



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:33 AM GMT

PDB ID : 2DD5
Title : Thiocyanate hydrolase (SCNase) from Thiobacillus thioparus native holo-enzyme
Authors : Arakawa, T.; Kawano, Y.; Kataoka, S.; Katayama, Y.; Kamiya, N.; Yohda, M.; Odaka, M.
Deposited on : 2006-01-19
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

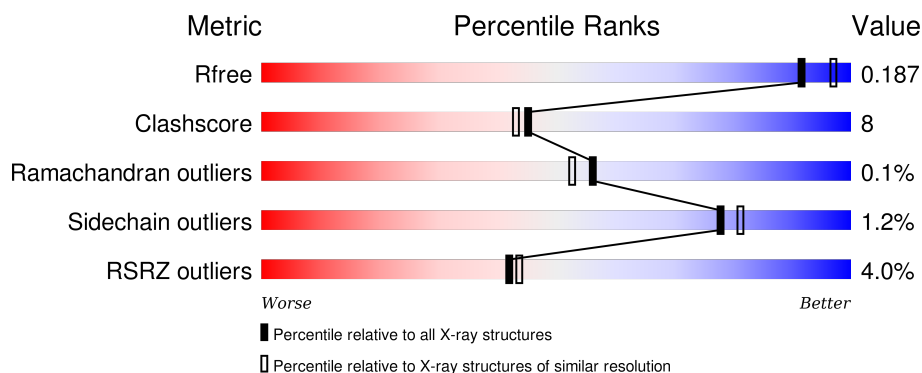
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	126	<div> <div>2%</div> <div>82% 12% 6%</div> </div>
1	D	126	<div> <div>6%</div> <div>84% 10% 6%</div> </div>
1	G	126	<div> <div>5%</div> <div>86% 10% 5%</div> </div>
1	J	126	<div> <div>4%</div> <div>89% 6% 5%</div> </div>
2	B	157	<div> <div>7%</div> <div>76% 20% ..</div> </div>

Continued on next page...

Continued from previous page...

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	SO4	I	3011	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 17962 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 alpha subunit.

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			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	INITIATING METHIONINE	UNP O66187
D	1	MET	-	INITIATING METHIONINE	UNP O66187
G	1	MET	-	INITIATING METHIONINE	UNP O66187
J	1	MET	-	INITIATING METHIONINE	UNP O66187

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

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			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	INITIATING METHIONINE	UNP O66186
E	1	MET	-	INITIATING METHIONINE	UNP O66186
H	1	MET	-	INITIATING METHIONINE	UNP O66186
K	1	MET	-	INITIATING METHIONINE	UNP O66186

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

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

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1	MET	-	INITIATING METHIONINE	UNP O66188
C	131	CSD	CYS	MODIFIED RESIDUE	UNP O66188
C	133	CSO	CYS	MODIFIED RESIDUE	UNP O66188
F	1	MET	-	INITIATING METHIONINE	UNP O66188
F	131	CSD	CYS	MODIFIED RESIDUE	UNP O66188
F	133	CSO	CYS	MODIFIED RESIDUE	UNP O66188
I	1	MET	-	INITIATING METHIONINE	UNP O66188
I	131	CSD	CYS	MODIFIED RESIDUE	UNP O66188
I	133	CSO	CYS	MODIFIED RESIDUE	UNP O66188
L	1	MET	-	INITIATING METHIONINE	UNP O66188
L	131	CSD	CYS	MODIFIED RESIDUE	UNP O66188
L	133	CSO	CYS	MODIFIED RESIDUE	UNP O66188

- Molecule 4 is COBALT (III) ION (three-letter code: 3CO) (formula: Co).

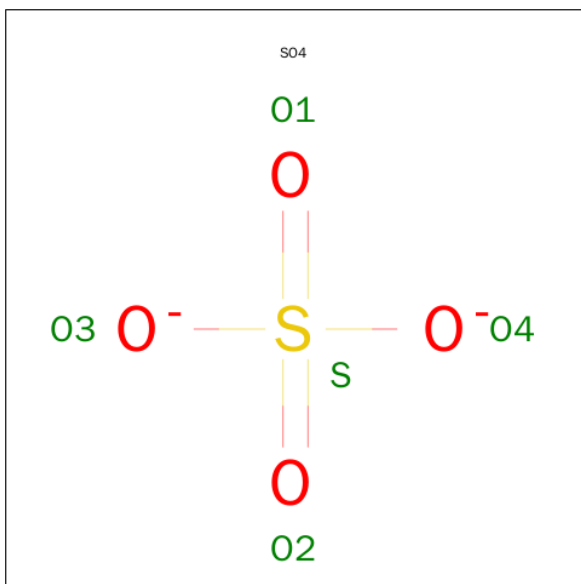
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	I	1	Total	Co	1	0
			1	1		
4	L	1	Total	Co	1	0
			1	1		
4	C	1	Total	Co	1	0
			1	1		

Continued on next page...

Continued from previous page...

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

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	O	S	0	0
			5	4	1		
5	F	1	Total	O	S	0	0
			5	4	1		
5	I	1	Total	O	S	0	0
			5	4	1		
5	L	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		
5	G	1	Total	O	S	0	0
			5	4	1		
5	J	1	Total	O	S	0	0
			5	4	1		
5	L	1	Total	O	S	0	0
			5	4	1		
5	L	1	Total	O	S	0	0
			5	4	1		

Continued on next page...

Continued from previous page...

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

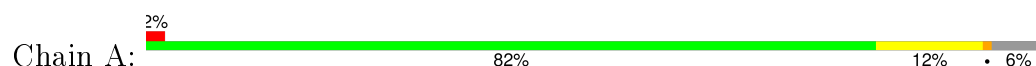
- Molecule 6 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	134	Total	O		0	0
			134	134			
6	B	161	Total	O		0	0
			161	161			
6	C	249	Total	O		0	0
			249	249			
6	D	103	Total	O		0	0
			103	103			
6	E	157	Total	O		0	0
			157	157			
6	F	233	Total	O		0	0
			233	233			
6	G	134	Total	O		0	0
			134	134			
6	H	157	Total	O		0	0
			157	157			
6	I	263	Total	O		0	0
			263	263			
6	J	148	Total	O		0	0
			148	148			
6	K	164	Total	O		0	0
			164	164			
6	L	287	Total	O		0	0
			287	287			

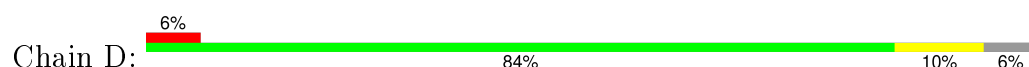
3 Residue-property plots [i](#)

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

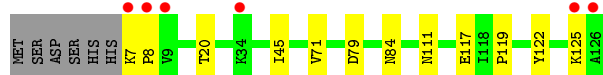
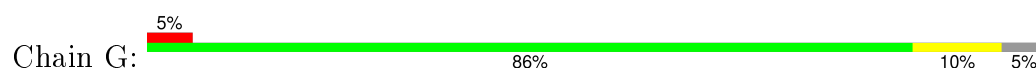
- Molecule 1: Thiocyanate hydrolase alpha subunit



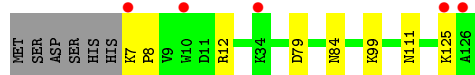
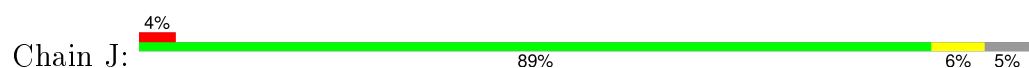
- Molecule 1: Thiocyanate hydrolase alpha subunit



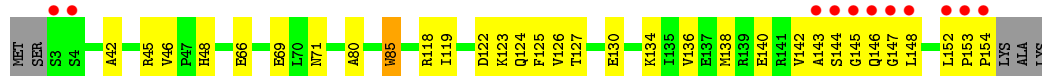
- Molecule 1: Thiocyanate hydrolase alpha subunit



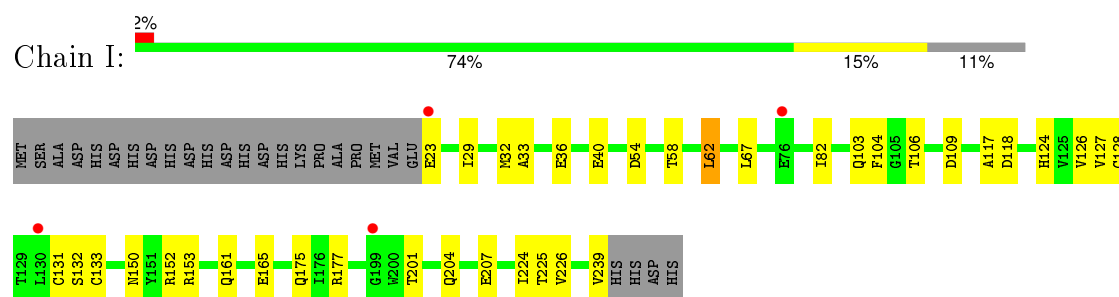
- Molecule 1: Thiocyanate hydrolase alpha subunit



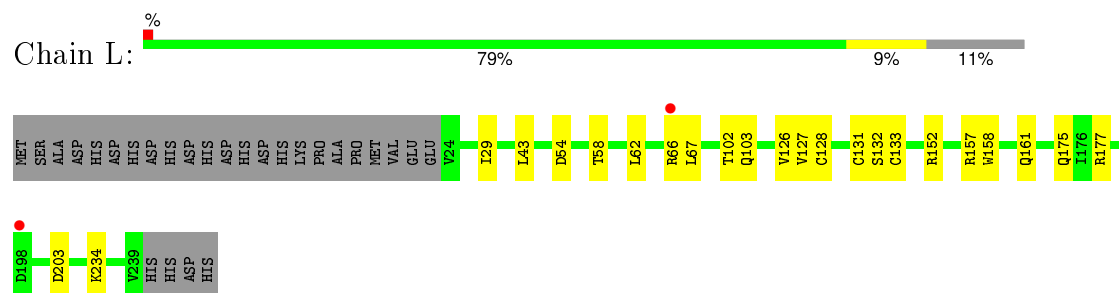
- Molecule 2: Thiocyanate hydrolase beta subunit



- Molecule 2: Thiocyanate hydrolase beta subunit



- Molecule 3: Thiocyanate hydrolase gamma subunit



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	170.19Å 170.19Å 282.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.80 – 2.00 37.80 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.3 (37.80-2.00) 99.9 (37.80-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.99 (at 2.00Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.185 , 0.205 0.187 , 0.187	Depositor DCC
R_{free} test set	13997 reflections (5.32%)	DCC
Wilson B-factor (Å ²)	20.6	Xtriage
Anisotropy	0.019	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 59.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 278076 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	17962	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.89% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CSD, 3CO, CSO, SO4

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	0.61	0/1342
1	D	0.32	0/991	0.59	0/1342
1	G	0.33	0/1000	0.60	0/1354
1	J	0.34	0/1000	0.61	0/1354
2	B	0.31	0/1264	0.58	0/1720
2	E	0.29	0/1258	0.56	0/1712
2	H	0.30	0/1294	0.58	0/1757
2	K	0.32	0/1264	0.59	0/1720
3	C	0.29	0/1752	0.60	0/2391
3	F	0.28	0/1743	0.59	0/2379
3	I	0.30	0/1752	0.61	0/2391
3	L	0.31	0/1743	0.62	0/2379
All	All	0.31	0/16052	0.59	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 Too-close contacts [i](#)

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	23	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	965	0	914	9	0
1	G	974	0	926	10	0
1	J	974	0	926	11	0
2	B	1232	0	1198	30	0
2	E	1226	0	1193	34	0
2	H	1262	0	1234	32	0
2	K	1232	0	1198	17	0
3	C	1724	0	1735	44	0
3	F	1715	0	1729	37	0
3	I	1724	0	1735	34	0
3	L	1715	0	1729	17	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	A	5	0	0	0	0
5	C	5	0	0	0	0
5	D	5	0	0	0	0
5	F	5	0	0	0	0
5	G	5	0	0	0	0
5	I	15	0	0	0	0
5	J	5	0	0	0	0
5	L	15	0	0	0	0
6	A	134	0	0	2	0
6	B	161	0	0	3	0
6	C	249	0	0	3	0
6	D	103	0	0	0	0
6	E	157	0	0	2	0
6	F	233	0	0	3	0
6	G	134	0	0	0	0
6	H	157	0	0	2	0
6	I	263	0	0	3	0
6	J	148	0	0	1	0
6	K	164	0	0	2	0
6	L	287	0	0	1	0
All	All	17962	0	15431	244	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 8.

All (244) 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)
2:H:148:LEU:HB3	3:I:32:MET:SD	2.06	0.95
1:A:26:GLN:HE21	1:A:26:GLN:H	1.01	0.94
3:I:36:GLU:O	3:I:40:GLU:HG3	1.69	0.93
3:I:82:ILE:HD11	3:I:117:ALA:HB2	1.51	0.90
2:B:148:LEU:HD11	3:C:32:MET:HE1	1.56	0.87
2:B:148:LEU:HG	3:C:32:MET:SD	2.16	0.85
2:E:148:LEU:HD11	3:F:32:MET:HE1	1.60	0.82
3:I:175:GLN:HE22	3:I:177:ARG:HH21	1.28	0.80
1:A:84:ASN:HD22	1:J:7:LYS:NZ	1.80	0.79
1:A:26:GLN:N	1:A:26:GLN:HE21	1.79	0.78
1:A:26:GLN:NE2	1:A:26:GLN:H	1.81	0.78
3:C:237:ARG:HH21	3:C:237:ARG:CG	1.98	0.77
2:H:58:ILE:HD11	2:H:60:TYR:CE1	2.20	0.76
3:C:237:ARG:HB2	3:C:237:ARG:HH21	1.50	0.76
6:C:3152:HOH:O	3:F:161:GLN:HG2	1.88	0.73
2:H:67:ILE:HD13	3:I:239:VAL:HA	1.71	0.72
3:C:237:ARG:HH21	3:C:237:ARG:CB	2.02	0.72
3:L:175:GLN:HE22	3:L:177:ARG:HH21	1.38	0.72
3:C:175:GLN:HE22	3:C:177:ARG:HH11	1.37	0.71
2:K:3:SER:O	2:K:7:GLU:HG3	1.90	0.71
2:H:67:ILE:CD1	3:I:239:VAL:HA	2.20	0.71
2:E:148:LEU:HD12	2:E:151:TYR:HB2	1.72	0.71
3:C:237:ARG:NH2	3:C:237:ARG:HB2	2.05	0.70
2:H:147:GLY:C	2:H:148:LEU:HD12	2.12	0.69
2:E:142:VAL:HG22	2:E:148:LEU:HG	1.75	0.69
2:E:124:GLN:HE21	1:G:84:ASN:ND2	1.91	0.68
2:B:148:LEU:CD1	3:C:32:MET:HE1	2.22	0.67
2:H:58:ILE:H	2:H:58:ILE:HD13	1.58	0.67
2:H:142:VAL:N	2:H:148:LEU:HD11	2.10	0.67
3:C:237:ARG:HH21	3:C:237:ARG:HG3	1.59	0.66
2:H:134:LYS:HE3	2:H:138:MET:HE1	1.78	0.66
1:D:11:ASP:OD2	1:D:14:HIS:HB2	1.96	0.66
1:A:86:GLU:H	1:A:86:GLU:CD	1.99	0.65
2:E:24:HIS:ND1	2:K:24:HIS:HD2	1.95	0.64
2:H:134:LYS:HE3	2:H:138:MET:CE	2.28	0.64
1:A:111:ASN:O	3:C:175:GLN:HG3	1.97	0.64
2:K:66:GLU:HB2	2:K:69:GLU:HG3	1.78	0.64
3:F:142:SER:OG	3:F:147:ARG:HD3	1.98	0.63
2:B:66:GLU:HB2	2:B:69:GLU:HG3	1.80	0.63
2:B:124:GLN:HE21	1:J:84:ASN:ND2	1.97	0.62
2:E:67:ILE:HG12	3:F:239:VAL:HB	1.80	0.62
2:E:136:VAL:O	2:E:140:GLU:HG3	2.00	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:82:ILE:CD1	3:I:117:ALA:HB2	2.28	0.61
2:E:148:LEU:HD21	3:F:32:MET:CE	2.30	0.61
2:H:148:LEU:HA	6:H:233:HOH:O	2.00	0.61
2:E:148:LEU:HD11	3:F:32:MET:CE	2.31	0.60
3:I:161:GLN:HG2	6:L:3108:HOH:O	2.00	0.60
2:B:136:VAL:O	2:B:140:GLU:HG3	2.02	0.60
1:G:111:ASN:O	3:I:175:GLN:HG3	2.02	0.59
3:F:238:PRO:O	3:F:239:VAL:HG23	2.02	0.59
1:G:7:LYS:HB2	1:G:8:PRO:HD3	1.83	0.59
1:A:84:ASN:HD22	1:J:7:LYS:HZ1	1.49	0.58
2:H:138:MET:O	2:H:148:LEU:HD21	2.03	0.58
2:B:148:LEU:HG	3:C:32:MET:CE	2.33	0.58
2:B:142:VAL:HG21	3:C:29:ILE:HD11	1.85	0.58
3:C:164:ALA:HB3	3:F:161:GLN:HE21	1.69	0.57
2:H:66:GLU:HB2	2:H:69:GLU:HG3	1.87	0.57
2:H:136:VAL:O	2:H:140:GLU:HG3	2.05	0.57
3:F:175:GLN:HE22	3:F:177:ARG:HH11	1.52	0.57
2:B:142:VAL:HG22	2:B:148:LEU:HD22	1.87	0.57
2:E:66:GLU:HB2	2:E:69:GLU:HG3	1.86	0.57
1:A:84:ASN:ND2	1:J:7:LYS:NZ	2.53	0.56
1:G:45:ILE:HD12	1:G:45:ILE:N	2.20	0.56
2:B:71:ASN:HD21	3:C:53:LYS:NZ	2.03	0.56
3:C:102:THR:O	3:C:103:GLN:HB2	2.06	0.56
2:B:138:MET:O	2:B:142:VAL:HG23	2.06	0.56
2:H:58:ILE:N	2:H:58:ILE:HD13	2.21	0.56
1:A:26:GLN:HE22	3:C:111:CYS:HB2	1.71	0.55
3:C:32:MET:O	3:C:36:GLU:HG3	2.08	0.54
2:B:42:ALA:O	2:B:45:ARG:HG2	2.08	0.54
2:E:67:ILE:CG1	3:F:239:VAL:HB	2.37	0.54
3:C:161:GLN:HE21	3:F:165:GLU:HG3	1.73	0.54
2:E:148:LEU:CD1	3:F:32:MET:SD	2.96	0.53
2:B:152:LEU:HA	6:B:226:HOH:O	2.06	0.53
3:I:224:ILE:N	3:I:224:ILE:HD12	2.23	0.53
3:C:207:GLU:HG2	3:C:225:THR:HG22	1.91	0.53
1:A:117:GLU:HG3	6:C:3011:HOH:O	2.07	0.53
3:L:127:VAL:HG22	3:L:128:CYS:N	2.24	0.53
3:I:207:GLU:HG2	3:I:225:THR:CG2	2.39	0.53
3:C:127:VAL:HG22	3:C:128:CYS:N	2.24	0.53
1:D:94:ILE:HD12	1:D:94:ILE:N	2.24	0.53
2:K:142:VAL:HG21	3:L:29:ILE:HD11	1.92	0.52
2:E:142:VAL:HG21	3:F:24:VAL:HG21	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:127:VAL:HG22	3:F:128:CYS:N	2.24	0.51
3:I:127:VAL:HG22	3:I:128:CYS:N	2.24	0.51
3:C:131:CSD:O	3:C:152:ARG:HD2	2.10	0.51
2:H:67:ILE:HD11	3:I:239:VAL:HA	1.93	0.51
1:D:79:ASP:HB3	1:D:84:ASN:O	2.10	0.51
3:C:75:PRO:O	3:C:79:LYS:HG3	2.10	0.51
1:G:79:ASP:HB3	1:G:84:ASN:O	2.11	0.51
3:I:23:GLU:HG2	3:I:23:GLU:O	2.10	0.51
3:L:131:CSD:O	3:L:152:ARG:HD2	2.10	0.51
6:K:247:HOH:O	3:L:234:LYS:HE3	2.11	0.51
3:F:102:THR:O	3:F:103:GLN:HB2	2.10	0.51
3:I:201:THR:OG1	3:I:204:GLN:HG3	2.11	0.50
2:B:148:LEU:CG	3:C:32:MET:HE1	2.40	0.50
2:B:148:LEU:CG	3:C:32:MET:CE	2.90	0.50
3:C:62:LEU:HB2	3:C:63:PRO:HD3	1.94	0.50
1:A:71:VAL:HG11	1:A:117:GLU:OE2	2.11	0.50
2:E:124:GLN:HE21	1:G:84:ASN:HD21	1.57	0.49
3:I:62:LEU:HB2	6:I:3045:HOH:O	2.11	0.49
2:B:145:GLY:HA2	6:B:281:HOH:O	2.12	0.49
2:H:46:VAL:HG12	2:H:96:CYS:SG	2.53	0.49
3:L:102:THR:O	3:L:103:GLN:HB2	2.13	0.49
3:L:62:LEU:O	3:L:66:ARG:HG2	2.13	0.48
1:A:125:LYS:O	1:A:125:LYS:HG3	2.11	0.48
2:K:116:ALA:O	2:K:119:ILE:HG22	2.13	0.48
3:F:201:THR:OG1	3:F:204:GLN:HG3	2.13	0.48
2:E:28:HIS:CE1	3:I:153:ARG:HH12	2.31	0.48
1:J:12:ARG:HD3	2:K:125:PHE:CZ	2.48	0.48
3:C:207:GLU:HG2	3:C:225:THR:CG2	2.44	0.48
3:I:131:CSD:O	3:I:152:ARG:HD2	2.13	0.48
2:K:5:ILE:N	2:K:5:ILE:HD12	2.29	0.48
2:E:45:ARG:NH1	2:E:100:GLN:HE22	2.11	0.48
2:E:148:LEU:CD1	2:E:151:TYR:HB2	2.42	0.48
2:E:148:LEU:HD13	3:F:32:MET:SD	2.54	0.48
1:G:45:ILE:CD1	1:G:45:ILE:N	2.77	0.47
2:K:46:VAL:CG1	2:K:96:CYS:SG	3.02	0.47
2:B:126:VAL:HG12	2:B:127:THR:O	2.13	0.47
2:B:147:GLY:N	2:B:154:PRO:HA	2.28	0.47
3:F:171:PRO:HB2	3:F:174:VAL:HG23	1.97	0.47
2:B:152:LEU:HD12	2:B:153:PRO:HD2	1.95	0.47
2:H:46:VAL:CG1	2:H:96:CYS:SG	3.02	0.47
3:F:173:GLU:CD	3:F:173:GLU:H	2.18	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:TYR:HA	2:B:46:VAL:HG11	1.96	0.47
3:I:54:ASP:O	3:I:58:THR:HG23	2.15	0.47
3:C:123:LYS:HD3	3:C:123:LYS:C	2.35	0.47
3:F:99:SER:HB2	3:F:100:PRO:HD3	1.97	0.47
2:K:118:ARG:HG3	2:K:122:ASP:OD2	2.15	0.47
3:C:175:GLN:HE22	3:C:177:ARG:NH1	2.09	0.46
3:C:170:LEU:HD13	3:C:176:ILE:HD11	1.97	0.46
2:B:146:GLN:O	2:B:146:GLN:HG2	2.16	0.46
3:C:127:VAL:HB	3:C:155:LEU:HD23	1.97	0.46
2:B:142:VAL:HG22	2:B:148:LEU:HD13	1.97	0.46
2:H:58:ILE:HD12	3:I:150:ASN:CG	2.36	0.46
3:F:126:VAL:HG12	3:F:127:VAL:N	2.30	0.46
3:C:237:ARG:NH2	3:C:237:ARG:HG3	2.28	0.46
3:C:126:VAL:HG12	3:C:127:VAL:N	2.31	0.46
6:B:191:HOH:O	1:J:79:ASP:HA	2.16	0.46
1:D:121:ARG:HG3	1:D:122:TYR:CD1	2.51	0.46
2:B:134:LYS:HE2	3:C:36:GLU:HB2	1.98	0.46
2:E:148:LEU:CD2	3:F:32:MET:SD	3.04	0.46
2:H:67:ILE:HG21	2:H:150:GLU:HG3	1.97	0.46
6:E:250:HOH:O	2:K:24:HIS:HE1	1.98	0.46
2:K:5:ILE:HD13	6:K:239:HOH:O	2.14	0.45
1:G:71:VAL:HG11	1:G:117:GLU:OE2	2.16	0.45
3:I:226:VAL:HG23	6:I:3114:HOH:O	2.15	0.45
2:E:118:ARG:HG3	2:E:122:ASP:OD2	2.17	0.45
1:A:12:ARG:HD3	2:B:125:PHE:CZ	2.52	0.45
1:A:9:VAL:HG23	1:A:9:VAL:O	2.16	0.45
3:F:131:CSD:O	3:F:152:ARG:HD3	2.16	0.45
2:E:144:SER:OG	2:E:146:GLN:HG3	2.16	0.45
2:H:118:ARG:HG3	2:H:122:ASP:OD2	2.17	0.45
1:G:20:THR:HA	3:I:104:PHE:HB3	1.98	0.45
3:I:165:GLU:HG3	3:L:161:GLN:HE21	1.82	0.45
2:K:137:GLU:OE2	2:K:141:ARG:NH2	2.33	0.45
2:E:66:GLU:CD	3:F:235:ALA:HB1	2.38	0.45
3:C:123:LYS:HG3	3:C:170:LEU:HD11	1.98	0.45
3:I:106:THR:OG1	3:I:109:ASP:HB2	2.16	0.44
2:E:4:SER:HB3	2:E:7:GLU:OE1	2.17	0.44
3:F:40:GLU:HG3	6:F:3098:HOH:O	2.17	0.44
1:A:28:PHE:HA	1:A:31:MET:HE3	1.99	0.44
3:L:54:ASP:O	3:L:58:THR:HG23	2.18	0.44
2:H:58:ILE:CD1	2:H:58:ILE:N	2.79	0.44
3:L:66:ARG:NH2	3:L:203:ASP:OD1	2.47	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:118:ASP:OD1	3:I:124:HIS:HD2	2.00	0.44
2:E:5:ILE:HD13	6:E:290:HOH:O	2.17	0.44
2:H:116:ALA:O	2:H:119:ILE:HG22	2.16	0.44
3:F:47:GLU:O	3:F:51:VAL:HG23	2.18	0.44
2:K:45:ARG:NH1	2:K:100:GLN:HE22	2.16	0.44
1:A:79:ASP:HA	6:A:3013:HOH:O	2.18	0.44
6:I:3120:HOH:O	3:L:161:GLN:HG2	2.17	0.44
2:B:80:ALA:HA	2:B:85:TRP:O	2.18	0.44
2:H:138:MET:HB3	3:I:29:ILE:HG23	2.00	0.44
1:D:92:TYR:HB2	1:D:94:ILE:HD11	1.99	0.44
1:A:79:ASP:HB3	1:A:84:ASN:O	2.18	0.44
3:F:150:ASN:OD1	3:F:154:ARG:HD3	2.18	0.44
2:H:134:LYS:HE3	2:H:138:MET:HE3	2.00	0.44
3:I:207:GLU:HG2	3:I:225:THR:HG22	1.99	0.44
1:A:104:GLU:HG3	6:C:3168:HOH:O	2.18	0.44
2:E:80:ALA:HA	2:E:85:TRP:O	2.17	0.43
3:F:67:LEU:C	3:F:67:LEU:HD23	2.39	0.43
2:B:119:ILE:HD11	2:B:123:LYS:HE3	1.98	0.43
2:K:120:LEU:HD22	3:L:43:LEU:CD1	2.48	0.43
3:C:164:ALA:HB3	3:F:161:GLN:NE2	2.31	0.43
2:B:142:VAL:HG21	3:C:24:VAL:HG21	2.00	0.43
2:E:116:ALA:O	2:E:119:ILE:HG22	2.19	0.43
2:H:80:ALA:HA	2:H:85:TRP:O	2.19	0.43
3:C:136:ARG:HB2	3:C:137:PRO:HD3	2.01	0.43
3:F:62:LEU:HB3	3:F:63:PRO:HD3	2.00	0.43
2:E:148:LEU:HB3	2:E:152:LEU:HB3	2.01	0.43
3:I:106:THR:HG1	3:I:109:ASP:HB2	1.84	0.43
3:C:171:PRO:HB2	3:C:174:VAL:HG23	2.01	0.43
1:A:12:ARG:NH2	6:A:3019:HOH:O	2.51	0.42
1:G:119:PRO:HG2	1:G:122:TYR:HD2	1.84	0.42
1:A:119:PRO:HG2	1:A:122:TYR:HD2	1.84	0.42
2:H:138:MET:CE	3:I:33:ALA:HA	2.50	0.42
2:H:41:ARG:HG2	2:K:12:HIS:HD2	1.84	0.42
2:H:142:VAL:HG22	2:H:148:LEU:HD13	2.00	0.42
3:L:126:VAL:HG12	3:L:127:VAL:N	2.35	0.42
3:F:116:LEU:HB3	3:F:124:HIS:CD2	2.55	0.42
1:D:84:ASN:ND2	2:H:124:GLN:HE21	2.17	0.42
3:F:100:PRO:HA	3:F:101:PRO:HD3	1.91	0.42
2:E:46:VAL:CG1	2:E:96:CYS:SG	3.08	0.42
3:L:157:ARG:HD3	3:L:158:TRP:CH2	2.54	0.42
3:C:54:ASP:O	3:C:58:THR:HG23	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:99:SER:HB2	3:C:100:PRO:HD3	2.02	0.42
3:I:132:SER:O	3:I:133:CSO:C	2.68	0.42
2:H:148:LEU:HD12	2:H:148:LEU:N	2.34	0.42
2:E:45:ARG:HH11	2:E:100:GLN:HE22	1.67	0.41
3:I:126:VAL:HG12	3:I:127:VAL:N	2.35	0.41
2:B:143:ALA:C	2:B:145:GLY:H	2.24	0.41
2:E:4:SER:HB3	2:E:7:GLU:CG	2.50	0.41
3:I:103:GLN:HG2	3:I:103:GLN:O	2.20	0.41
2:H:26:GLN:NE2	6:H:220:HOH:O	2.53	0.41
2:B:118:ARG:HG3	2:B:122:ASP:OD2	2.20	0.41
3:C:161:GLN:HG2	6:F:3070:HOH:O	2.21	0.41
1:A:84:ASN:HD22	1:J:7:LYS:CE	2.33	0.41
3:I:67:LEU:C	3:I:67:LEU:HD23	2.41	0.41
3:C:99:SER:N	3:C:100:PRO:CD	2.84	0.41
3:F:125:VAL:HA	3:F:216:GLY:HA3	2.02	0.41
2:E:148:LEU:N	2:E:152:LEU:O	2.54	0.41
3:L:132:SER:O	3:L:133:CSO:C	2.68	0.41
3:C:132:SER:O	3:C:133:CSO:C	2.69	0.41
1:D:50:ASP:O	1:D:51:LEU:C	2.60	0.41
3:C:100:PRO:HA	3:C:101:PRO:HD3	1.96	0.41
3:F:123:LYS:HG3	3:F:170:LEU:HD11	2.03	0.41
2:H:148:LEU:HD23	3:I:32:MET:SD	2.61	0.40
2:E:4:SER:HB3	2:E:7:GLU:HG3	2.03	0.40
3:L:67:LEU:HD23	3:L:67:LEU:C	2.41	0.40
3:F:154:ARG:NH2	3:F:165:GLU:OE2	2.43	0.40
2:K:152:LEU:HD12	2:K:153:PRO:HD2	2.03	0.40
3:F:157:ARG:HD3	3:F:158:TRP:CH2	2.56	0.40
1:D:71:VAL:HG11	1:D:117:GLU:OE2	2.21	0.40
2:E:61:HIS:HE1	6:F:3056:HOH:O	2.04	0.40
1:D:93:SER:C	1:D:94:ILE:HD12	2.42	0.40
1:J:7:LYS:HA	1:J:8:PRO:HD3	1.92	0.40
1:J:111:ASN:O	3:L:175:GLN:HG3	2.21	0.40
2:B:126:VAL:HG13	2:B:130:GLU:HB2	2.03	0.40
2:K:127:THR:OG1	2:K:130:GLU:HG3	2.22	0.40
3:F:160:ARG:NE	3:F:176:ILE:HD12	2.36	0.40
1:A:84:ASN:ND2	1:J:7:LYS:HZ3	2.19	0.40
2:E:127:THR:OG1	2:E:130:GLU:HG3	2.22	0.40
1:J:125:LYS:HG3	6:J:3134:HOH:O	2.21	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
1	D	117/126 (93%)	108 (92%)	9 (8%)	0	100	100
1	G	118/126 (94%)	114 (97%)	4 (3%)	0	100	100
1	J	118/126 (94%)	114 (97%)	4 (3%)	0	100	100
2	B	150/157 (96%)	144 (96%)	5 (3%)	1 (1%)	26	19
2	E	149/157 (95%)	142 (95%)	7 (5%)	0	100	100
2	H	154/157 (98%)	147 (96%)	7 (4%)	0	100	100
2	K	150/157 (96%)	146 (97%)	4 (3%)	0	100	100
3	C	213/243 (88%)	205 (96%)	8 (4%)	0	100	100
3	F	212/243 (87%)	204 (96%)	8 (4%)	0	100	100
3	I	213/243 (88%)	205 (96%)	8 (4%)	0	100	100
3	L	212/243 (87%)	205 (97%)	7 (3%)	0	100	100
All	All	1923/2104 (91%)	1845 (96%)	77 (4%)	1 (0%)	56	53

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	144	SER

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%)	100 (99%)	1 (1%)	82	85
1	D	101/108 (94%)	101 (100%)	0	100	100
1	G	102/108 (94%)	101 (99%)	1 (1%)	82	85
1	J	102/108 (94%)	101 (99%)	1 (1%)	82	85
2	B	130/134 (97%)	128 (98%)	2 (2%)	72	75
2	E	129/134 (96%)	126 (98%)	3 (2%)	58	60
2	H	133/134 (99%)	128 (96%)	5 (4%)	40	36
2	K	130/134 (97%)	128 (98%)	2 (2%)	72	75
3	C	188/212 (89%)	186 (99%)	2 (1%)	80	83
3	F	187/212 (88%)	185 (99%)	2 (1%)	80	83
3	I	188/212 (89%)	187 (100%)	1 (0%)	92	94
3	L	187/212 (88%)	187 (100%)	0	100	100
All	All	1678/1816 (92%)	1658 (99%)	20 (1%)	78	81

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

Mol	Chain	Res	Type
1	A	26	GLN
2	B	48	HIS
2	B	85	TRP
3	C	198	ASP
3	C	237	ARG
2	E	48	HIS
2	E	70	LEU
2	E	85	TRP
3	F	37	LEU
3	F	239	VAL
1	G	125	LYS
2	H	39	LEU
2	H	48	HIS
2	H	58	ILE
2	H	85	TRP
2	H	137	GLU
3	I	62	LEU
1	J	99	LYS
2	K	48	HIS
2	K	85	TRP

Some 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	84	ASN
1	A	111	ASN
2	B	26	GLN
2	B	37	HIS
2	B	71	ASN
2	B	100	GLN
3	C	175	GLN
2	E	26	GLN
2	E	61	HIS
2	E	94	GLN
2	E	100	GLN
2	E	146	GLN
3	F	49	HIS
3	F	161	GLN
3	F	175	GLN
1	G	14	HIS
1	G	84	ASN
1	G	87	ASN
2	H	28	HIS
2	H	61	HIS
2	H	100	GLN
2	H	124	GLN
3	I	103	GLN
3	I	112	ASN
3	I	124	HIS
3	I	141	GLN
3	I	169	GLN
3	I	175	GLN
1	J	84	ASN
1	J	87	ASN
2	K	12	HIS
2	K	24	HIS
2	K	26	GLN
2	K	100	GLN
3	L	112	ASN
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	CSD	C	131	3,4	3,7,8	0.77	0	3,8,10	1.76	1 (33%)
3	CSO	C	133	3,4	3,6,7	0.70	0	1,6,8	1.69	0
3	CSD	F	131	3,4	3,7,8	0.85	0	3,8,10	1.70	1 (33%)
3	CSO	F	133	3,4	3,6,7	0.62	0	1,6,8	1.75	0
3	CSD	I	131	3,4	3,7,8	0.75	0	3,8,10	1.75	1 (33%)
3	CSO	I	133	3,4	3,6,7	0.67	0	1,6,8	1.81	0
3	CSD	L	131	3,4	3,7,8	0.77	0	3,8,10	1.73	1 (33%)
3	CSO	L	133	3,4	3,6,7	0.71	0	1,6,8	1.78	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	CSD	C	131	3,4	-	1/2/6/8	0/0/0/0
3	CSO	C	133	3,4	-	0/1/5/7	0/0/0/0
3	CSD	F	131	3,4	-	1/2/6/8	0/0/0/0
3	CSO	F	133	3,4	-	0/1/5/7	0/0/0/0
3	CSD	I	131	3,4	-	1/2/6/8	0/0/0/0
3	CSO	I	133	3,4	-	0/1/5/7	0/0/0/0
3	CSD	L	131	3,4	-	1/2/6/8	0/0/0/0
3	CSO	L	133	3,4	-	0/1/5/7	0/0/0/0

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	131	CSD	OD1-SG-CB	2.36	109.34	105.40
3	I	131	CSD	OD1-SG-CB	2.43	109.46	105.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	131	CSD	OD1-SG-CB	2.46	109.50	105.40
3	C	131	CSD	OD1-SG-CB	2.46	109.50	105.40

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	I	131	CSD	CA-CB-SG-OD1
3	C	131	CSD	CA-CB-SG-OD1
3	L	131	CSD	CA-CB-SG-OD1
3	F	131	CSD	CA-CB-SG-OD1

There are no ring outliers.

7 monomers are involved in 7 short contacts:

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 4 are monoatomic - leaving 12 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	SO4	A	3005	-	4,4,4	0.24	0	6,6,6	0.09	0
5	SO4	C	3001	-	4,4,4	0.15	0	6,6,6	0.11	0
5	SO4	D	3006	-	4,4,4	0.23	0	6,6,6	0.07	0
5	SO4	F	3002	-	4,4,4	0.16	0	6,6,6	0.10	0
5	SO4	G	3007	-	4,4,4	0.22	0	6,6,6	0.07	0
5	SO4	I	3003	-	4,4,4	0.14	0	6,6,6	0.10	0
5	SO4	I	3011	-	4,4,4	0.29	0	6,6,6	0.09	0
5	SO4	I	3012	-	4,4,4	0.38	0	6,6,6	0.16	0
5	SO4	J	3008	-	4,4,4	0.24	0	6,6,6	0.08	0
5	SO4	L	3004	-	4,4,4	0.19	0	6,6,6	0.07	0
5	SO4	L	3009	-	4,4,4	0.19	0	6,6,6	0.08	0
5	SO4	L	3010	-	4,4,4	0.27	0	6,6,6	0.09	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	SO4	A	3005	-	-	0/0/0/0	0/0/0/0
5	SO4	C	3001	-	-	0/0/0/0	0/0/0/0
5	SO4	D	3006	-	-	0/0/0/0	0/0/0/0
5	SO4	F	3002	-	-	0/0/0/0	0/0/0/0
5	SO4	G	3007	-	-	0/0/0/0	0/0/0/0
5	SO4	I	3003	-	-	0/0/0/0	0/0/0/0
5	SO4	I	3011	-	-	0/0/0/0	0/0/0/0
5	SO4	I	3012	-	-	0/0/0/0	0/0/0/0
5	SO4	J	3008	-	-	0/0/0/0	0/0/0/0
5	SO4	L	3004	-	-	0/0/0/0	0/0/0/0
5	SO4	L	3009	-	-	0/0/0/0	0/0/0/0
5	SO4	L	3010	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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%)	-0.25	2 (1%) 73 73	12, 19, 32, 40	0
1	D	119/126 (94%)	0.18	7 (5%) 26 27	17, 26, 42, 50	0
1	G	120/126 (95%)	0.06	6 (5%) 32 34	13, 21, 37, 57	0
1	J	120/126 (95%)	-0.16	5 (4%) 40 41	11, 19, 34, 43	0
2	B	152/157 (96%)	0.11	11 (7%) 18 20	11, 18, 46, 57	0
2	E	151/157 (96%)	0.08	9 (5%) 25 27	13, 20, 49, 58	0
2	H	156/157 (99%)	0.45	16 (10%) 9 9	12, 20, 55, 67	0
2	K	152/157 (96%)	-0.38	2 (1%) 79 80	10, 16, 29, 43	0
3	C	215/243 (88%)	0.04	9 (4%) 40 41	10, 22, 37, 49	0
3	F	214/243 (88%)	0.16	5 (2%) 64 64	15, 24, 35, 48	0
3	I	215/243 (88%)	-0.10	4 (1%) 70 70	10, 17, 30, 47	0
3	L	214/243 (88%)	-0.27	2 (0%) 85 86	9, 16, 26, 33	0
All	All	1947/2104 (92%)	-0.01	78 (4%) 42 44	9, 20, 36, 67	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	156	ALA	13.7
2	H	157	LYS	11.1
2	H	148	LEU	8.6
2	H	3	SER	8.6
3	F	239	VAL	8.3
2	B	152	LEU	7.6
2	H	2	SER	7.6
2	B	154	PRO	7.6
2	H	154	PRO	7.6
2	B	148	LEU	7.6
2	E	153	PRO	7.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	153	PRO	7.2
2	B	144	SER	7.1
2	H	152	LEU	6.4
2	H	153	PRO	6.3
2	E	148	LEU	6.2
2	E	154	PRO	6.1
2	H	147	GLY	5.9
2	E	147	GLY	5.6
2	H	144	SER	5.4
2	H	155	LYS	5.3
2	B	147	GLY	5.2
1	A	126	ALA	5.1
2	K	3	SER	5.1
2	E	144	SER	5.0
3	C	198	ASP	4.9
1	G	126	ALA	4.9
2	B	146	GLN	4.4
3	C	23	GLU	4.3
2	E	145	GLY	4.3
2	E	152	LEU	4.3
1	G	7	LYS	4.2
1	D	9	VAL	3.9
3	F	76	GLU	3.8
2	E	146	GLN	3.7
1	D	126	ALA	3.7
2	H	146	GLN	3.5
2	H	145	GLY	3.5
2	B	3	SER	3.4
1	D	8	PRO	3.4
2	B	143	ALA	3.1
1	D	125	LYS	3.1
2	B	145	GLY	3.0
1	A	125	LYS	3.0
3	F	198	ASP	3.0
3	C	173	GLU	2.8
2	H	4	SER	2.8
1	G	8	PRO	2.7
1	J	34	LYS	2.7
1	G	125	LYS	2.7
3	I	23	GLU	2.5
1	G	9	VAL	2.5
3	C	199	GLY	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	F	127	VAL	2.4
3	C	234	LYS	2.4
1	J	126	ALA	2.4
3	F	79	LYS	2.4
3	I	130	LEU	2.3
3	I	199	GLY	2.3
3	C	200	TRP	2.3
1	D	17	LYS	2.3
1	G	34	LYS	2.3
3	C	239	VAL	2.3
1	D	86	GLU	2.2
2	B	4	SER	2.2
3	L	66	ARG	2.2
2	H	143	ALA	2.2
1	J	125	LYS	2.2
1	J	10	TRP	2.2
1	J	7	LYS	2.1
2	E	143	ALA	2.1
3	C	57	HIS	2.1
3	I	76	GLU	2.1
1	D	11	ASP	2.1
3	C	229	LYS	2.1
3	L	198	ASP	2.1
2	K	4	SER	2.0
2	H	140	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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	CSO	L	133	7/8	0.96	0.16	-	6,9,13,15	1
3	CSO	F	133	7/8	0.80	0.21	-	13,14,18,19	1
3	CSO	I	133	7/8	0.85	0.22	-	10,12,17,18	1
3	CSD	L	131	8/9	0.97	0.17	-	5,9,10,12	2
3	CSD	C	131	8/9	0.93	0.19	-	8,11,13,15	2
3	CSO	C	133	7/8	0.94	0.13	-	9,11,16,16	1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	CSD	I	131	8/9	0.94	0.21	-	8,10,13,14	2
3	CSD	F	131	8/9	0.89	0.21	-	11,14,15,17	2

6.3 Carbohydrates [i](#)

There are no carbohydrates 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. 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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	SO4	I	3011	5/5	0.94	0.19	2.80	49,49,50,52	0
5	SO4	I	3012	5/5	0.96	0.12	1.75	51,51,51,53	0
5	SO4	L	3010	5/5	0.92	0.21	1.61	49,49,50,52	0
5	SO4	L	3004	5/5	0.97	0.14	0.95	30,34,37,37	0
5	SO4	A	3005	5/5	0.96	0.12	0.35	42,42,44,45	0
5	SO4	I	3003	5/5	0.97	0.16	-0.05	33,34,35,36	0
5	SO4	L	3009	5/5	0.96	0.14	-0.28	47,48,49,50	0
5	SO4	D	3006	5/5	0.98	0.10	-0.31	37,37,38,39	0
5	SO4	F	3002	5/5	0.97	0.14	-0.33	37,37,40,40	0
5	SO4	J	3008	5/5	0.98	0.11	-0.39	46,46,47,47	0
5	SO4	G	3007	5/5	0.97	0.10	-0.86	41,41,41,42	0
5	SO4	C	3001	5/5	0.98	0.10	-1.10	32,34,36,37	0
4	3CO	C	301	1/1	-	-	-	14,14,14,14	1
4	3CO	I	301	1/1	-	-	-	13,13,13,13	1
4	3CO	L	301	1/1	-	-	-	12,12,12,12	1
4	3CO	F	301	1/1	-	-	-	18,18,18,18	1

6.5 Other polymers [i](#)

There are no such residues in this entry.