:HB3	2.01	0.41
1:G:7:LYS:HB2	1:G:8:PRO:HD3	2.01	0.41
1:J:67:ILE:HD12	1:J:92:TYR:CB	2.48	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:113:LEU:HD11	3:C:188:ILE:HG12	2.03	0.41
2:E:67:ILE:HD11	3:F:239:VAL:CA	2.51	0.41
2:K:69:GLU:HB3	2:K:109:TYR:CD1	2.56	0.41
3:C:106:THR:HG1	3:C:109:ASP:HB2	1.85	0.41
2:E:136:VAL:O	2:E:140:GLU:HG3	2.20	0.41
3:L:208:ILE:C	3:L:208:ILE:CD1	2.88	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
6:C:3155:HOH:O	3:F:161:GLN:HG2	2.20	0.41
2:B:137:GLU:HB3	6:B:228:HOH:O	2.21	0.41
3:I:127:VAL:HB	3:I:155:LEU:HD23	2.03	0.41
2:H:116:ALA:O	2:H:119:ILE:HG22	2.21	0.41
3:L:157:ARG:HD3	3:L:158:TRP:CH2	2.56	0.41
3:L:99:SER:N	3:L:100:PRO:CD	2.84	0.41
2:B:58:ILE:HD12	3:C:150:ASN:ND2	2.36	0.41
3:C:221:LYS:HE2	6:C:3214:HOH:O	2.21	0.40
2:E:108:TYR:CZ	3:F:147:ARG:HD2	2.56	0.40
1:D:43:VAL:HG22	1:D:67:ILE:HD11	2.03	0.40
3:C:54:ASP:O	3:C:58:THR:HG23	2.21	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:F:102:THR:HB	3:F:104:PHE:CE2	2.56	0.40
3:I:160:ARG:CD	3:I:176:ILE:HD12	2.52	0.40
1:G:7:LYS:N	1:G:8:PRO:CD	2.84	0.40
3:C:66:ARG:HD2	6:C:3116:HOH:O	2.21	0.40
1:J:92:TYR:O	1:J:94:ILE:HD12	2.21	0.40
2:E:48:HIS:HB2	3:F:130:LEU:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	117/126 (93%)	111 (95%)	6 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	68	61
1	D	101/108 (94%)	100 (99%)	1 (1%)	85	84
1	G	102/108 (94%)	102 (100%)	0	100	100
1	J	102/108 (94%)	101 (99%)	1 (1%)	85	84
2	B	130/134 (97%)	126 (97%)	4 (3%)	52	41
2	E	129/134 (96%)	125 (97%)	4 (3%)	52	41
2	H	133/134 (99%)	129 (97%)	4 (3%)	53	42
2	K	130/134 (97%)	127 (98%)	3 (2%)	63	55
3	C	188/212 (89%)	187 (100%)	1 (0%)	94	94
3	F	187/212 (88%)	187 (100%)	0	100	100
3	I	188/212 (89%)	186 (99%)	2 (1%)	84	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	L	187/212 (88%)	186 (100%)	1 (0%)	94	94
All	All	1678/1816 (92%)	1655 (99%)	23 (1%)	78	75

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	MET
1	A	26	GLN
2	B	48	HIS
2	B	58	ILE
2	B	85	TRP
2	B	150	GLU
3	C	198	ASP
1	D	25	PRO
2	E	46	VAL
2	E	48	HIS
2	E	85	TRP
2	E	119	ILE
2	H	39	LEU
2	H	48	HIS
2	H	58	ILE
2	H	85	TRP
3	I	66	ARG
3	I	188	ILE
1	J	99	LYS
2	K	48	HIS
2	K	85	TRP
2	K	119	ILE
3	L	215	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	84	ASN
1	A	111	ASN
2	B	28	HIS
2	B	37	HIS
2	B	71	ASN
2	B	100	GLN
2	B	124	GLN

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Mol	Chain	Res	Type
3	C	141	GLN
3	C	175	GLN
1	D	84	ASN
2	E	94	GLN
2	E	100	GLN
2	E	124	GLN
2	E	146	GLN
3	F	49	HIS
3	F	175	GLN
1	G	14	HIS
1	G	87	ASN
2	H	61	HIS
2	H	100	GLN
2	H	146	GLN
3	I	112	ASN
3	I	124	HIS
3	I	141	GLN
3	I	169	GLN
3	I	175	GLN
3	I	236	ASN
2	K	12	HIS
2	K	24	HIS
2	K	100	GLN
2	K	146	GLN
3	L	112	ASN
3	L	175	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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	CSD	C	131	4	7,7,8	6.82	3 (42%)	6,8,10	2.64	3 (50%)
3	CSO	C	133	4	6,6,7	7.24	2 (33%)	3,6,8	1.72	1 (33%)
3	CSD	F	131	4	7,7,8	6.96	3 (42%)	6,8,10	3.19	3 (50%)
3	CSO	F	133	4	6,6,7	7.24	3 (50%)	3,6,8	1.66	1 (33%)
3	CSD	I	131	4	7,7,8	6.84	3 (42%)	6,8,10	2.69	2 (33%)
3	CSO	I	133	4	6,6,7	7.40	3 (50%)	3,6,8	1.48	0
3	CSD	L	131	4	7,7,8	6.79	3 (42%)	6,8,10	2.93	2 (33%)
3	CSO	L	133	4	6,6,7	7.39	3 (50%)	3,6,8	1.53	1 (33%)

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	CSD	C	131	4	-	0/3/6/8	0/0/0/0
3	CSO	C	133	4	-	0/2/5/7	0/0/0/0
3	CSD	F	131	4	-	0/3/6/8	0/0/0/0
3	CSO	F	133	4	-	0/2/5/7	0/0/0/0
3	CSD	I	131	4	-	0/3/6/8	0/0/0/0
3	CSO	I	133	4	-	0/2/5/7	0/0/0/0
3	CSD	L	131	4	-	0/3/6/8	0/0/0/0
3	CSO	L	133	4	-	0/2/5/7	0/0/0/0

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	131	CSD	O-C	17.84	1.23	1.11
3	L	133	CSO	O-C	17.69	1.23	1.11
3	I	133	CSO	O-C	17.68	1.23	1.11
3	C	131	CSD	O-C	17.54	1.23	1.11
3	I	131	CSD	O-C	17.41	1.23	1.11
3	L	131	CSD	O-C	17.38	1.23	1.11
3	C	133	CSO	O-C	17.34	1.23	1.11
3	F	133	CSO	O-C	17.28	1.23	1.11
3	I	131	CSD	OD1-SG	-3.98	1.42	1.47
3	F	131	CSD	OD1-SG	-3.75	1.42	1.47
3	L	131	CSD	OD1-SG	-3.59	1.42	1.47
3	C	131	CSD	OD1-SG	-3.33	1.43	1.47
3	C	133	CSO	OD-SG	-3.07	1.49	1.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	133	CSO	OD-SG	-2.97	1.49	1.62
3	L	133	CSO	OD-SG	-2.86	1.50	1.62
3	I	133	CSO	OD-SG	-2.83	1.50	1.62
3	I	131	CSD	CA-C	2.51	1.53	1.48
3	I	133	CSO	CA-C	2.47	1.52	1.48
3	L	133	CSO	CA-C	2.39	1.52	1.48
3	F	133	CSO	CA-C	2.38	1.52	1.48
3	L	131	CSD	CA-C	2.35	1.52	1.48
3	F	131	CSD	CA-C	2.28	1.52	1.48
3	C	131	CSD	CA-C	2.25	1.52	1.48

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	131	CSD	C-CA-N	6.31	120.13	113.83
3	L	131	CSD	C-CA-N	5.94	119.76	113.83
3	I	131	CSD	C-CA-N	5.10	118.92	113.83
3	C	131	CSD	C-CA-N	4.66	118.49	113.83
3	L	131	CSD	OD2-SG-CB	3.00	109.51	97.42
3	I	131	CSD	OD2-SG-CB	2.99	109.46	97.42
3	C	131	CSD	OD2-SG-CB	2.90	109.08	97.42
3	F	131	CSD	OD2-SG-CB	2.85	108.88	97.42
3	F	131	CSD	CB-CA-N	2.60	114.34	110.16
3	C	131	CSD	CB-CA-N	2.50	114.18	110.16
3	C	133	CSO	C-CA-N	-2.16	111.67	113.83
3	L	133	CSO	CB-CA-N	2.13	113.88	110.27
3	F	133	CSO	C-CA-N	-2.01	111.82	113.83

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates 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	C	3001	-	9,9,9	1.89	3 (33%)	12,12,12	0.80	0
5	TLA	E	3002	-	9,9,9	1.80	3 (33%)	12,12,12	0.83	0
5	TLA	I	3003	-	9,9,9	2.01	4 (44%)	12,12,12	0.90	0
5	TLA	L	3004	-	9,9,9	1.93	2 (22%)	12,12,12	0.81	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	C	3001	-	-	0/12/12/12	0/0/0/0
5	TLA	E	3002	-	-	0/12/12/12	0/0/0/0
5	TLA	I	3003	-	-	0/12/12/12	0/0/0/0
5	TLA	L	3004	-	-	0/12/12/12	0/0/0/0

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	I	3003	TLA	O2-C2	3.57	1.49	1.42
5	L	3004	TLA	O2-C2	3.39	1.49	1.42
5	C	3001	TLA	O2-C2	3.16	1.48	1.42
5	E	3002	TLA	O1-C1	2.61	1.31	1.22
5	E	3002	TLA	O2-C2	2.56	1.47	1.42
5	I	3003	TLA	O1-C1	2.42	1.30	1.22
5	L	3004	TLA	O1-C1	2.41	1.30	1.22
5	C	3001	TLA	O1-C1	2.31	1.30	1.22
5	C	3001	TLA	O11-C1	-2.24	1.22	1.30
5	I	3003	TLA	C3-C4	-2.12	1.49	1.52
5	E	3002	TLA	O11-C1	-2.08	1.22	1.30
5	I	3003	TLA	C2-C1	2.03	1.55	1.52

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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%)	-0.18	3 (2%) 54 56	9, 15, 31, 36	0
1	D	119/126 (94%)	-0.23	3 (2%) 54 56	9, 13, 29, 31	0
1	G	120/126 (95%)	-0.19	2 (1%) 67 69	9, 15, 29, 41	0
1	J	120/126 (95%)	-0.33	1 (0%) 83 85	9, 12, 27, 42	0
2	B	152/157 (96%)	-0.30	3 (1%) 62 63	8, 12, 26, 31	0
2	E	151/157 (96%)	-0.18	7 (4%) 31 31	8, 13, 31, 40	0
2	H	156/157 (99%)	-0.20	6 (3%) 38 40	8, 12, 26, 56	0
2	K	152/157 (96%)	-0.22	8 (5%) 25 26	8, 12, 28, 39	0
3	C	217/243 (89%)	-0.25	3 (1%) 72 74	8, 13, 25, 44	0
3	F	216/243 (88%)	-0.07	5 (2%) 57 59	9, 16, 30, 39	0
3	I	217/243 (89%)	-0.26	3 (1%) 72 74	8, 13, 23, 42	0
3	L	216/243 (88%)	-0.26	2 (0%) 81 83	8, 13, 26, 40	0
All	All	1955/2104 (92%)	-0.22	46 (2%) 56 57	8, 13, 27, 56	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	239	VAL	7.0
2	H	157	LYS	6.9
2	H	156	ALA	5.6
3	I	239	VAL	5.6
3	L	239	VAL	5.4
3	F	239	VAL	5.3
2	H	2	SER	4.0
2	K	3	SER	3.9
2	H	155	LYS	3.7
2	B	150	GLU	3.6
2	H	3	SER	3.6

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Mol	Chain	Res	Type	RSRZ
1	G	126	ALA	3.5
3	I	23	GLU	3.4
2	H	28	HIS	3.3
3	C	23	GLU	3.2
2	E	152	LEU	3.0
1	A	126	ALA	3.0
1	A	125	LYS	2.8
2	K	146	GLN	2.8
2	K	153	PRO	2.7
2	K	154	PRO	2.6
1	D	126	ALA	2.6
2	E	147	GLY	2.6
2	E	153	PRO	2.5
2	E	146	GLN	2.5
3	F	198	ASP	2.5
3	F	103	GLN	2.4
2	B	154	PRO	2.4
2	K	152	LEU	2.4
2	E	145	GLY	2.4
2	E	148	LEU	2.3
3	L	103	GLN	2.3
3	I	57	HIS	2.2
3	F	199	GLY	2.2
1	D	34	LYS	2.2
2	K	144	SER	2.2
1	D	50	ASP	2.1
2	B	153	PRO	2.1
2	E	154	PRO	2.1
1	G	34	LYS	2.1
1	A	50	ASP	2.1
2	K	145	GLY	2.1
1	J	126	ALA	2.1
2	K	147	GLY	2.0
3	C	198	ASP	2.0
3	F	195	GLU	2.0

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

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	CSO	I	133	7/8	0.13	0.64	11,11,13,17	1
3	CSD	C	131	8/9	0.11	-0.19	9,11,13,13	2
3	CSD	L	131	8/9	0.09	-0.27	9,11,14,15	2
3	CSD	F	131	8/9	0.10	-0.43	11,13,14,15	2
3	CSO	C	133	7/8	0.11	-0.62	10,11,14,17	1
3	CSO	L	133	7/8	0.09	-0.66	9,10,14,14	1
3	CSD	I	131	8/9	0.09	-1.06	10,12,13,14	1
3	CSO	F	133	7/8	0.10	-1.12	11,13,16,17	1

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	TLA	L	3004	10/10	0.38	22.00	32,36,39,41	0
5	TLA	E	3002	10/10	0.41	20.16	34,41,46,46	0
5	TLA	I	3003	10/10	0.51	18.55	44,46,50,51	0
5	TLA	C	3001	10/10	0.30	10.06	27,31,31,35	0
4	3CO	C	301	1/1	0.04	-2.96	6,6,6,6	1
4	3CO	L	301	1/1	0.04	-2.99	9,9,9,9	1
4	3CO	F	301	1/1	0.09	-3.40	14,14,14,14	1
4	3CO	I	301	1/1	0.04	-3.81	7,7,7,7	1

6.5 Other polymers

There are no such residues in this entry.