



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 01:53 AM GMT

PDB ID : 4L5S
Title : p202 HIN1 in complex with 12-mer dsDNA
Authors : Yin, Q.; Tian, Y.; Wu, H.
Deposited on : 2013-06-11
Resolution : 2.94 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>

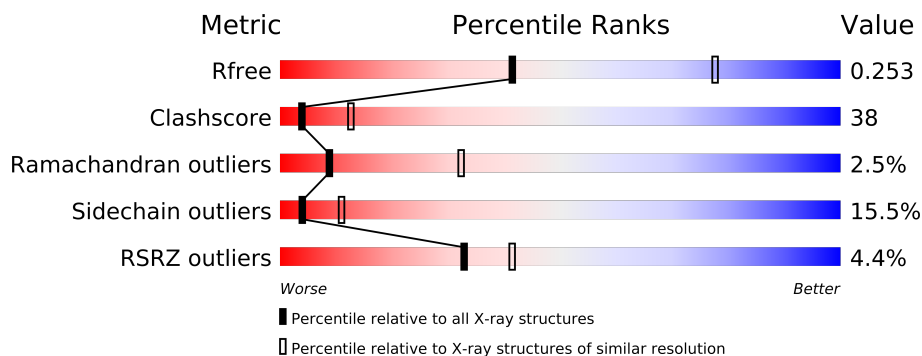
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.94 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	1424 (2.98-2.90)
Clashscore	79885	1761 (2.98-2.90)
Ramachandran outliers	78287	1708 (2.98-2.90)
Sidechain outliers	78261	1710 (2.98-2.90)
RSRZ outliers	66119	1425 (2.98-2.90)

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	199	
1	B	199	
2	C	12	
2	D	12	
2	E	12	
2	F	12	
2	G	12	
2	H	12	
2	I	12	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	SO4	A	301	-	X
3	SO4	A	302	-	X
3	SO4	D	101	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4705 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 Interferon-activable protein 202.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	199	Total	C	N	O	S	0	0	0
			1597	1022	268	302	5			
1	B	198	Total	C	N	O	S	0	0	0
			1589	1018	268	298	5			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	45	SER	-	EXPRESSION TAG	UNP Q9R002
A	92	LYS	GLN	VARIANT	UNP Q9R002
A	111	GLN	LYS	VARIANT	UNP Q9R002
A	141	MET	ILE	VARIANT	UNP Q9R002
A	142	PHE	ILE	VARIANT	UNP Q9R002
A	204	GLU	LYS	VARIANT	UNP Q9R002
B	45	SER	-	EXPRESSION TAG	UNP Q9R002
B	92	LYS	GLN	VARIANT	UNP Q9R002
B	111	GLN	LYS	VARIANT	UNP Q9R002
B	141	MET	ILE	VARIANT	UNP Q9R002
B	142	PHE	ILE	VARIANT	UNP Q9R002
B	204	GLU	LYS	VARIANT	UNP Q9R002

- Molecule 2 is a DNA chain called 12-mer DNA.

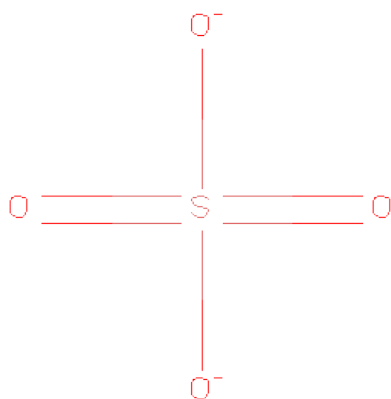
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	11	Total	C	N	O	P	0	0	0
			213	102	38	63	10			
2	D	12	Total	C	N	O	P	0	0	0
			243	117	45	70	11			
2	E	11	Total	C	N	O	P	0	0	0
			222	107	40	65	10			
2	F	9	Total	C	N	O	P	0	0	0
			175	83	30	53	9			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	9	Total	C	N	O	P	0	0	0
			183	88	35	52	8			
2	H	12	Total	C	N	O	P	0	0	0
			226	107	40	68	11			
2	I	12	Total	C	N	O	P	0	0	0
			225	107	40	67	11			

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



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	O	0	0
			3	3		

Continued on next page...

Continued from previous page...

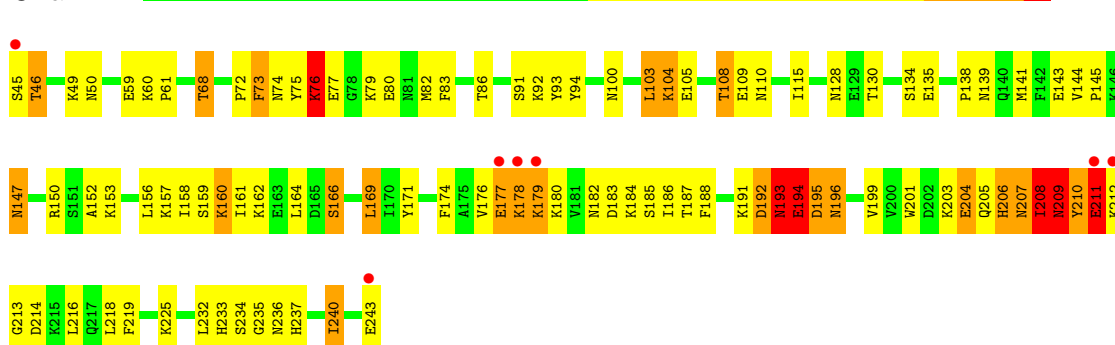
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	3	Total 3	O 3	0	0
4	I	1	Total 1	O 1	0	0

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.

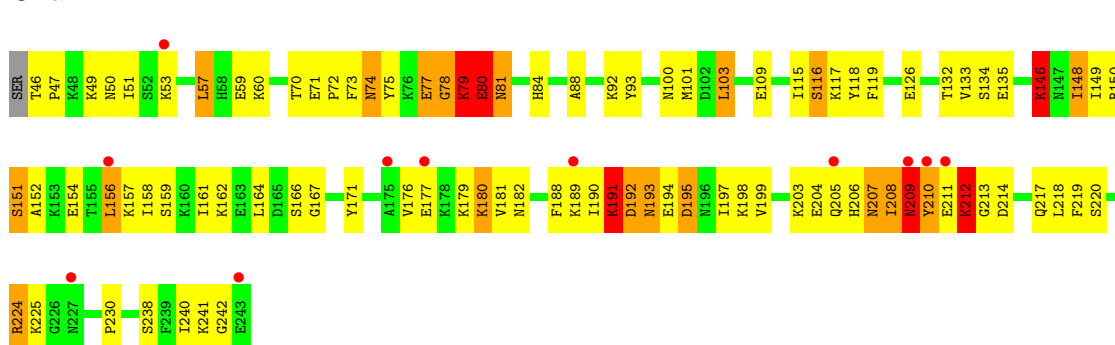
• Molecule 1: Interferon-activable protein 202

Chain A:



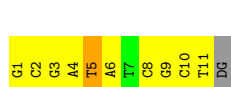
• Molecule 1: Interferon-activable protein 202

Chain B:



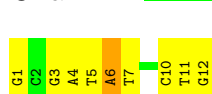
• Molecule 2: 12-mer DNA

Chain C:

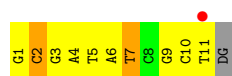


• Molecule 2: 12-mer DNA

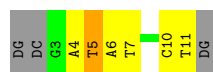
Chain D:



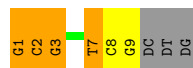
● Molecule 2: 12-mer DNA

Chain E: 

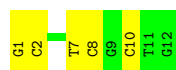
● Molecule 2: 12-mer DNA

Chain F: 

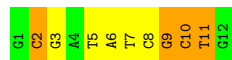
● Molecule 2: 12-mer DNA

Chain G: 

● Molecule 2: 12-mer DNA

Chain H: 

● Molecule 2: 12-mer DNA

Chain I: 

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	111.31Å 156.12Å 117.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.97 – 2.94 46.97 – 2.94	Depositor EDS
% Data completeness (in resolution range)	99.7 (46.97-2.94) 99.8 (46.97-2.94)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 2.96Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.7.1.743)	Depositor
R, R_{free}	0.204 , 0.255 0.219 , 0.253	Depositor DCC
R_{free} test set	1128 reflections (5.12%)	DCC
Wilson B-factor (Å ²)	61.5	Xtriage
Anisotropy	0.409	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 45.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 22048 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4705	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.94% 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: 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	0.49	0/1628	0.67	0/2186
1	B	0.46	0/1620	0.68	1/2175 (0.0%)
2	C	0.70	0/238	1.59	4/365 (1.1%)
2	D	0.73	0/272	1.87	11/419 (2.6%)
2	E	0.70	0/248	1.77	10/381 (2.6%)
2	F	0.65	0/195	1.19	1/298 (0.3%)
2	G	0.74	0/205	1.65	5/315 (1.6%)
2	H	0.65	0/252	1.53	6/388 (1.5%)
2	I	0.89	0/251	1.87	9/385 (2.3%)
All	All	0.57	0/4909	1.15	47/6912 (0.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	8
1	B	0	6
All	All	0	14

There are no bond length outliers.

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	8	DC	O4'-C1'-N1	-13.37	98.64	108.00
2	I	11	DT	C6-C5-C7	-11.54	115.97	122.90
2	I	11	DT	C4-C5-C7	8.87	124.32	119.00
2	D	6	DA	O4'-C1'-N9	-8.76	101.87	108.00
2	G	3	DG	O4'-C1'-N9	8.18	113.73	108.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	4	DA	O4'-C1'-N9	-8.08	102.34	108.00
2	I	10	DC	O4'-C4'-C3'	-7.76	101.34	106.00
2	E	2	DC	O4'-C1'-C2'	-7.74	99.71	105.90
2	E	2	DC	C1'-O4'-C4'	-7.70	102.40	110.10
2	G	3	DG	C1'-O4'-C4'	-7.42	102.68	110.10
2	H	10	DC	O4'-C1'-N1	7.21	113.04	108.00
2	D	4	DA	O4'-C4'-C3'	-6.96	101.72	104.50
2	E	2	DC	C5-C6-N1	-6.81	117.60	121.00
2	D	10	DC	C1'-O4'-C4'	-6.80	103.30	110.10
2	C	10	DC	O4'-C4'-C3'	-6.78	101.79	104.50
2	D	10	DC	O4'-C1'-N1	-6.77	103.26	108.00
2	D	1	DG	O4'-C4'-C3'	-6.73	101.81	104.50
2	D	4	DA	O4'-C1'-N9	-6.52	103.44	108.00
2	D	5	DT	O4'-C1'-N1	-6.42	103.50	108.00
1	B	78	GLY	N-CA-C	-6.35	97.22	113.10
2	F	5	DT	C1'-O4'-C4'	-6.32	103.78	110.10
2	G	1	DG	O4'-C1'-N9	-6.32	103.58	108.00
2	I	11	DT	P-O5'-C5'	-6.20	110.99	120.90
2	E	7	DT	C1'-O4'-C4'	-6.11	103.99	110.10
2	D	5	DT	N3-C4-O4	6.10	123.56	119.90
2	E	1	DG	O4'-C1'-C2'	-6.09	101.03	105.90
2	I	9	DG	O4'-C1'-N9	6.06	112.24	108.00
2	H	7	DT	N3-C4-O4	5.99	123.49	119.90
2	H	2	DC	O4'-C1'-C2'	-5.88	101.19	105.90
2	E	1	DG	C8-N9-C4	-5.87	104.05	106.40
2	I	11	DT	C1'-O4'-C4'	-5.84	104.26	110.10
2	D	3	DG	O4'-C1'-N9	-5.73	103.99	108.00
2	D	7	DT	O4'-C1'-N1	-5.57	104.10	108.00
2	H	2	DC	O4'-C1'-N1	-5.50	104.15	108.00
2	E	1	DG	N7-C8-N9	5.38	115.79	113.10
2	G	7	DT	N3-C4-O4	5.37	123.12	119.90
2	C	5	DT	N3-C4-O4	5.30	123.08	119.90
2	H	8	DC	O4'-C1'-C2'	-5.28	101.68	105.90
2	I	2	DC	C1'-O4'-C4'	-5.27	104.83	110.10
2	D	5	DT	C5-C4-O4	-5.21	121.25	124.90
2	I	11	DT	O4'-C1'-N1	5.19	111.64	108.00
2	E	7	DT	O4'-C1'-C2'	-5.15	101.78	105.90
2	E	2	DC	C6-N1-C2	5.08	122.33	120.30
2	G	2	DC	C1'-O4'-C4'	-5.08	105.02	110.10
2	I	11	DT	C3'-C2'-C1'	-5.07	96.42	102.50
2	H	10	DC	O4'-C1'-C2'	-5.05	101.86	105.90
2	E	5	DT	C6-C5-C7	-5.05	119.87	122.90

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	193	ASN	Peptide
1	A	194	GLU	Peptide
1	A	196	ASN	Peptide
1	A	208	ILE	Peptide
1	A	209	ASN	Peptide
1	A	210	TYR	Peptide
1	A	211	GLU	Peptide
1	A	76	LYS	Peptide
1	B	146	LYS	Peptide
1	B	191	LYS	Peptide
1	B	192	ASP	Peptide
1	B	206	HIS	Peptide
1	B	77	GLU	Peptide
1	B	79	LYS	Peptide

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	1597	0	1612	116	0
1	B	1589	0	1609	177	2
2	C	213	0	120	9	1
2	D	243	0	134	2	0
2	E	222	0	126	10	0
2	F	175	0	97	9	1
2	G	183	0	103	15	0
2	H	226	0	125	1	0
2	I	225	0	125	10	0
3	A	10	0	0	1	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	D	5	0	0	0	1
4	A	3	0	0	1	0
4	B	3	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	I	1	0	0	0	0
All	All	4705	0	4051	324	3

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 38.

All (324) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:211:GLU:N	1:B:212:LYS:HB3	1.34	1.42
1:B:188:PHE:CE1	1:B:210:TYR:OH	1.73	1.42
1:B:211:GLU:CA	1:B:212:LYS:HB3	1.58	1.31
1:B:211:GLU:N	1:B:212:LYS:CB	1.96	1.28
1:B:188:PHE:HE1	1:B:210:TYR:OH	0.90	1.21
1:A:177:GLU:CG	1:A:178:LYS:HE3	1.72	1.19
1:B:78:GLY:C	1:B:80:GLU:HG3	1.65	1.15
1:B:211:GLU:CB	1:B:212:LYS:HB3	1.77	1.14
1:B:212:LYS:HG3	1:B:213:GLY:H	1.07	1.11
1:B:210:TYR:O	1:B:212:LYS:HE2	1.49	1.10
1:B:210:TYR:C	1:B:212:LYS:HG2	1.73	1.08
1:A:209:ASN:HA	1:A:210:TYR:HB2	1.08	1.07
1:B:157:LYS:HZ1	1:B:194:GLU:HB2	0.93	1.07
1:B:211:GLU:N	1:B:212:LYS:CG	2.17	1.06
1:A:178:LYS:HD2	1:A:178:LYS:N	1.62	1.04
1:B:210:TYR:C	1:B:212:LYS:HE2	1.77	1.03
1:B:79:LYS:HE2	1:B:79:LYS:HA	1.41	1.02
1:A:178:LYS:HD2	1:A:178:LYS:H	1.09	1.02
1:B:210:TYR:O	1:B:212:LYS:HG2	1.60	1.00
1:B:211:GLU:H	1:B:212:LYS:HB3	1.17	0.99
1:A:177:GLU:HG3	1:A:178:LYS:HE3	1.40	0.99
1:B:208:ILE:O	1:B:209:ASN:ND2	1.95	0.98
1:B:157:LYS:NZ	1:B:194:GLU:HB2	1.76	0.98
1:B:211:GLU:H	1:B:212:LYS:CB	1.68	0.95
1:B:212:LYS:CG	1:B:213:GLY:H	1.79	0.94
1:A:240:ILE:O	2:I:11:DT:H73	1.67	0.94
1:B:210:TYR:HD2	1:B:212:LYS:H	1.13	0.94
1:A:209:ASN:HA	1:A:210:TYR:CB	1.98	0.94
1:A:209:ASN:CA	1:A:210:TYR:HB2	1.99	0.93
2:C:2:DC:H5	2:E:9:DG:H1	1.00	0.92
1:B:211:GLU:H	1:B:212:LYS:CG	1.75	0.91
1:A:193:ASN:O	1:A:193:ASN:ND2	2.03	0.91
1:B:135:GLU:N	1:B:135:GLU:OE1	2.02	0.91
1:B:210:TYR:CD2	1:B:212:LYS:N	2.39	0.90

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:211:GLU:H	1:B:212:LYS:CD	1.87	0.88
1:A:178:LYS:CD	1:A:178:LYS:H	1.75	0.88
1:B:211:GLU:N	1:B:212:LYS:HE2	1.88	0.88
1:A:177:GLU:HG2	1:A:178:LYS:HE3	1.55	0.88
1:A:59:GLU:HG2	1:A:60:LYS:H	1.39	0.87
1:A:79:LYS:HB2	1:A:80:GLU:HG2	1.57	0.86
1:B:212:LYS:HG3	1:B:213:GLY:N	1.88	0.86
2:C:9:DG:H1	2:E:2:DC:H5	1.23	0.84
1:B:211:GLU:N	1:B:212:LYS:CE	2.41	0.84
1:A:72:PRO:O	1:A:82:MET:O	1.94	0.84
1:B:208:ILE:HG13	1:B:209:ASN:N	1.92	0.84
1:A:177:GLU:OE1	1:A:191:LYS:CD	2.25	0.83
1:B:209:ASN:OD1	1:B:211:GLU:HA	1.78	0.83
1:B:211:GLU:H	1:B:212:LYS:CE	1.92	0.82
1:B:208:ILE:HG13	1:B:209:ASN:H	1.42	0.82
1:B:224:ARG:HH22	2:G:3:DG:H21	1.27	0.82
1:A:208:ILE:H	1:A:208:ILE:HD12	1.45	0.82
1:B:210:TYR:C	1:B:212:LYS:CG	2.47	0.80
1:B:210:TYR:O	1:B:212:LYS:CE	2.30	0.80
1:B:212:LYS:CG	1:B:213:GLY:N	2.42	0.80
1:A:46:THR:HG23	2:D:6:DA:OP1	1.82	0.79
1:B:211:GLU:CB	1:B:212:LYS:CB	2.59	0.78
1:B:78:GLY:CA	1:B:80:GLU:HG3	2.12	0.78
1:B:207:ASN:HB3	1:B:208:ILE:O	1.83	0.78
1:B:79:LYS:HE2	1:B:79:LYS:CA	2.14	0.78
1:B:57:LEU:HB2	1:B:119:PHE:CE2	2.19	0.77
1:B:50:ASN:HD21	1:B:79:LYS:CD	1.99	0.76
1:B:78:GLY:CA	1:B:80:GLU:CG	2.62	0.76
1:A:59:GLU:HG2	1:A:60:LYS:N	2.00	0.76
1:A:195:ASP:HA	1:A:196:ASN:HB2	1.68	0.76
1:A:164:LEU:O	1:A:225:LYS:HE3	1.86	0.76
2:C:2:DC:H5	2:E:9:DG:N1	1.79	0.76
1:B:74:ASN:OD1	1:B:74:ASN:N	2.20	0.74
1:B:74:ASN:HB3	1:B:80:GLU:CA	2.17	0.74
1:B:166:SER:OG	1:B:225:LYS:NZ	2.20	0.74
1:B:210:TYR:HB2	1:B:212:LYS:C	2.06	0.74
1:A:77:GLU:OE1	1:A:204:GLU:OE1	2.06	0.74
1:A:203:LYS:HE3	1:A:235:GLY:O	1.87	0.73
1:B:75:TYR:CD1	1:B:80:GLU:O	2.40	0.73
1:A:176:VAL:CG2	1:A:216:LEU:HB2	2.19	0.72
1:A:72:PRO:HA	1:A:83:PHE:HB3	1.69	0.72
1:B:157:LYS:HZ1	1:B:194:GLU:CB	1.89	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:195:ASP:HB3	1:A:196:ASN:O	1.90	0.72
1:B:50:ASN:HD21	1:B:79:LYS:HD2	1.55	0.72
1:A:204:GLU:HG3	1:A:206:HIS:CE1	2.24	0.71
1:B:210:TYR:HB2	1:B:212:LYS:N	2.06	0.71
2:E:2:DC:O2	2:E:2:DC:H2'	1.90	0.70
1:A:158:ILE:HG13	1:A:192:ASP:HB3	1.71	0.70
1:B:78:GLY:C	1:B:80:GLU:CG	2.53	0.70
1:B:79:LYS:N	1:B:80:GLU:HG3	2.06	0.70
1:B:78:GLY:H	1:B:80:GLU:HG2	1.57	0.70
1:B:74:ASN:HB3	1:B:80:GLU:HA	1.74	0.69
1:A:194:GLU:O	1:A:195:ASP:OD1	2.10	0.69
1:B:77:GLU:HG2	1:B:77:GLU:O	1.93	0.69
1:A:162:LYS:NZ	1:A:195:ASP:OD2	2.24	0.69
1:A:147:ASN:OD1	4:A:402:HOH:O	2.10	0.68
1:A:46:THR:HG22	1:A:49:LYS:HB2	1.75	0.68
1:A:177:GLU:HB3	1:A:178:LYS:HD2	1.74	0.68
1:B:188:PHE:CZ	1:B:210:TYR:OH	2.42	0.68
1:B:224:ARG:NH2	2:G:3:DG:H21	1.92	0.68
1:B:210:TYR:HB3	1:B:214:ASP:H	1.59	0.68
1:B:74:ASN:HA	1:B:80:GLU:O	1.94	0.67
1:B:50:ASN:ND2	1:B:79:LYS:HD2	2.09	0.67
1:B:78:GLY:CA	1:B:80:GLU:HG2	2.25	0.66
1:B:72:PRO:HB3	1:B:101:MET:CE	2.26	0.66
1:A:158:ILE:HG13	1:A:192:ASP:CB	2.27	0.65
1:A:240:ILE:O	2:I:11:DT:C7	2.42	0.65
1:B:53:LYS:HD2	2:F:11:DT:H5''	1.78	0.65
1:A:212:LYS:O	1:A:214:ASP:N	2.30	0.65
1:B:79:LYS:CE	1:B:79:LYS:HA	2.09	0.65
1:A:59:GLU:HG2	1:A:60:LYS:HG3	1.78	0.65
1:B:177:GLU:OE1	1:B:189:LYS:HG2	1.95	0.65
1:A:192:ASP:O	1:A:193:ASN:ND2	2.31	0.64
1:B:78:GLY:N	1:B:80:GLU:HG2	2.12	0.64
1:B:217:GLN:OE1	1:B:241:LYS:HE3	1.97	0.64
2:C:1:DG:H4'	2:C:2:DC:H5'	1.78	0.64
1:B:188:PHE:HE1	1:B:210:TYR:HH	0.70	0.64
1:B:73:PHE:O	1:B:81:ASN:HA	1.98	0.64
1:A:150:ARG:HA	1:A:153:LYS:HE2	1.80	0.63
1:B:177:GLU:HB2	1:B:189:LYS:HB3	1.80	0.63
1:B:135:GLU:CD	1:B:135:GLU:H	1.91	0.62
1:B:59:GLU:HG2	1:B:60:LYS:HG3	1.81	0.62
1:B:225:LYS:HG2	1:B:230:PRO:HB3	1.81	0.62
1:A:206:HIS:N	1:A:206:HIS:CD2	2.66	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:210:TYR:HB2	1:B:212:LYS:CA	2.29	0.62
1:B:75:TYR:CE1	1:B:80:GLU:O	2.53	0.62
1:B:210:TYR:O	1:B:212:LYS:CG	2.43	0.62
1:A:204:GLU:CG	1:A:206:HIS:CE1	2.82	0.62
1:B:78:GLY:H	1:B:80:GLU:CG	2.13	0.62
1:A:218:LEU:HD22	1:A:240:ILE:HG22	1.82	0.62
1:A:191:LYS:HA	1:A:195:ASP:O	2.00	0.61
1:B:74:ASN:HB3	1:B:80:GLU:HB3	1.81	0.61
2:C:5:DT:H2''	2:C:6:DA:C8	2.36	0.61
1:B:50:ASN:OD1	1:B:79:LYS:CG	2.49	0.60
1:B:72:PRO:HB3	1:B:101:MET:HE1	1.82	0.60
1:B:74:ASN:HB3	1:B:80:GLU:CB	2.32	0.60
1:A:177:GLU:HG3	1:A:178:LYS:CE	2.23	0.60
1:A:204:GLU:HG2	1:A:206:HIS:NE2	2.17	0.60
2:E:10:DC:H2''	2:E:11:DT:H5'	1.83	0.60
1:B:207:ASN:HB3	1:B:208:ILE:HA	1.83	0.60
2:I:8:DC:H2''	2:I:9:DG:C8	2.37	0.60
1:B:207:ASN:CB	1:B:208:ILE:HA	2.32	0.59
1:A:176:VAL:HG12	1:A:177:GLU:N	2.16	0.59
2:I:10:DC:H4'	2:I:11:DT:OP1	2.02	0.59
1:B:207:ASN:HB3	1:B:208:ILE:C	2.23	0.59
1:B:210:TYR:HB3	1:B:214:ASP:HB2	1.85	0.59
1:B:224:ARG:NH2	2:G:3:DG:OP2	2.35	0.59
1:A:176:VAL:HG12	1:A:177:GLU:H	1.66	0.58
2:F:6:DA:H1'	2:F:7:DT:H5'	1.84	0.58
1:A:82:MET:HE1	1:A:237:HIS:HB3	1.85	0.58
1:B:93:TYR:CD2	1:B:152:ALA:HB2	2.38	0.58
1:B:207:ASN:HB3	1:B:208:ILE:CA	2.34	0.58
1:A:182:ASN:O	1:A:183:ASP:C	2.42	0.57
1:A:188:PHE:HB2	1:A:199:VAL:HB	1.86	0.57
1:B:93:TYR:CG	1:B:152:ALA:HB2	2.39	0.57
1:B:177:GLU:HG3	1:B:191:LYS:HG2	1.86	0.57
1:A:73:PHE:HA	2:I:11:DT:O5'	2.04	0.57
1:B:78:GLY:N	1:B:80:GLU:CG	2.68	0.56
1:B:210:TYR:HA	1:B:214:ASP:OD2	2.05	0.56
1:B:53:LYS:HD2	2:F:11:DT:C5'	2.35	0.56
1:A:135:GLU:N	3:A:301:SO4:O3	2.28	0.56
1:B:210:TYR:CB	1:B:212:LYS:N	2.68	0.56
1:A:176:VAL:HG22	1:A:216:LEU:HB2	1.85	0.56
1:B:78:GLY:HA2	1:B:80:GLU:CG	2.34	0.56
1:A:204:GLU:CG	1:A:206:HIS:NE2	2.69	0.56
1:A:177:GLU:OE1	1:A:191:LYS:CG	2.53	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:50:ASN:HD21	1:B:79:LYS:HD3	1.70	0.56
1:A:93:TYR:CG	1:A:152:ALA:HB2	2.41	0.56
1:B:207:ASN:CB	1:B:208:ILE:CA	2.84	0.56
1:A:45:SER:HB2	1:A:49:LYS:HD3	1.88	0.55
1:A:68:THR:HB	1:A:86:THR:HB	1.88	0.55
1:A:177:GLU:CB	1:A:178:LYS:HE3	2.36	0.55
1:A:158:ILE:HB	1:A:195:ASP:HB2	1.88	0.54
1:B:148:ILE:HA	1:B:151:SER:HB3	1.88	0.54
1:B:203:LYS:O	1:B:204:GLU:HG3	2.07	0.54
1:B:220:SER:O	1:B:238:SER:HB3	2.07	0.54
2:E:2:DC:O2	2:E:2:DC:C2'	2.55	0.54
1:B:210:TYR:H	1:B:211:GLU:C	2.11	0.53
1:B:210:TYR:H	1:B:211:GLU:CA	2.21	0.53
1:B:218:LEU:HD23	1:B:240:ILE:HG22	1.90	0.53
2:C:9:DG:N1	2:E:2:DC:H5	1.98	0.53
1:A:219:PHE:CD1	1:A:219:PHE:N	2.75	0.53
2:G:8:DC:O3'	2:G:9:DG:H4'	2.07	0.53
1:B:210:TYR:H	1:B:211:GLU:HA	1.72	0.53
1:B:210:TYR:CG	1:B:212:LYS:N	2.77	0.53
1:A:195:ASP:HB3	1:A:196:ASN:C	2.29	0.53
1:A:201:TRP:CE2	1:A:203:LYS:HB2	2.44	0.53
1:B:49:LYS:O	1:B:50:ASN:HB2	2.09	0.52
1:A:72:PRO:O	1:A:73:PHE:CD1	2.61	0.52
1:B:78:GLY:HA2	1:B:80:GLU:HG2	1.91	0.51
1:B:50:ASN:ND2	1:B:79:LYS:CD	2.71	0.51
1:A:75:TYR:O	1:A:76:LYS:C	2.49	0.51
1:A:203:LYS:O	1:A:204:GLU:HB3	2.09	0.51
2:F:10:DC:C5	2:G:1:DG:C4	2.98	0.51
2:G:7:DT:H2''	2:G:8:DC:H5'	1.93	0.51
1:A:147:ASN:N	1:A:147:ASN:OD1	2.39	0.51
1:A:192:ASP:O	1:A:193:ASN:CG	2.49	0.51
1:B:190:ILE:HG12	1:B:197:ILE:HG22	1.93	0.51
1:B:208:ILE:HG12	1:B:242:GLY:H	1.76	0.51
1:B:192:ASP:O	1:B:192:ASP:CG	2.49	0.51
1:B:72:PRO:HB3	1:B:101:MET:HE2	1.93	0.50
1:B:77:GLU:O	1:B:77:GLU:CG	2.59	0.50
1:B:161:ILE:HA	1:B:164:LEU:HD23	1.93	0.50
1:A:210:TYR:O	1:A:211:GLU:C	2.49	0.50
1:B:100:ASN:O	1:B:103:LEU:HB2	2.11	0.50
1:B:210:TYR:CD1	1:B:210:TYR:N	2.80	0.50
1:B:210:TYR:CG	1:B:211:GLU:C	2.86	0.49
2:C:5:DT:H2''	2:C:6:DA:H8	1.75	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:207:ASN:N	1:B:207:ASN:OD1	2.45	0.49
1:A:176:VAL:HG21	1:A:216:LEU:HB2	1.93	0.49
1:A:109:GLU:O	1:A:110:ASN:HB2	2.12	0.49
1:A:193:ASN:O	1:A:194:GLU:HB2	2.11	0.49
1:A:75:TYR:HE1	1:A:82:MET:HB3	1.77	0.49
1:B:158:ILE:HB	1:B:195:ASP:HB3	1.93	0.49
1:B:209:ASN:C	1:B:210:TYR:CD1	2.85	0.49
1:A:171:TYR:CD2	1:A:219:PHE:HA	2.47	0.49
2:G:7:DT:H1'	2:G:8:DC:H5'	1.93	0.49
1:B:134:SER:HA	1:B:135:GLU:OE1	2.13	0.49
1:A:158:ILE:CG1	1:A:192:ASP:HB3	2.41	0.49
1:B:210:TYR:CD2	1:B:211:GLU:C	2.85	0.48
2:G:7:DT:C2'	2:G:8:DC:H5'	2.43	0.48
1:B:50:ASN:OD1	1:B:79:LYS:HD2	2.13	0.48
1:A:162:LYS:NZ	1:A:196:ASN:O	2.41	0.48
1:B:151:SER:O	1:B:154:GLU:N	2.42	0.48
1:B:151:SER:O	1:B:154:GLU:HB2	2.13	0.48
1:A:193:ASN:O	1:A:194:GLU:CB	2.61	0.48
1:A:179:LYS:HE3	1:A:179:LYS:HB3	1.71	0.47
1:B:74:ASN:HA	1:B:80:GLU:C	2.33	0.47
1:B:157:LYS:HD3	1:B:159:SER:OG	2.14	0.47
1:A:61:PRO:HA	1:A:115:ILE:O	2.13	0.47
1:A:206:HIS:H	1:A:206:HIS:CD2	2.31	0.47
1:B:88:ALA:HB1	1:B:148:ILE:HD11	1.96	0.47
1:B:116:SER:O	1:B:117:LYS:HB2	2.14	0.47
1:A:166:SER:HB2	1:B:150:ARG:NH2	2.30	0.47
1:A:104:LYS:O	1:A:104:LYS:HD2	2.15	0.47
2:G:8:DC:H2''	2:G:9:DG:O4'	2.14	0.47
1:B:46:THR:N	1:B:47:PRO:CD	2.78	0.47
2:C:2:DC:H2''	2:C:3:DG:C5'	2.45	0.47
1:B:53:LYS:HD2	2:F:11:DT:H3'	1.97	0.46
1:B:176:VAL:HG12	1:B:177:GLU:O	2.16	0.46
1:B:157:LYS:NZ	1:B:194:GLU:OE1	2.48	0.46
1:A:233:HIS:HD2	1:A:234:SER:O	1.99	0.46
1:B:224:ARG:NH2	2:G:2:DC:H2''	2.30	0.46
1:B:59:GLU:H	1:B:59:GLU:CD	2.17	0.46
1:B:50:ASN:CG	1:B:79:LYS:HD2	2.36	0.46
2:G:7:DT:C2	2:G:8:DC:H6	2.34	0.46
1:A:105:GLU:HA	2:H:1:DG:H5'	1.96	0.46
1:A:177:GLU:HB3	1:A:178:LYS:CD	2.45	0.46
1:A:92:LYS:HD3	1:A:94:TYR:CZ	2.51	0.46
1:A:186:ILE:HD11	1:A:205:GLN:HE21	1.81	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:93:TYR:C	1:A:93:TYR:CD1	2.90	0.45
1:A:74:ASN:HB2	2:I:10:DC:O3'	2.17	0.45
1:B:100:ASN:ND2	1:B:103:LEU:HD22	2.32	0.45
1:B:146:LYS:O	1:B:149:ILE:HB	2.17	0.45
2:E:6:DA:C2	2:E:7:DT:C2	3.04	0.45
1:B:210:TYR:CB	1:B:211:GLU:C	2.85	0.45
1:A:192:ASP:N	1:A:195:ASP:O	2.45	0.45
1:A:161:ILE:O	1:A:164:LEU:HB2	2.17	0.45
2:I:5:DT:H2''	2:I:6:DA:O5'	2.16	0.45
1:A:75:TYR:CD1	1:A:80:GLU:O	2.70	0.45
2:E:2:DC:H2''	2:E:3:DG:C8	2.52	0.44
1:A:182:ASN:HB2	1:A:185:SER:OG	2.16	0.44
1:B:115:ILE:HG22	1:B:133:VAL:HG22	1.99	0.44
1:B:70:THR:CG2	1:B:84:HIS:HB2	2.48	0.44
1:B:92:LYS:HE3	2:C:11:DT:OP1	2.17	0.44
1:B:208:ILE:HD11	1:B:242:GLY:HA3	2.00	0.44
1:A:100:ASN:HB3	1:A:103:LEU:HD22	2.00	0.44
1:B:117:LYS:NZ	1:B:132:THR:HG23	2.33	0.44
1:B:180:LYS:HG3	1:B:181:VAL:N	2.33	0.44
1:A:174:PHE:N	1:A:216:LEU:O	2.42	0.44
1:B:57:LEU:HB2	1:B:119:PHE:CD2	2.53	0.44
1:A:178:LYS:N	1:A:178:LYS:CD	2.41	0.43
2:F:5:DT:H2''	2:F:6:DA:C8	2.54	0.43
1:B:210:TYR:HB3	1:B:214:ASP:N	2.30	0.43
1:A:157:LYS:O	1:A:160:LYS:N	2.51	0.43
2:G:8:DC:O2	2:G:9:DG:C8	2.71	0.43
1:B:118:TYR:H	1:B:118:TYR:HD1	1.63	0.43
1:B:210:TYR:CD2	1:B:211:GLU:O	2.71	0.43
1:B:49:LYS:HD2	1:B:50:ASN:H	1.84	0.43
1:B:156:LEU:HD22	1:B:157:LYS:H	1.82	0.43
1:B:156:LEU:CD2	1:B:157:LYS:H	2.31	0.43
1:A:75:TYR:HE2	1:A:76:LYS:HD3	1.84	0.43
2:I:2:DC:H2''	2:I:3:DG:C8	2.53	0.43
1:A:128:ASN:OD1	1:A:130:THR:HB	2.19	0.43
1:B:210:TYR:CG	1:B:211:GLU:O	2.72	0.43
1:B:50:ASN:OD1	1:B:79:LYS:HG2	2.18	0.43
1:A:166:SER:HB2	1:B:150:ARG:HH22	1.84	0.43
2:I:6:DA:H1'	2:I:7:DT:H5'	2.00	0.43
1:A:169:LEU:HD12	1:A:169:LEU:HA	1.70	0.42
1:B:51:ILE:HG23	1:B:126:GLU:OE1	2.19	0.42
1:B:188:PHE:HB2	1:B:199:VAL:HB	2.01	0.42
1:B:162:LYS:HD3	1:B:230:PRO:HG2	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:177:GLU:HB2	1:B:189:LYS:O	2.19	0.42
2:E:3:DG:H2"	2:E:4:DA:C8	2.54	0.42
2:G:2:DC:O2	2:G:2:DC:H2'	2.19	0.42
1:B:103:LEU:HD12	1:B:103:LEU:HA	1.71	0.42
1:B:208:ILE:CG1	1:B:242:GLY:H	2.32	0.42
1:A:207:ASN:ND2	1:A:208:ILE:N	2.68	0.41
1:A:59:GLU:CG	1:A:60:LYS:H	2.21	0.41
1:A:199:VAL:HG22	1:A:232:LEU:HB2	2.02	0.41
1:B:211:GLU:N	1:B:212:LYS:CD	2.61	0.41
2:F:5:DT:H2"	2:F:6:DA:H5'	2.01	0.41
1:B:210:TYR:N	1:B:211:GLU:CA	2.82	0.41
1:A:156:LEU:HA	1:A:156:LEU:HD23	1.87	0.41
1:B:53:LYS:CD	2:F:11:DT:H3'	2.50	0.41
1:A:177:GLU:OE1	1:A:191:LYS:HG3	2.21	0.41
1:A:208:ILE:CD1	1:A:208:ILE:H	2.15	0.41
2:D:11:DT:H1'	2:D:12:DG:H5'	2.02	0.41
1:B:210:TYR:N	1:B:211:GLU:C	2.72	0.41
1:A:144:VAL:HA	1:A:145:PRO:HD3	1.86	0.41
1:B:171:TYR:CD2	1:B:219:PHE:HA	2.56	0.41
1:B:210:TYR:HB3	1:B:214:ASP:CB	2.50	0.41
1:A:208:ILE:HB	1:A:210:TYR:CE2	2.56	0.41
1:A:74:ASN:HB2	2:I:11:DT:OP2	2.20	0.41
1:A:108:THR:O	1:A:109:GLU:C	2.59	0.41
1:A:158:ILE:HG13	1:A:192:ASP:HB2	2.02	0.40
1:A:75:TYR:CE2	1:A:76:LYS:HD3	2.56	0.40
1:B:224:ARG:HH21	2:G:3:DG:P	2.44	0.40
1:B:157:LYS:HE3	1:B:159:SER:OG	2.21	0.40
1:B:208:ILE:CD1	1:B:242:GLY:H	2.34	0.40
2:F:6:DA:C2	2:F:7:DT:C2	3.09	0.40
1:A:182:ASN:O	1:A:184:LYS:N	2.55	0.40
1:B:161:ILE:O	1:B:164:LEU:HB2	2.20	0.40
1:A:138:PRO:HA	1:A:141:MET:SD	2.61	0.40
1:B:167:GLY:HA2	2:G:3:DG:OP1	2.21	0.40
1:B:210:TYR:CA	1:B:211:GLU:C	2.89	0.40
1:A:194:GLU:C	1:A:195:ASP:OD1	2.60	0.40
1:A:49:LYS:O	1:A:50:ASN:HB2	2.21	0.40
1:B:59:GLU:HG2	1:B:60:LYS:H	1.87	0.40
1:B:190:ILE:CG1	1:B:197:ILE:HG22	2.51	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:11:DT:O3'	3:D:101:SO4:O2[3_554]	1.37	0.83
1:B:205:GLN:OE1	1:B:211:GLU:CB[4_555]	2.06	0.14
1:B:198:LYS:NZ	2:F:4:DA:OP2[3_554]	2.19	0.01

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	197/199 (99%)	173 (88%)	20 (10%)	4 (2%)	11	40
1	B	196/199 (98%)	175 (89%)	15 (8%)	6 (3%)	7	25
All	All	393/398 (99%)	348 (88%)	35 (9%)	10 (2%)	9	32

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	79	LYS
1	B	209	ASN
1	B	212	LYS
1	A	73	PHE
1	A	194	GLU
1	B	193	ASN
1	B	80	GLU
1	B	146	LYS
1	A	211	GLU
1	A	213	GLY

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	178/180 (99%)	147 (83%)	31 (17%)	3	8

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	177/180 (98%)	153 (86%)	24 (14%)	5	15
All	All	355/360 (99%)	300 (84%)	55 (16%)	4	11

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	THR
1	A	68	THR
1	A	76	LYS
1	A	91	SER
1	A	103	LEU
1	A	104	LYS
1	A	108	THR
1	A	134	SER
1	A	139	ASN
1	A	143	GLU
1	A	147	ASN
1	A	159	SER
1	A	160	LYS
1	A	166	SER
1	A	169	LEU
1	A	177	GLU
1	A	178	LYS
1	A	179	LYS
1	A	180	LYS
1	A	187	THR
1	A	192	ASP
1	A	193	ASN
1	A	195	ASP
1	A	204	GLU
1	A	206	HIS
1	A	207	ASN
1	A	208	ILE
1	A	209	ASN
1	A	236	ASN
1	A	240	ILE
1	A	243	GLU
1	B	57	LEU
1	B	71	GLU
1	B	74	ASN
1	B	79	LYS
1	B	80	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	81	ASN
1	B	103	LEU
1	B	109	GLU
1	B	116	SER
1	B	148	ILE
1	B	151	SER
1	B	156	LEU
1	B	179	LYS
1	B	180	LYS
1	B	182	ASN
1	B	191	LYS
1	B	193	ASN
1	B	195	ASP
1	B	207	ASN
1	B	208	ILE
1	B	209	ASN
1	B	210	TYR
1	B	212	LYS
1	B	224	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	206	HIS
1	A	207	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

5 ligands 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	SO4	A	301	-	4,4,4	0.21	0	6,6,6	0.08	0
3	SO4	A	302	-	4,4,4	1.56	0	6,6,6	1.64	1 (16%)
3	SO4	B	301	-	4,4,4	0.27	0	6,6,6	0.08	0
3	SO4	C	101	-	4,4,4	0.14	0	6,6,6	0.11	0
3	SO4	D	101	-	4,4,4	1.56	0	6,6,6	1.64	1 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SO4	A	301	-	-	0/0/0/0	0/0/0/0
3	SO4	A	302	-	-	0/0/0/0	0/0/0/0
3	SO4	B	301	-	-	0/0/0/0	0/0/0/0
3	SO4	C	101	-	-	0/0/0/0	0/0/0/0
3	SO4	D	101	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	101	SO4	O4-S-O3	3.86	125.39	109.08
3	A	302	SO4	O4-S-O3	3.86	125.39	109.08

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	199/199 (100%)	0.15	7 (3%) 42 51	27, 50, 110, 180	0
1	B	198/199 (99%)	0.35	11 (5%) 24 30	26, 66, 121, 154	0
2	C	11/12 (91%)	-0.23	0 100 100	58, 72, 103, 103	0
2	D	12/12 (100%)	-0.28	0 100 100	39, 49, 125, 139	0
2	E	11/12 (91%)	0.24	1 (9%) 9 12	47, 63, 129, 162	0
2	F	9/12 (75%)	-0.10	0 100 100	20, 86, 108, 122	0
2	G	9/12 (75%)	0.17	0 100 100	59, 88, 132, 167	0
2	H	12/12 (100%)	-0.29	0 100 100	52, 58, 72, 82	0
2	I	12/12 (100%)	-0.25	0 100 100	46, 53, 65, 76	0
All	All	473/482 (98%)	0.19	19 (4%) 33 45	20, 59, 120, 180	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	209	ASN	6.2
1	B	227	ASN	6.1
1	B	210	TYR	5.2
1	A	179	LYS	3.5
1	B	177	GLU	3.5
2	E	11	DT	3.5
1	B	189	LYS	3.3
1	B	243	GLU	3.2
1	A	178	LYS	3.1
1	A	211	GLU	2.9
1	B	211	GLU	2.6
1	A	243	GLU	2.4
1	B	205	GLN	2.3
1	A	212	LYS	2.3
1	B	53	LYS	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	156	LEU	2.2
1	B	175	ALA	2.1
1	A	45	SER	2.1
1	A	177	GLU	2.1

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

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

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(Å ²)	Q<0.9
3	SO4	A	302	5/5	0.63	12.32	30,30,30,30	0
3	SO4	D	101	5/5	0.47	7.65	30,30,30,30	0
3	SO4	A	301	5/5	0.30	3.09	109,113,117,117	0
3	SO4	B	301	5/5	0.26	1.88	133,138,142,146	0
3	SO4	C	101	5/5	0.21	0.89	104,111,113,116	0

6.5 Other polymers ⓘ

There are no such residues in this entry.