



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 17, 2021 – 05:17 AM EDT

PDB ID : 1KKM
Title : L.casei HprK/P in complex with B.subtilis P-Ser-HPr
Authors : Fieulaine, S.; Morera, S.; Poncet, S.; Galinier, A.; Janin, J.; Deutscher, J.; Nessler, S.
Deposited on : 2001-12-10
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.23.2
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

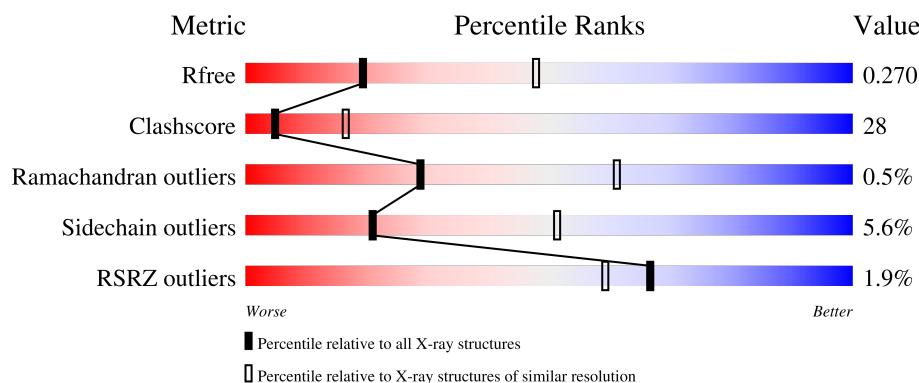
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	205	<div> <div>5%</div> <div> <div></div> <div>53%</div> <div>30%</div> <div>•</div> <div>14%</div> </div> </div>
1	B	205	<div> <div>%</div> <div> <div></div> <div>54%</div> <div>29%</div> <div>•</div> <div>14%</div> </div> </div>
1	C	205	<div> <div></div> <div> <div></div> <div>52%</div> <div>30%</div> <div>•</div> <div>15%</div> </div> </div>
2	H	100	<div> <div>%</div> <div> <div></div> <div>47%</div> <div>34%</div> <div>5%</div> <div>•</div> <div>13%</div> </div> </div>
2	I	100	<div> <div></div> <div> <div></div> <div>48%</div> <div>33%</div> <div>•</div> <div>•</div> <div>13%</div> </div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	J	100	

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
4	PO4	A	501	-	-	X	-
4	PO4	B	502	-	-	X	-
4	PO4	C	503	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6051 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 HprK protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	176	Total	C	N	O	S	0	0	0
			1336	847	233	252	4			
1	B	177	Total	C	N	O	S	0	0	0
			1337	848	233	252	4			
1	C	175	Total	C	N	O	S	0	0	0
			1331	844	232	251	4			

There are 39 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	115	MET	-	expression tag	UNP Q9RE09
A	116	ARG	-	expression tag	UNP Q9RE09
A	117	GLY	-	expression tag	UNP Q9RE09
A	118	SER	-	expression tag	UNP Q9RE09
A	119	HIS	-	expression tag	UNP Q9RE09
A	120	HIS	-	expression tag	UNP Q9RE09
A	121	HIS	-	expression tag	UNP Q9RE09
A	122	HIS	-	expression tag	UNP Q9RE09
A	123	HIS	-	expression tag	UNP Q9RE09
A	124	HIS	-	expression tag	UNP Q9RE09
A	125	GLY	-	expression tag	UNP Q9RE09
A	126	SER	-	expression tag	UNP Q9RE09
A	127	MET	-	expression tag	UNP Q9RE09
B	115	MET	-	expression tag	UNP Q9RE09
B	116	ARG	-	expression tag	UNP Q9RE09
B	117	GLY	-	expression tag	UNP Q9RE09
B	118	SER	-	expression tag	UNP Q9RE09
B	119	HIS	-	expression tag	UNP Q9RE09
B	120	HIS	-	expression tag	UNP Q9RE09
B	121	HIS	-	expression tag	UNP Q9RE09
B	122	HIS	-	expression tag	UNP Q9RE09
B	123	HIS	-	expression tag	UNP Q9RE09
B	124	HIS	-	expression tag	UNP Q9RE09

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	125	GLY	-	expression tag	UNP Q9RE09
B	126	SER	-	expression tag	UNP Q9RE09
B	127	MET	-	expression tag	UNP Q9RE09
C	115	MET	-	expression tag	UNP Q9RE09
C	116	ARG	-	expression tag	UNP Q9RE09
C	117	GLY	-	expression tag	UNP Q9RE09
C	118	SER	-	expression tag	UNP Q9RE09
C	119	HIS	-	expression tag	UNP Q9RE09
C	120	HIS	-	expression tag	UNP Q9RE09
C	121	HIS	-	expression tag	UNP Q9RE09
C	122	HIS	-	expression tag	UNP Q9RE09
C	123	HIS	-	expression tag	UNP Q9RE09
C	124	HIS	-	expression tag	UNP Q9RE09
C	125	GLY	-	expression tag	UNP Q9RE09
C	126	SER	-	expression tag	UNP Q9RE09
C	127	MET	-	expression tag	UNP Q9RE09

- Molecule 2 is a protein called PHOSPHOCARRIER PROTEIN HPR.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	H	87	Total	C	N	O	P	S	0	0	0
			618	376	102	136	1	3			
2	I	87	Total	C	N	O	P	S	0	0	0
			618	376	102	136	1	3			
2	J	87	Total	C	N	O	P	S	0	0	0
			622	379	103	136	1	3			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	-11	MET	-	expression tag	UNP P08877
H	-10	ARG	-	expression tag	UNP P08877
H	-9	GLY	-	expression tag	UNP P08877
H	-8	SER	-	expression tag	UNP P08877
H	-7	HIS	-	expression tag	UNP P08877
H	-6	HIS	-	expression tag	UNP P08877
H	-5	HIS	-	expression tag	UNP P08877
H	-4	HIS	-	expression tag	UNP P08877
H	-3	HIS	-	expression tag	UNP P08877
H	-2	HIS	-	expression tag	UNP P08877
H	-1	GLY	-	expression tag	UNP P08877
H	0	SER	-	expression tag	UNP P08877

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
H	46	SEP	SER	modified residue	UNP P08877
H	85	ARG	GLY	engineered mutation	UNP P08877
I	-11	MET	-	expression tag	UNP P08877
I	-10	ARG	-	expression tag	UNP P08877
I	-9	GLY	-	expression tag	UNP P08877
I	-8	SER	-	expression tag	UNP P08877
I	-7	HIS	-	expression tag	UNP P08877
I	-6	HIS	-	expression tag	UNP P08877
I	-5	HIS	-	expression tag	UNP P08877
I	-4	HIS	-	expression tag	UNP P08877
I	-3	HIS	-	expression tag	UNP P08877
I	-2	HIS	-	expression tag	UNP P08877
I	-1	GLY	-	expression tag	UNP P08877
I	0	SER	-	expression tag	UNP P08877
I	46	SEP	SER	modified residue	UNP P08877
I	85	ARG	GLY	engineered mutation	UNP P08877
J	-11	MET	-	expression tag	UNP P08877
J	-10	ARG	-	expression tag	UNP P08877
J	-9	GLY	-	expression tag	UNP P08877
J	-8	SER	-	expression tag	UNP P08877
J	-7	HIS	-	expression tag	UNP P08877
J	-6	HIS	-	expression tag	UNP P08877
J	-5	HIS	-	expression tag	UNP P08877
J	-4	HIS	-	expression tag	UNP P08877
J	-3	HIS	-	expression tag	UNP P08877
J	-2	HIS	-	expression tag	UNP P08877
J	-1	GLY	-	expression tag	UNP P08877
J	0	SER	-	expression tag	UNP P08877
J	46	SEP	SER	modified residue	UNP P08877
J	85	ARG	GLY	engineered mutation	UNP P08877

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Ca 1 1	0	0
3	B	1	Total Ca 1 1	0	0
3	C	1	Total Ca 1 1	0	0

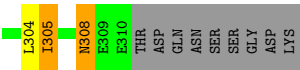
- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



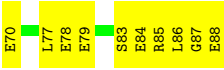
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			5	4	1		
4	B	1	Total	O	P	1	0
			5	4	1		
4	C	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	39	Total	O	0	0
			39	39		
5	B	48	Total	O	0	0
			48	48		
5	C	40	Total	O	0	0
			40	40		
5	H	14	Total	O	0	0
			14	14		
5	I	14	Total	O	0	0
			14	14		
5	J	16	Total	O	0	0
			16	16		



• Molecule 2: PHOSPHOCARRIER PROTEIN HPR



• Molecule 2: PHOSPHOCARRIER PROTEIN HPR



• Molecule 2: PHOSPHOCARRIER PROTEIN HPR



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 1 2	Depositor
Cell constants a, b, c, α , β , γ	80.83Å 80.83Å 252.49Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.80 19.96 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.1 (30.00-2.80) 99.3 (19.96-2.80)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	9.31 (at 2.79Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.200 , 0.257 0.226 , 0.270	Depositor DCC
R_{free} test set	1133 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	55.0	Xtriage
Anisotropy	0.365	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 65.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.053 for -h,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6051	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.82% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, CA, SEP

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	0.37	0/1357	0.72	3/1843 (0.2%)
1	B	0.37	0/1358	0.72	3/1845 (0.2%)
1	C	0.38	0/1352	0.90	3/1836 (0.2%)
2	H	0.74	1/611 (0.2%)	0.98	4/827 (0.5%)
2	I	0.52	1/611 (0.2%)	0.84	3/827 (0.4%)
2	J	0.63	1/615 (0.2%)	0.81	1/831 (0.1%)
All	All	0.47	3/5904 (0.1%)	0.82	17/8009 (0.2%)

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
2	H	0	1
2	I	0	1
2	J	0	1
All	All	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	47	ILE	C-N	-14.32	1.01	1.34
2	J	47	ILE	C-N	-11.68	1.07	1.34
2	I	47	ILE	C-N	-7.96	1.15	1.34

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	285	ARG	NE-CZ-NH1	-18.84	110.88	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	47	ILE	O-C-N	-18.10	93.74	122.70
1	C	285	ARG	NE-CZ-NH2	17.95	129.27	120.30
2	I	47	ILE	O-C-N	-14.83	98.97	122.70
2	J	47	ILE	O-C-N	-12.30	103.02	122.70
1	A	285	ARG	NE-CZ-NH2	-9.81	115.40	120.30
1	A	285	ARG	NE-CZ-NH1	9.64	125.12	120.30
1	B	285	ARG	NE-CZ-NH1	9.33	124.97	120.30
1	C	285	ARG	CD-NE-CZ	9.08	136.31	123.60
1	B	285	ARG	NE-CZ-NH2	-8.99	115.80	120.30
2	H	47	ILE	CA-C-N	7.40	133.47	117.20
2	I	47	ILE	CA-C-N	6.49	131.47	117.20
2	H	47	ILE	CA-C-O	6.04	132.78	120.10
2	H	48	MET	CG-SD-CE	5.47	108.95	100.20
2	I	48	MET	CG-SD-CE	5.17	108.48	100.20
1	A	285	ARG	CD-NE-CZ	5.12	130.77	123.60
1	B	285	ARG	CD-NE-CZ	5.02	130.63	123.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	46	SEP	Mainchain
2	I	46	SEP	Mainchain
2	J	46	SEP	Mainchain

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	1336	0	1342	67	0
1	B	1337	0	1338	80	0
1	C	1331	0	1340	83	0
2	H	618	0	581	47	0
2	I	618	0	582	46	0
2	J	622	0	593	27	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1	0	0	0	0
4	A	5	0	0	3	0
4	B	5	0	0	3	0
4	C	5	0	0	3	0
5	A	39	0	0	1	0
5	B	48	0	0	2	0
5	C	40	0	0	2	0
5	H	14	0	0	0	0
5	I	14	0	0	2	0
5	J	16	0	0	0	0
All	All	6051	0	5776	322	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 28.

All (322) 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:I:47:ILE:O	2:I:48:MET:C	1.70	1.19
2:J:47:ILE:O	2:J:48:MET:C	1.69	1.17
2:I:23:VAL:HG11	2:I:47:ILE:HD13	1.45	0.96
1:C:143:LEU:HD11	1:C:228:ILE:HD11	1.49	0.94
1:C:301:LEU:O	1:C:305:ILE:HD13	1.66	0.94
1:B:152:LEU:HB3	1:B:231:ILE:HD13	1.48	0.94
2:I:47:ILE:O	2:I:49:GLY:N	2.01	0.92
1:A:191:ILE:HD11	1:A:258:VAL:HB	1.51	0.92
1:C:143:LEU:HD21	1:C:228:ILE:HD12	1.50	0.92
2:H:67:GLY:O	2:H:70:GLU:HG3	1.69	0.91
1:A:273:LEU:O	1:A:277:ILE:HD13	1.71	0.90
2:H:47:ILE:HD12	2:H:50:VAL:HB	1.54	0.90
2:H:19:ALA:HB1	2:H:47:ILE:HD11	1.53	0.88
1:B:152:LEU:HB3	1:B:231:ILE:CD1	2.04	0.86
2:I:23:VAL:CG1	2:I:47:ILE:HD13	2.08	0.82
1:A:166:LEU:HD21	1:C:279:VAL:HG21	1.63	0.81
1:A:191:ILE:HG22	1:A:228:ILE:HD13	1.62	0.80
1:B:279:VAL:HG21	1:C:166:LEU:HD21	1.64	0.80
2:I:67:GLY:H	2:I:70:GLU:HG3	1.46	0.80
2:I:47:ILE:HD12	2:I:50:VAL:HB	1.63	0.79
1:C:230:LEU:HD11	1:C:263:ILE:HD13	1.65	0.78
2:I:63:ILE:HG21	2:I:77:LEU:HD13	1.67	0.77
1:B:230:LEU:HD11	1:B:263:ILE:HD13	1.66	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:176:ILE:HD13	1:B:223:ARG:O	1.85	0.76
1:C:238:THR:HB	1:C:241:LYS:HE2	1.67	0.75
2:I:19:ALA:HB1	2:I:47:ILE:HD11	1.69	0.75
1:C:152:LEU:HB3	1:C:231:ILE:CD1	2.17	0.74
1:B:309:GLU:HB3	2:J:56:ALA:HB1	1.68	0.74
2:H:9:THR:HG23	2:H:87:GLY:HA2	1.70	0.74
2:H:35:LEU:HG	2:H:63:ILE:CD1	2.18	0.74
1:A:136:ARG:HG2	1:A:184:TYR:HB3	1.71	0.73
1:A:191:ILE:HD13	1:A:255:ILE:HB	1.70	0.73
2:I:67:GLY:H	2:I:70:GLU:CG	2.03	0.72
1:C:152:LEU:HD23	1:C:231:ILE:HD12	1.71	0.72
1:C:272:ASN:C	1:C:272:ASN:HD22	1.92	0.72
2:J:47:ILE:O	2:J:49:GLY:N	2.23	0.72
1:A:255:ILE:HD12	1:A:260:VAL:HG21	1.72	0.72
1:B:272:ASN:C	1:B:272:ASN:HD22	1.93	0.71
2:H:47:ILE:HG23	2:H:48:MET:N	2.04	0.71
1:C:161:LYS:HG3	4:C:503:PO4:O2	1.89	0.71
2:H:23:VAL:HG11	2:H:47:ILE:HD13	1.71	0.71
1:A:272:ASN:C	1:A:272:ASN:HD22	1.93	0.71
1:C:191:ILE:HD11	1:C:255:ILE:O	1.91	0.70
1:C:176:ILE:HG12	1:C:226:THR:HG22	1.73	0.70
1:A:279:VAL:HG21	1:B:166:LEU:HD21	1.73	0.68
1:B:176:ILE:HG13	1:B:226:THR:HG22	1.75	0.68
2:I:67:GLY:O	2:I:70:GLU:HG3	1.94	0.68
1:A:198:ILE:HD13	1:C:304:LEU:HD22	1.74	0.68
2:I:47:ILE:HG23	2:I:48:MET:N	2.09	0.67
1:B:146:ILE:HD13	1:B:173:HIS:CB	2.25	0.67
1:A:176:ILE:HG12	1:A:226:THR:HG22	1.76	0.66
1:B:176:ILE:HD12	1:B:225:ASP:CA	2.25	0.66
2:H:37:TYR:CE1	2:H:55:ILE:HA	2.31	0.66
1:B:254:LEU:O	1:B:255:ILE:HD13	1.95	0.66
1:C:305:ILE:HD11	2:H:54:GLY:HA2	1.77	0.66
1:C:146:ILE:HD13	1:C:173:HIS:HB3	1.77	0.65
1:C:143:LEU:HD21	1:C:228:ILE:CD1	2.26	0.65
1:C:152:LEU:HB3	1:C:231:ILE:HD13	1.78	0.65
2:I:35:LEU:HG	2:I:63:ILE:CD1	2.27	0.65
1:B:146:ILE:HD13	1:B:173:HIS:HB3	1.77	0.65
1:A:146:ILE:HD13	1:A:173:HIS:HB3	1.79	0.64
1:B:145:ASP:CG	1:B:174:ARG:NH1	2.51	0.64
2:I:47:ILE:C	2:I:49:GLY:N	2.48	0.63
1:C:230:LEU:CD1	1:C:263:ILE:HD13	2.29	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:ILE:HD13	1:A:173:HIS:CB	2.30	0.62
1:B:269:VAL:HG12	1:C:269:VAL:HG12	1.81	0.62
1:B:191:ILE:HD13	1:B:258:VAL:HB	1.81	0.62
1:C:164:THR:HG21	1:C:277:ILE:HD12	1.82	0.62
1:B:309:GLU:HG3	1:B:310:GLU:OE2	2.00	0.62
1:C:305:ILE:CD1	2:H:54:GLY:HA2	2.30	0.61
2:H:20:THR:O	2:H:24:GLN:HB2	2.00	0.61
2:I:32:ASP:O	2:I:65:ALA:HA	2.00	0.61
1:B:152:LEU:HD23	1:B:231:ILE:HD12	1.82	0.61
2:I:44:LEU:HD11	2:I:63:ILE:HD12	1.82	0.61
1:B:176:ILE:HD12	1:B:225:ASP:HA	1.82	0.61
1:B:230:LEU:CD1	1:B:263:ILE:HD13	2.29	0.60
2:H:44:LEU:CD1	2:H:63:ILE:HD12	2.31	0.60
1:C:159:VAL:CG2	1:C:267:VAL:HG21	2.32	0.59
1:B:263:ILE:HA	5:B:508:HOH:O	2.02	0.59
2:H:23:VAL:CG1	2:H:47:ILE:HD13	2.33	0.59
2:I:8:VAL:HG21	2:I:55:ILE:CG2	2.33	0.59
1:A:198:ILE:HD13	1:C:304:LEU:CD2	2.32	0.59
1:C:166:LEU:HD22	1:C:205:ILE:CD1	2.33	0.59
2:J:2:ALA:HB1	2:J:74:LEU:HD23	1.85	0.58
1:B:166:LEU:HD22	1:B:205:ILE:CD1	2.33	0.58
1:A:238:THR:OG1	1:A:241:LYS:HG3	2.03	0.58
1:A:166:LEU:HD22	1:A:205:ILE:CD1	2.34	0.58
1:C:146:ILE:HD13	1:C:173:HIS:CB	2.34	0.58
2:H:79:GLU:O	2:H:83:SER:HB2	2.03	0.58
1:C:191:ILE:HD13	1:C:255:ILE:HB	1.86	0.58
1:C:238:THR:HG22	1:C:240:ASP:H	1.69	0.58
2:J:19:ALA:O	2:J:23:VAL:HG13	2.04	0.58
1:C:166:LEU:HD22	1:C:205:ILE:HD13	1.84	0.58
2:J:67:GLY:O	2:J:70:GLU:HG2	2.04	0.58
1:A:269:VAL:HG12	1:B:269:VAL:HG12	1.86	0.58
2:I:44:LEU:CD1	2:I:63:ILE:HD12	2.33	0.58
1:B:166:LEU:HD22	1:B:205:ILE:HD13	1.85	0.58
1:B:191:ILE:CG2	1:B:228:ILE:HD12	2.33	0.57
1:C:159:VAL:HG12	4:C:503:PO4:O2	2.03	0.57
2:H:14:ILE:HD12	2:H:55:ILE:HG21	1.85	0.57
1:A:191:ILE:CD1	1:A:255:ILE:HB	2.34	0.57
1:B:146:ILE:HD13	1:B:173:HIS:CG	2.39	0.57
1:B:272:ASN:HB2	5:C:517:HOH:O	2.04	0.57
1:C:191:ILE:CD1	1:C:258:VAL:HB	2.33	0.57
2:J:32:ASP:O	2:J:65:ALA:HA	2.03	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:164:THR:HG21	1:B:277:ILE:HD12	1.85	0.57
2:H:47:ILE:CG2	2:H:48:MET:N	2.67	0.57
1:A:159:VAL:CG2	1:A:267:VAL:HG21	2.35	0.57
1:A:166:LEU:HD22	1:A:205:ILE:HD13	1.87	0.57
1:C:301:LEU:CD1	1:C:305:ILE:HD11	2.35	0.57
2:H:44:LEU:HD12	2:H:63:ILE:HD12	1.86	0.57
1:B:256:PHE:O	1:B:257:ASP:HB2	2.03	0.57
2:I:35:LEU:HG	2:I:63:ILE:HD13	1.86	0.57
1:A:146:ILE:HD13	1:A:173:HIS:CG	2.40	0.56
1:B:252:THR:HG23	1:B:253:GLN:N	2.20	0.56
1:C:243:PHE:CZ	1:C:266:PRO:HB3	2.40	0.56
1:C:252:THR:HG21	1:C:259:PRO:HB3	1.87	0.56
1:C:301:LEU:HD12	1:C:305:ILE:CD1	2.36	0.56
2:I:16:ALA:O	2:I:20:THR:HG23	2.06	0.56
2:I:66:SER:HA	2:I:70:GLU:HG2	1.87	0.56
2:J:2:ALA:HB1	2:J:74:LEU:CD2	2.34	0.56
1:C:191:ILE:HD11	1:C:258:VAL:HB	1.87	0.56
2:I:69:ASP:HB2	2:I:72:ASP:HB2	1.86	0.56
1:C:152:LEU:HB3	1:C:231:ILE:HD12	1.88	0.55
1:C:256:PHE:O	1:C:257:ASP:HB2	2.06	0.55
2:H:35:LEU:HG	2:H:63:ILE:HD11	1.89	0.55
2:I:85:ARG:HD2	5:I:96:HOH:O	2.06	0.55
1:B:136:ARG:HG3	1:B:136:ARG:HH11	1.72	0.54
1:C:305:ILE:CD1	1:C:305:ILE:N	2.71	0.54
1:B:158:GLY:H	4:B:502:PO4:P	2.31	0.54
1:A:269:VAL:HG12	1:C:269:VAL:HG12	1.90	0.54
2:I:67:GLY:N	2:I:70:GLU:HG3	2.21	0.53
1:C:262:LYS:C	1:C:263:ILE:HD12	2.29	0.53
2:J:19:ALA:HB1	2:J:47:ILE:HD11	1.91	0.53
2:H:84:GLU:HB2	2:H:86:LEU:HG	1.90	0.52
1:A:228:ILE:HD12	1:A:228:ILE:N	2.24	0.52
1:C:271:ARG:HH11	1:C:271:ARG:HG2	1.75	0.52
1:B:308:ASN:C	1:B:310:GLU:H	2.12	0.52
2:I:47:ILE:CG2	2:I:48:MET:N	2.72	0.52
1:B:145:ASP:OD1	1:B:174:ARG:NH1	2.43	0.52
1:B:271:ARG:HG2	1:B:271:ARG:HH11	1.75	0.52
2:J:47:ILE:HD12	2:J:50:VAL:HB	1.92	0.52
1:B:146:ILE:HG23	1:B:173:HIS:CE1	2.45	0.52
2:I:26:ALA:HB1	2:I:33:VAL:HG11	1.92	0.51
1:B:245:ARG:NH2	2:J:46:SEP:HA	2.25	0.51
2:H:66:SER:HA	2:H:70:GLU:OE2	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:136:ARG:HG2	1:B:184:TYR:HB3	1.91	0.51
1:B:245:ARG:NH1	1:C:204:GLU:OE1	2.44	0.51
2:J:47:ILE:HG23	2:J:48:MET:N	2.25	0.51
1:C:255:ILE:HD13	1:C:260:VAL:CG2	2.40	0.51
1:C:182:ASP:OD2	1:C:196:PRO:HG3	2.11	0.51
1:C:157:SER:HA	4:C:503:PO4:O1	2.11	0.51
1:C:191:ILE:CD1	1:C:255:ILE:HB	2.40	0.51
1:C:253:GLN:O	1:C:255:ILE:HD12	2.11	0.51
2:H:19:ALA:HB1	2:H:47:ILE:CD1	2.32	0.51
2:I:47:ILE:CD1	2:I:50:VAL:HB	2.38	0.51
1:A:159:VAL:HG12	4:A:501:PO4:O2	2.10	0.50
1:C:301:LEU:HD12	1:C:305:ILE:HD11	1.94	0.50
2:H:36:GLU:HA	2:H:40:LYS:O	2.11	0.50
2:I:35:LEU:HB2	2:I:44:LEU:HG	1.93	0.50
1:B:257:ASP:O	1:B:259:PRO:HD3	2.10	0.50
1:B:245:ARG:HH22	2:J:46:SEP:HA	1.75	0.50
1:A:238:THR:C	1:A:240:ASP:H	2.14	0.50
1:B:153:ILE:HD12	1:B:153:ILE:N	2.26	0.50
1:A:210:ILE:CD1	2:H:48:MET:SD	3.00	0.50
2:H:14:ILE:HD12	2:H:55:ILE:CG2	2.42	0.50
1:C:272:ASN:HD21	1:C:274:ALA:HB3	1.77	0.50
2:J:37:TYR:CE1	2:J:59:ALA:HB1	2.47	0.50
1:B:191:ILE:HD13	1:B:258:VAL:CB	2.42	0.49
1:C:185:GLN:NE2	1:C:258:VAL:HG23	2.26	0.49
2:I:14:ILE:CD1	2:I:86:LEU:HD22	2.42	0.49
2:I:3:GLN:HB3	2:I:64:SER:HB3	1.93	0.49
1:B:262:LYS:C	1:B:263:ILE:HD12	2.32	0.49
2:I:35:LEU:HG	2:I:63:ILE:HD11	1.94	0.49
1:A:238:THR:O	1:A:240:ASP:N	2.46	0.49
1:A:193:GLY:N	1:A:228:ILE:HD11	2.28	0.49
1:B:272:ASN:C	1:B:272:ASN:ND2	2.65	0.49
2:H:3:GLN:HG2	2:H:64:SER:HB3	1.93	0.49
2:H:35:LEU:HG	2:H:63:ILE:HD13	1.94	0.49
1:A:234:LEU:HD21	1:A:277:ILE:HD11	1.95	0.49
1:B:276:ILE:HD12	1:C:205:ILE:HG21	1.95	0.49
1:A:185:GLN:OE1	1:A:256:PHE:O	2.31	0.49
1:A:271:ARG:HH11	1:A:271:ARG:HG2	1.76	0.48
1:A:251:GLN:HG3	1:A:262:LYS:O	2.13	0.48
2:I:33:VAL:HG21	2:I:77:LEU:HD11	1.95	0.48
1:A:157:SER:HA	4:A:501:PO4:O1	2.13	0.48
1:A:228:ILE:HD12	1:A:228:ILE:H	1.79	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:256:PHE:O	1:B:257:ASP:CB	2.61	0.48
2:H:23:VAL:HG11	2:H:47:ILE:CD1	2.40	0.48
1:A:210:ILE:HD11	2:H:48:MET:SD	2.53	0.48
1:C:228:ILE:HD13	1:C:228:ILE:N	2.28	0.48
1:C:238:THR:HB	1:C:241:LYS:CE	2.40	0.48
1:B:252:THR:CG2	1:B:253:GLN:N	2.75	0.48
1:A:171:ARG:NH1	1:A:278:GLU:OE2	2.47	0.48
1:A:187:ASP:OD1	1:A:190:THR:HB	2.14	0.47
1:A:272:ASN:HD21	1:A:274:ALA:HB3	1.80	0.47
2:J:63:ILE:HG21	2:J:77:LEU:HD13	1.96	0.47
1:A:182:ASP:OD2	1:A:196:PRO:HG3	2.13	0.47
1:B:176:ILE:HG13	1:B:226:THR:CG2	2.44	0.47
2:H:35:LEU:O	2:H:41:THR:HA	2.14	0.47
2:I:2:ALA:O	2:I:74:LEU:HD11	2.14	0.47
1:A:203:LEU:HD12	1:A:211:ILE:HD11	1.96	0.47
2:H:7:LYS:N	2:H:88:GLU:O	2.39	0.47
2:J:47:ILE:HD11	2:J:51:MET:HG3	1.95	0.47
1:C:146:ILE:HG23	1:C:173:HIS:CE1	2.48	0.47
2:H:38:ASN:N	2:H:38:ASN:HD22	2.13	0.47
1:B:176:ILE:CD1	1:B:223:ARG:HB3	2.45	0.47
2:H:23:VAL:HG12	2:H:50:VAL:HG21	1.97	0.47
1:A:275:ILE:HG23	1:B:170:GLN:OE1	2.15	0.46
1:B:309:GLU:HB3	2:J:56:ALA:CB	2.42	0.46
1:A:145:ASP:HB2	1:A:176:ILE:HD11	1.96	0.46
1:C:272:ASN:C	1:C:272:ASN:ND2	2.64	0.46
1:B:236:ASN:HA	1:B:267:VAL:HB	1.98	0.46
1:C:301:LEU:HD11	1:C:305:ILE:HD11	1.98	0.46
2:I:67:GLY:N	2:I:70:GLU:CG	2.77	0.46
2:J:18:PRO:HA	2:J:21:VAL:HG12	1.97	0.46
1:A:256:PHE:O	1:A:257:ASP:HB2	2.16	0.46
1:C:144:VAL:HG11	1:C:146:ILE:HD11	1.98	0.46
2:I:23:VAL:HG11	2:I:47:ILE:CD1	2.31	0.46
2:H:43:ASN:OD1	2:H:45:LYS:HB2	2.16	0.46
1:B:157:SER:CB	2:I:46:SEP:O2P	2.64	0.45
1:B:171:ARG:NH2	5:B:511:HOH:O	2.49	0.45
1:B:204:GLU:HB2	2:I:48:MET:CG	2.46	0.45
1:B:145:ASP:CG	1:B:174:ARG:HH11	2.20	0.45
1:C:145:ASP:OD2	1:C:145:ASP:C	2.54	0.45
2:H:6:PHE:CE2	2:H:78:GLU:HG3	2.51	0.45
2:J:17:ARG:O	2:J:20:THR:HB	2.17	0.45
1:C:185:GLN:HE21	1:C:258:VAL:HG23	1.82	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:37:TYR:HE1	2:J:59:ALA:HB1	1.81	0.45
1:A:145:ASP:CG	1:A:174:ARG:NH1	2.70	0.45
1:C:272:ASN:CG	1:C:275:ILE:HG12	2.37	0.45
2:H:67:GLY:H	2:H:70:GLU:CG	2.30	0.45
2:I:47:ILE:C	2:I:49:GLY:H	2.19	0.45
2:J:47:ILE:HG13	2:J:51:MET:HE2	1.99	0.45
1:B:243:PHE:CE2	1:B:266:PRO:HB3	2.52	0.45
2:I:71:ASN:ND2	5:I:101:HOH:O	2.50	0.45
1:B:139:MET:SD	1:B:255:ILE:HD12	2.57	0.45
1:B:182:ASP:OD2	1:B:196:PRO:HG3	2.16	0.44
2:H:29:TYR:O	2:H:45:LYS:NZ	2.37	0.44
1:B:272:ASN:HD21	1:B:274:ALA:HB3	1.83	0.44
2:H:47:ILE:CD1	2:H:50:VAL:HB	2.38	0.44
1:B:171:ARG:NH1	1:B:278:GLU:OE2	2.49	0.44
1:A:230:LEU:HD12	1:A:231:ILE:H	1.82	0.44
1:C:142:VAL:HG11	1:C:165:ALA:HB2	2.00	0.44
2:I:18:PRO:HB3	2:I:86:LEU:HD21	1.98	0.44
2:I:6:PHE:HD1	2:I:88:GLU:HA	1.82	0.44
1:A:272:ASN:C	1:A:272:ASN:ND2	2.65	0.44
1:A:201:HIS:HD2	5:A:526:HOH:O	2.01	0.44
2:J:37:TYR:O	2:J:38:ASN:HB2	2.18	0.44
1:C:240:ASP:OD2	1:C:240:ASP:N	2.51	0.43
2:H:37:TYR:CD1	2:H:55:ILE:HG12	2.53	0.43
2:J:18:PRO:HB3	2:J:86:LEU:HD21	2.00	0.43
1:B:159:VAL:HG12	4:B:502:PO4:O2	2.18	0.43
1:A:183:VAL:HA	1:A:192:VAL:O	2.19	0.43
2:I:14:ILE:HD11	2:I:86:LEU:HB3	2.00	0.43
1:B:143:LEU:HB3	1:B:176:ILE:HB	2.00	0.43
1:B:191:ILE:HG22	1:B:228:ILE:HD12	2.00	0.43
1:B:306:GLU:O	1:B:309:GLU:HG2	2.18	0.43
2:H:67:GLY:N	2:H:70:GLU:HG2	2.34	0.43
1:A:272:ASN:CG	1:A:275:ILE:HG12	2.39	0.43
1:C:203:LEU:HD12	1:C:211:ILE:HD11	2.00	0.43
1:C:301:LEU:HD12	1:C:305:ILE:HD13	2.00	0.43
1:B:191:ILE:HG21	1:B:228:ILE:HD12	2.00	0.43
1:C:308:ASN:HD22	1:C:308:ASN:HA	1.56	0.43
2:J:47:ILE:C	2:J:49:GLY:N	2.68	0.43
1:A:145:ASP:HB3	1:A:174:ARG:HB2	2.01	0.43
1:A:309:GLU:O	1:A:310:GLU:C	2.57	0.43
1:A:147:TYR:CE2	1:A:173:HIS:HE1	2.36	0.42
1:B:272:ASN:CG	1:B:275:ILE:HG12	2.39	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:ASP:C	1:A:246:LEU:H	2.22	0.42
1:C:143:LEU:HB3	1:C:176:ILE:HB	2.01	0.42
1:C:258:VAL:HA	1:C:259:PRO:HD3	1.73	0.42
1:A:276:ILE:HD12	1:B:205:ILE:HG21	2.00	0.42
1:B:176:ILE:HD12	1:B:225:ASP:N	2.33	0.42
1:C:242:THR:C	1:C:243:PHE:CD1	2.93	0.42
2:I:37:TYR:CZ	2:I:38:ASN:ND2	2.87	0.42
2:J:33:VAL:HG22	2:J:65:ALA:HB2	2.01	0.42
1:A:171:ARG:HH11	1:A:278:GLU:CD	2.23	0.42
2:H:69:ASP:O	2:H:70:GLU:C	2.58	0.42
1:A:161:LYS:HG3	4:A:501:PO4:O2	2.19	0.42
1:C:136:ARG:HD2	1:C:184:TYR:HB3	2.02	0.42
1:C:170:GLN:NE2	5:C:520:HOH:O	2.53	0.42
2:H:19:ALA:O	2:H:23:VAL:HG22	2.20	0.42
2:H:23:VAL:HG23	2:H:24:GLN:N	2.35	0.42
1:A:203:LEU:HB2	1:A:211:ILE:HD11	2.02	0.42
1:A:211:ILE:HD12	1:A:211:ILE:C	2.40	0.42
1:A:275:ILE:O	1:A:279:VAL:HG23	2.20	0.42
1:B:171:ARG:HH11	1:B:278:GLU:CD	2.22	0.42
1:C:246:LEU:C	1:C:248:SER:H	2.22	0.42
1:A:308:ASN:C	1:A:310:GLU:H	2.23	0.42
1:B:157:SER:HA	2:I:46:SEP:O2P	2.19	0.41
1:C:196:PRO:O	1:C:197:PRO:C	2.58	0.41
2:H:44:LEU:HD11	2:H:63:ILE:HD12	2.01	0.41
2:I:33:VAL:HA	2:I:64:SER:O	2.20	0.41
1:C:272:ASN:ND2	1:C:275:ILE:HG12	2.34	0.41
1:C:254:LEU:C	1:C:255:ILE:HD12	2.41	0.41
1:A:153:ILE:HD11	1:A:277:ILE:HG21	2.02	0.41
1:A:196:PRO:O	1:A:197:PRO:C	2.59	0.41
1:A:240:ASP:O	1:A:241:LYS:C	2.58	0.41
1:B:238:THR:CG2	1:B:239:PRO:HD2	2.51	0.41
1:C:185:GLN:HE21	1:C:258:VAL:CG2	2.34	0.41
2:H:63:ILE:HG21	2:H:77:LEU:HD13	2.03	0.41
1:B:269:VAL:HG12	1:C:269:VAL:CG1	2.49	0.41
1:B:140:HIS:CD2	2:I:43:ASN:HD22	2.38	0.41
1:C:171:ARG:NH1	1:C:278:GLU:OE2	2.53	0.41
1:C:179:ASP:CG	2:J:46:SEP:O3P	2.58	0.41
1:A:210:ILE:HD12	2:H:48:MET:SD	2.61	0.41
1:B:161:LYS:N	4:B:502:PO4:O3	2.53	0.41
1:C:146:ILE:HD13	1:C:173:HIS:CG	2.56	0.41
1:B:245:ARG:C	1:B:246:LEU:HD12	2.42	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:243:PHE:CE2	1:C:266:PRO:HB3	2.56	0.40
2:I:66:SER:HA	2:I:70:GLU:CG	2.51	0.40
1:A:272:ASN:ND2	1:A:275:ILE:HG12	2.36	0.40
2:H:14:ILE:HD12	2:H:55:ILE:CB	2.51	0.40
1:A:210:ILE:HD12	2:H:48:MET:CE	2.52	0.40
1:B:183:VAL:HA	1:B:192:VAL:O	2.22	0.40
1:C:211:ILE:HD12	1:C:211:ILE:C	2.41	0.40
1:A:242:THR:CG2	1:A:243:PHE:N	2.85	0.40
1:B:191:ILE:CD1	1:B:258:VAL:HB	2.51	0.40
1:B:230:LEU:HD12	1:B:231:ILE:H	1.86	0.40
1:C:164:THR:HG21	1:C:277:ILE:CD1	2.51	0.40
2:J:10:ALA:HB2	2:J:86:LEU:HA	2.02	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	174/205 (85%)	160 (92%)	13 (8%)	1 (1%)	25	56
1	B	175/205 (85%)	165 (94%)	9 (5%)	1 (1%)	25	56
1	C	173/205 (84%)	162 (94%)	11 (6%)	0	100	100
2	H	84/100 (84%)	73 (87%)	10 (12%)	1 (1%)	13	39
2	I	84/100 (84%)	70 (83%)	13 (16%)	1 (1%)	13	39
2	J	84/100 (84%)	76 (90%)	8 (10%)	0	100	100
All	All	774/915 (85%)	706 (91%)	64 (8%)	4 (0%)	29	61

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	239	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	48	MET
2	I	48	MET
1	B	309	GLU

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	143/174 (82%)	134 (94%)	9 (6%)	18	46
1	B	142/174 (82%)	135 (95%)	7 (5%)	25	57
1	C	143/174 (82%)	134 (94%)	9 (6%)	18	46
2	H	61/78 (78%)	57 (93%)	4 (7%)	16	44
2	I	61/78 (78%)	57 (93%)	4 (7%)	16	44
2	J	62/78 (80%)	61 (98%)	1 (2%)	62	88
All	All	612/756 (81%)	578 (94%)	34 (6%)	21	51

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	143	LEU
1	A	174	ARG
1	A	180	ARG
1	A	198	ILE
1	A	240	ASP
1	A	251	GLN
1	A	252	THR
1	A	272	ASN
1	A	277	ILE
1	B	143	LEU
1	B	174	ARG
1	B	244	ASP
1	B	245	ARG
1	B	252	THR
1	B	272	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	308	ASN
1	C	143	LEU
1	C	174	ARG
1	C	180	ARG
1	C	191	ILE
1	C	214	MET
1	C	252	THR
1	C	272	ASN
1	C	305	ILE
1	C	308	ASN
2	H	35	LEU
2	H	36	GLU
2	H	44	LEU
2	H	85	ARG
2	I	3	GLN
2	I	44	LEU
2	I	74	LEU
2	I	84	GLU
2	J	44	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	251	GLN
1	A	272	ASN
1	A	283	ASN
1	A	300	ASN
1	A	308	ASN
1	B	140	HIS
1	B	189	GLN
1	B	201	HIS
1	B	272	ASN
1	B	283	ASN
1	B	300	ASN
1	B	302	ASN
1	B	308	ASN
1	C	185	GLN
1	C	272	ASN
1	C	283	ASN
1	C	300	ASN
1	C	303	HIS
1	C	307	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	308	ASN
2	H	3	GLN
2	H	38	ASN
2	I	38	ASN
2	I	71	ASN
2	J	24	GLN
2	J	34	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 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	$\# Z > 2$
2	SEP	H	46	2,3	8,9,10	0.77	0	8,12,14	1.81	2 (25%)
2	SEP	J	46	2,3	8,9,10	0.69	0	8,12,14	2.68	3 (37%)
2	SEP	I	46	2,3	8,9,10	0.74	0	8,12,14	2.09	4 (50%)

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
2	SEP	H	46	2,3	-	1/5/8/10	-
2	SEP	J	46	2,3	-	1/5/8/10	-
2	SEP	I	46	2,3	-	2/5/8/10	-

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	46	SEP	OG-CB-CA	5.94	113.93	108.14
2	I	46	SEP	OG-CB-CA	3.45	111.50	108.14
2	H	46	SEP	OG-P-O1P	-3.08	97.84	106.47
2	J	46	SEP	OG-P-O1P	-2.33	99.94	106.47
2	I	46	SEP	O3P-P-O2P	2.28	116.37	107.64
2	J	46	SEP	O3P-P-O2P	2.27	116.31	107.64
2	H	46	SEP	O3P-P-O2P	2.27	116.30	107.64
2	I	46	SEP	O2P-P-OG	-2.24	100.78	106.73
2	I	46	SEP	OG-P-O1P	-2.06	100.69	106.47

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	46	SEP	N-CA-CB-OG
2	I	46	SEP	N-CA-CB-OG
2	J	46	SEP	N-CA-CB-OG
2	I	46	SEP	CB-OG-P-O3P

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	46	SEP	3	0
2	I	46	SEP	2	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 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	$\# Z > 2$
4	PO4	A	501	-	4,4,4	1.68	0	6,6,6	0.46	0
4	PO4	C	503	3	4,4,4	1.76	1 (25%)	6,6,6	0.46	0
4	PO4	B	502	-	4,4,4	1.82	1 (25%)	6,6,6	0.44	0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	502	PO4	P-O2	-2.16	1.48	1.54
4	C	503	PO4	P-O2	-2.06	1.48	1.54

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	501	PO4	3	0
4	C	503	PO4	3	0
4	B	502	PO4	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	I	1
2	J	1
2	H	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	47:ILE	C	48:MET	N	1.15
1	J	47:ILE	C	48:MET	N	1.07
1	H	47:ILE	C	48:MET	N	1.01

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	176/205 (85%)	-0.14	11 (6%) 20 12	25, 48, 80, 97	0
1	B	177/205 (86%)	-0.31	2 (1%) 80 75	27, 45, 75, 89	0
1	C	175/205 (85%)	-0.40	1 (0%) 89 86	27, 45, 79, 94	0
2	H	86/100 (86%)	-0.29	1 (1%) 79 73	38, 56, 77, 88	0
2	I	86/100 (86%)	-0.29	0 100 100	44, 57, 76, 95	0
2	J	86/100 (86%)	-0.25	0 100 100	38, 53, 71, 79	0
All	All	786/915 (85%)	-0.28	15 (1%) 66 59	25, 50, 78, 97	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	248	SER	4.0
1	A	242	THR	3.8
1	A	244	ASP	3.6
1	A	247	GLY	3.5
1	A	249	GLY	3.4
1	B	244	ASP	3.0
1	A	239	PRO	2.9
1	B	248	SER	2.7
1	A	246	LEU	2.6
1	A	240	ASP	2.6
1	A	135	GLU	2.6
1	A	189	GLN	2.4
1	C	244	ASP	2.3
2	H	58	GLY	2.1
1	A	241	LYS	2.1

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	SEP	J	46	10/11	0.90	0.21	53,57,59,59	4
2	SEP	I	46	10/11	0.91	0.22	58,63,72,73	4
2	SEP	H	46	10/11	0.94	0.19	52,57,65,66	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	CA	A	401	1/1	0.86	0.16	57,57,57,57	0
4	PO4	A	501	5/5	0.90	0.34	96,96,97,98	0
3	CA	B	402	1/1	0.94	0.15	48,48,48,48	0
3	CA	C	403	1/1	0.96	0.09	45,45,45,45	0
4	PO4	C	503	5/5	0.96	0.22	43,44,47,48	5
4	PO4	B	502	5/5	0.97	0.19	39,41,42,43	5

6.5 Other polymers [i](#)

There are no such residues in this entry.