Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 08:30 PM GMT

PDB ID	:	1KKL
Title	:	L.casei HprK/P in complex with B.subtilis 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

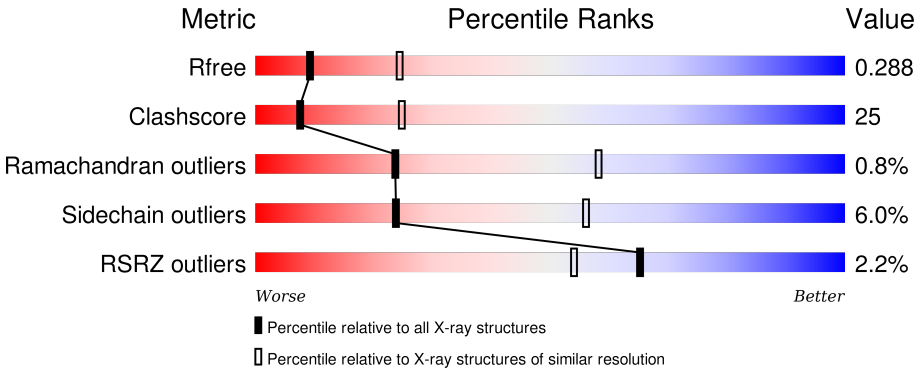
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (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 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 <=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	2% 50% 30% • 19%
1	B	205	3% 55% 24% • 19%
1	C	205	% 57% 24% • 18%
2	H	100	50% 33% • 14%
2	I	100	47% 34% 6% 13%

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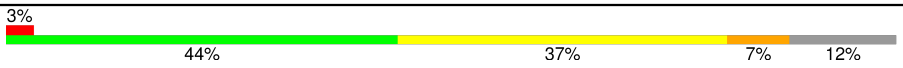
Mol	Chain	Length	Quality of chain
2	J	100	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5870 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	167	Total	C	N	O	S	0	0	0
			1275	809	223	239	4			
1	B	166	Total	C	N	O	S	0	0	0
			1255	798	219	234	4			
1	C	168	Total	C	N	O	S	0	0	0
			1275	809	223	239	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

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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	86	Total	C	N	O	S	0	0	0
			625	385	105	132	3			
2	I	87	Total	C	N	O	S	0	0	0
			630	388	106	133	3			
2	J	88	Total	C	N	O	S	0	0	0
			629	388	104	134	3			

There are 39 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

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Chain	Residue	Modelled	Actual	Comment	Reference
H	85	ARG	GLY	ENGINEERED	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	85	ARG	GLY	ENGINEERED	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	85	ARG	GLY	ENGINEERED	UNP P08877

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

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

- Molecule 4 is water.

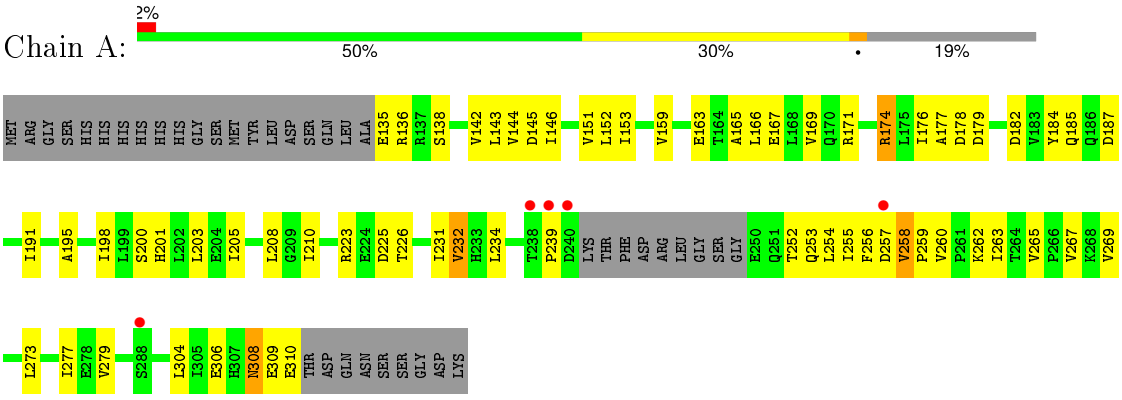
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	47	Total O 47 47	0	0
4	B	32	Total O 32 32	0	0
4	C	51	Total O 51 51	0	0
4	H	19	Total O 19 19	0	0
4	I	15	Total O 15 15	0	0
4	J	14	Total O 14 14	0	0

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.

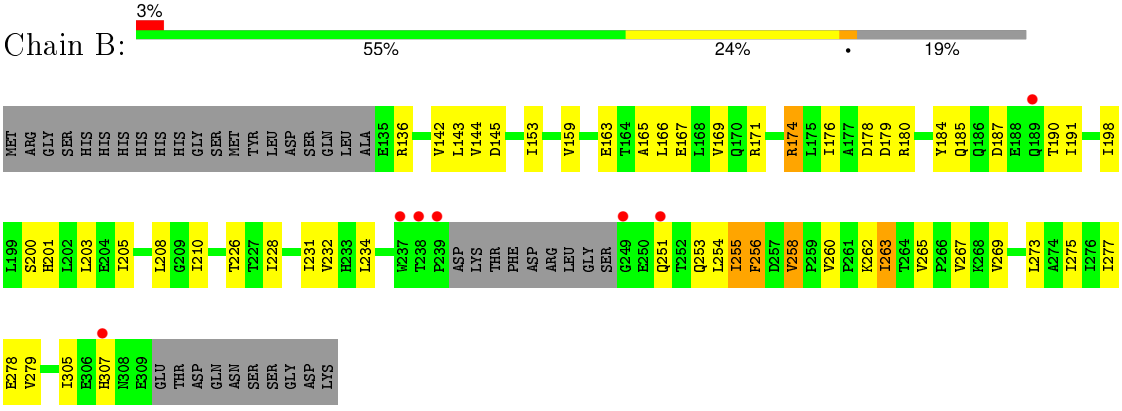
- Molecule 1: HprK protein

Chain A:



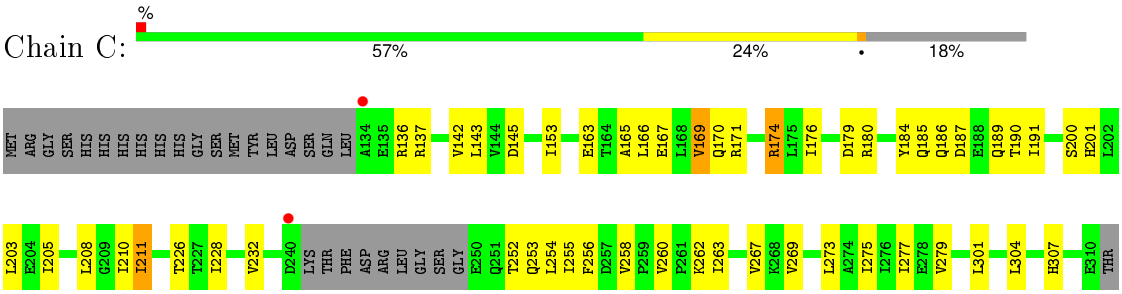
- Molecule 1: HprK protein

Chain B:



- Molecule 1: HprK protein

Chain C:

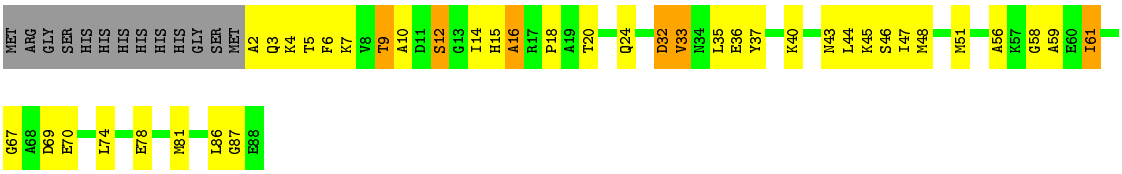


- Molecule 2: PHOSPHOCARRIER PROTEIN HPR

Chain H:

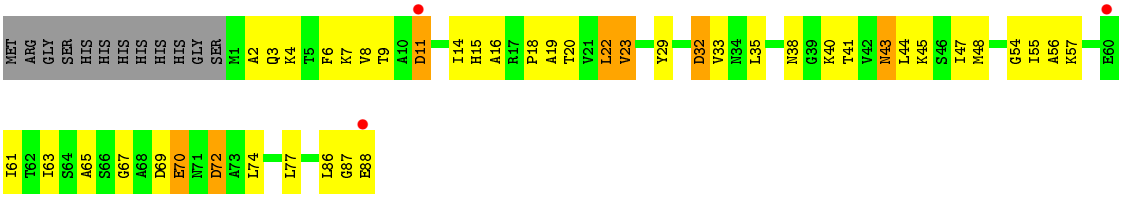
- Molecule 2: PHOSPHOCARRIER PROTEIN HPR

Chain I:



- Molecule 2: PHOSPHOCARRIER PROTEIN HPR

Chain J:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 1 2	Depositor
Cell constants a, b, c, α, β, γ	81.14Å 81.14Å 253.19Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.80 19.72 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.2 (20.00-2.80) 98.6 (19.72-2.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.33 (at 2.79Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.213 , 0.264 0.247 , 0.288	Depositor DCC
R_{free} test set	1135 reflections (4.82%)	DCC
Wilson B-factor (Å^2)	54.5	Xtriage
Anisotropy	0.360	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 60.6	EDS
Estimated twinning fraction	0.043 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 23554 reflections	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	5870	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.16% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.38	0/1294	0.65	0/1757
1	B	0.37	0/1274	0.66	0/1731
1	C	0.38	0/1294	0.65	0/1758
2	H	0.35	0/629	0.60	0/847
2	I	0.36	0/634	0.61	0/854
2	J	0.35	0/633	0.57	0/854
All	All	0.37	0/5758	0.63	0/7801

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

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	1275	0	1286	74	0
1	B	1255	0	1266	69	0
1	C	1275	0	1283	58	0
2	H	625	0	623	34	0
2	I	630	0	628	34	0
2	J	629	0	622	47	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	47	0	0	3	0
4	B	32	0	0	1	0
4	C	51	0	0	0	0
4	H	19	0	0	0	0
4	I	15	0	0	0	0
4	J	14	0	0	0	0
All	All	5870	0	5708	289	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 25.

All (289) 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:J:4:LYS:HE3	2:J:74:LEU:HB3	1.41	1.01
1:A:191:ILE:HD11	1:A:258:VAL:HG11	1.41	0.98
1:A:176:ILE:HD13	1:A:223:ARG:O	1.70	0.91
2:H:61:ILE:HD13	2:H:61:ILE:H	1.34	0.91
1:C:273:LEU:O	1:C:277:ILE:HD13	1.71	0.91
1:A:273:LEU:O	1:A:277:ILE:HD13	1.71	0.90
1:B:273:LEU:O	1:B:277:ILE:HD13	1.71	0.90
1:A:191:ILE:HD11	1:A:258:VAL:CG1	2.00	0.89
2:J:9:THR:HG23	2:J:87:GLY:HA2	1.54	0.88
2:I:61:ILE:H	2:I:61:ILE:HD13	1.39	0.88
2:H:26:ALA:HB1	2:H:33:VAL:HG21	1.56	0.88
2:H:8:VAL:HG23	2:H:61:ILE:HD12	1.57	0.84
2:I:9:THR:HG23	2:I:87:GLY:HA2	1.62	0.82
1:C:166:LEU:HD22	1:C:205:ILE:HD13	1.63	0.81
2:I:67:GLY:O	2:I:70:GLU:HB2	1.80	0.80
1:C:145:ASP:HB3	1:C:174:ARG:HB2	1.64	0.80
1:C:179:ASP:OD2	2:J:48:MET:HB2	1.81	0.79
1:A:255:ILE:HD13	1:A:260:VAL:CG2	2.13	0.78
1:A:145:ASP:HB3	1:A:174:ARG:HB2	1.65	0.78
1:B:145:ASP:HB3	1:B:174:ARG:HB2	1.66	0.77
2:J:63:ILE:HG21	2:J:77:LEU:HD13	1.66	0.77
1:A:255:ILE:O	1:A:258:VAL:HG13	1.84	0.77
1:A:232:VAL:HG21	1:A:277:ILE:HG13	1.67	0.77
1:A:166:LEU:HD22	1:A:205:ILE:HD13	1.66	0.77
1:C:166:LEU:HD22	1:C:205:ILE:CD1	2.16	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:203:LEU:O	1:C:211:ILE:HD13	1.86	0.76
2:I:33:VAL:HG22	2:I:44:LEU:HB3	1.68	0.75
1:B:136:ARG:HG2	1:B:136:ARG:HH21	1.50	0.75
1:A:198:ILE:HD12	1:C:304:LEU:HD23	1.67	0.75
1:A:255:ILE:HD13	1:A:260:VAL:HG23	1.68	0.75
2:I:18:PRO:HB3	2:I:86:LEU:HD21	1.67	0.74
1:B:166:LEU:HD22	1:B:205:ILE:HD13	1.69	0.74
2:H:67:GLY:O	2:H:70:GLU:HB2	1.88	0.74
2:H:61:ILE:H	2:H:61:ILE:CD1	2.00	0.73
1:B:251:GLN:HE21	1:B:262:LYS:HD2	1.52	0.73
1:B:255:ILE:HD13	1:B:260:VAL:CG2	2.17	0.73
1:A:198:ILE:HD12	1:C:304:LEU:CD2	2.18	0.72
1:C:167:GLU:O	1:C:171:ARG:HG3	1.89	0.72
1:A:191:ILE:CD1	1:A:258:VAL:HG11	2.19	0.72
1:C:187:ASP:OD1	1:C:190:THR:HB	1.89	0.72
1:B:254:LEU:HD22	4:B:430:HOH:O	1.91	0.71
2:J:3:GLN:HG2	2:J:4:LYS:N	2.06	0.71
1:C:136:ARG:HH11	1:C:136:ARG:HG3	1.56	0.71
2:I:20:THR:HG22	2:I:47:ILE:CD1	2.22	0.70
1:A:179:ASP:OD2	2:H:48:MET:HB2	1.90	0.70
1:A:167:GLU:O	1:A:171:ARG:HG3	1.92	0.69
1:B:167:GLU:O	1:B:171:ARG:HG3	1.92	0.69
2:H:34:ASN:HD22	2:H:41:THR:CG2	2.06	0.68
2:I:20:THR:HG22	2:I:47:ILE:HD12	1.76	0.68
1:B:253:GLN:HB2	1:B:262:LYS:HE3	1.76	0.67
2:H:8:VAL:CG2	2:H:61:ILE:HD12	2.24	0.67
1:A:166:LEU:HD22	1:A:205:ILE:CD1	2.24	0.67
1:B:166:LEU:HD22	1:B:205:ILE:CD1	2.24	0.67
2:J:67:GLY:O	2:J:70:GLU:HB2	1.95	0.66
1:A:279:VAL:HG21	1:B:166:LEU:HD21	1.76	0.66
1:A:176:ILE:HD12	1:A:225:ASP:CA	2.25	0.66
1:B:231:ILE:HD11	1:B:255:ILE:HD11	1.78	0.65
1:A:152:LEU:HB3	1:A:231:ILE:CD1	2.27	0.65
1:B:185:GLN:HA	1:B:191:ILE:HD13	1.79	0.65
2:H:35:LEU:HB2	2:H:44:LEU:HG	1.78	0.65
1:B:305:ILE:HD13	2:J:54:GLY:C	2.17	0.65
2:I:2:ALA:O	2:I:74:LEU:HD11	1.97	0.64
1:A:269:VAL:HG12	1:C:269:VAL:HG12	1.79	0.64
2:J:18:PRO:HB3	2:J:86:LEU:HD21	1.76	0.64
1:A:166:LEU:HD21	1:C:279:VAL:HG21	1.79	0.64
1:B:254:LEU:HD23	1:B:254:LEU:H	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:269:VAL:HG12	1:C:269:VAL:HG12	1.80	0.63
2:J:19:ALA:O	2:J:23:VAL:HG13	1.97	0.63
1:A:176:ILE:HD12	1:A:225:ASP:HA	1.81	0.63
2:I:37:TYR:CE1	2:I:59:ALA:HB1	2.33	0.63
2:H:6:PHE:CD1	2:H:63:ILE:HD13	2.34	0.63
2:H:34:ASN:HD22	2:H:41:THR:HG22	1.62	0.63
1:C:205:ILE:HD12	1:C:211:ILE:CD1	2.29	0.62
2:I:16:ALA:O	2:I:20:THR:HG23	1.99	0.62
1:B:231:ILE:CD1	1:B:255:ILE:HD11	2.30	0.62
1:B:255:ILE:HD12	1:B:255:ILE:N	2.14	0.62
1:C:185:GLN:HE21	1:C:258:VAL:CG2	2.12	0.61
1:C:255:ILE:HD13	1:C:260:VAL:CG2	2.30	0.61
2:J:2:ALA:HB1	2:J:74:LEU:HD12	1.82	0.61
1:B:251:GLN:NE2	1:B:262:LYS:HD2	2.15	0.61
1:A:254:LEU:C	1:A:255:ILE:HD12	2.20	0.61
1:B:185:GLN:HE21	1:B:258:VAL:HG12	1.65	0.61
2:H:19:ALA:O	2:H:23:VAL:HG13	2.00	0.60
1:A:253:GLN:HB2	1:A:262:LYS:HE3	1.82	0.60
2:H:6:PHE:HB2	2:H:61:ILE:HD11	1.83	0.60
1:A:310:GLU:HG2	4:A:441:HOH:O	2.02	0.59
2:J:6:PHE:CD2	2:J:63:ILE:HD13	2.37	0.59
1:B:255:ILE:HD13	1:B:260:VAL:HG21	1.85	0.58
1:A:304:LEU:CD2	1:B:198:ILE:HD12	2.34	0.58
1:A:252:THR:HG21	1:A:259:PRO:HB2	1.86	0.58
1:A:152:LEU:HB3	1:A:231:ILE:HD13	1.85	0.57
1:A:269:VAL:HG12	1:B:269:VAL:HG12	1.87	0.57
2:I:14:ILE:HD13	2:I:86:LEU:HD22	1.86	0.57
2:J:18:PRO:O	2:J:22:LEU:HD22	2.04	0.57
1:A:306:GLU:HG3	4:A:420:HOH:O	2.05	0.57
1:A:255:ILE:HD12	1:A:255:ILE:N	2.19	0.57
2:I:15:HIS:O	2:I:18:PRO:HG2	2.04	0.57
1:A:304:LEU:HD22	1:B:198:ILE:HD12	1.85	0.57
2:J:11:ASP:HA	2:J:57:LYS:HD2	1.87	0.57
1:B:262:LYS:HG2	1:B:263:ILE:N	2.19	0.57
1:A:239:PRO:HD2	4:A:434:HOH:O	2.05	0.56
2:J:15:HIS:O	2:J:18:PRO:HG2	2.05	0.56
2:I:14:ILE:CD1	2:I:86:LEU:HD22	2.35	0.56
1:A:309:GLU:HG3	2:I:56:ALA:HB1	1.88	0.56
2:H:5:THR:HG22	2:H:6:PHE:N	2.21	0.56
1:C:191:ILE:CG2	1:C:228:ILE:HD12	2.36	0.56
2:H:9:THR:HG23	2:H:87:GLY:HA2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:69:ASP:O	2:J:70:GLU:C	2.44	0.56
2:H:6:PHE:O	2:H:61:ILE:HD13	2.05	0.56
2:J:33:VAL:HG11	2:J:77:LEU:HD11	1.87	0.55
2:I:61:ILE:CD1	2:I:61:ILE:H	2.14	0.55
1:B:234:LEU:HD23	1:B:265:VAL:CG2	2.36	0.55
2:H:63:ILE:HD12	2:H:63:ILE:N	2.21	0.55
1:A:208:LEU:CD2	1:C:263:ILE:HD12	2.36	0.55
1:C:136:ARG:NH1	1:C:136:ARG:HG3	2.21	0.55
1:C:137:ARG:HG3	1:C:256:PHE:CZ	2.42	0.55
1:C:262:LYS:HG2	1:C:263:ILE:N	2.20	0.54
1:A:262:LYS:HG2	1:A:263:ILE:N	2.21	0.54
2:J:63:ILE:HD12	2:J:63:ILE:N	2.22	0.54
2:J:8:VAL:HG21	2:J:56:ALA:O	2.06	0.54
2:I:6:PHE:O	2:I:61:ILE:HD13	2.08	0.54
1:B:255:ILE:N	1:B:255:ILE:CD1	2.69	0.54
1:C:205:ILE:HD12	1:C:211:ILE:HD11	1.90	0.54
1:B:187:ASP:HB2	1:B:190:THR:HB	1.89	0.54
1:B:255:ILE:O	1:B:258:VAL:HG13	2.08	0.54
1:C:253:GLN:HB2	1:C:262:LYS:HE3	1.89	0.54
1:C:254:LEU:C	1:C:255:ILE:HD12	2.29	0.54
1:B:136:ARG:HG2	1:B:136:ARG:NH2	2.22	0.54
1:A:234:LEU:HD23	1:A:265:VAL:CG2	2.38	0.53
2:I:32:ASP:OD2	2:I:32:ASP:N	2.39	0.53
2:J:14:ILE:HD12	2:J:55:ILE:CD1	2.39	0.53
1:B:179:ASP:OD2	2:I:48:MET:HB2	2.08	0.53
2:J:61:ILE:HD12	2:J:63:ILE:HD11	1.91	0.53
1:B:263:ILE:HD13	1:C:208:LEU:CD2	2.39	0.53
2:I:3:GLN:O	2:I:4:LYS:HG3	2.08	0.53
2:J:14:ILE:HD12	2:J:55:ILE:HG21	1.91	0.52
2:H:17:ARG:O	2:H:20:THR:HB	2.10	0.52
1:C:136:ARG:HG2	1:C:184:TYR:HB3	1.92	0.52
1:A:263:ILE:HD12	1:B:208:LEU:CD2	2.39	0.52
2:J:2:ALA:HB3	2:J:70:GLU:HG2	1.91	0.52
1:A:255:ILE:HD13	1:A:260:VAL:HG21	1.91	0.52
1:B:153:ILE:N	1:B:153:ILE:HD12	2.25	0.52
2:H:6:PHE:HD1	2:H:63:ILE:HD13	1.74	0.52
1:B:305:ILE:O	1:B:307:HIS:N	2.42	0.52
1:B:191:ILE:HD11	1:B:258:VAL:CG1	2.40	0.52
2:J:43:ASN:ND2	2:J:45:LYS:H	2.08	0.52
1:A:185:GLN:OE1	1:A:256:PHE:O	2.28	0.52
2:J:6:PHE:HA	2:J:88:GLU:OE2	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:205:ILE:HD12	1:C:211:ILE:HD12	1.92	0.51
2:J:32:ASP:O	2:J:65:ALA:HA	2.10	0.51
2:H:31:ALA:HB2	2:H:69:ASP:HB2	1.92	0.51
1:C:255:ILE:HD13	1:C:260:VAL:HG23	1.92	0.51
1:A:153:ILE:HD12	1:A:153:ILE:N	2.24	0.51
1:C:142:VAL:HG11	1:C:165:ALA:HB2	1.93	0.51
2:H:30:ASP:N	2:H:69:ASP:OD1	2.44	0.51
1:B:279:VAL:HG21	1:C:166:LEU:HD21	1.92	0.51
2:I:43:ASN:OD1	2:I:45:LYS:HB2	2.11	0.51
1:B:255:ILE:HD13	1:B:260:VAL:HG23	1.93	0.51
1:A:176:ILE:HG13	1:A:226:THR:HG22	1.92	0.50
2:J:6:PHE:HD2	2:J:63:ILE:HD13	1.77	0.50
1:B:145:ASP:CG	1:B:174:ARG:HH11	2.15	0.50
1:A:135:GLU:O	1:A:184:TYR:HA	2.11	0.50
2:J:8:VAL:HA	2:J:87:GLY:HA3	1.94	0.50
2:J:43:ASN:C	2:J:43:ASN:HD22	2.15	0.50
1:C:145:ASP:CG	1:C:174:ARG:HH11	2.15	0.49
1:B:191:ILE:HD11	1:B:258:VAL:HG11	1.93	0.49
2:I:20:THR:O	2:I:24:GLN:HB2	2.12	0.49
2:J:2:ALA:HB1	2:J:74:LEU:CD1	2.42	0.49
1:A:145:ASP:CG	1:A:174:ARG:HH11	2.16	0.49
2:I:35:LEU:HD12	2:I:44:LEU:HD13	1.95	0.49
1:A:308:ASN:C	1:A:310:GLU:H	2.15	0.49
1:A:185:GLN:HG3	1:A:191:ILE:HD13	1.94	0.49
2:J:7:LYS:HE3	2:J:8:VAL:O	2.12	0.49
2:J:20:THR:HA	2:J:47:ILE:HD13	1.94	0.49
2:J:35:LEU:HD12	2:J:44:LEU:HD13	1.95	0.49
2:J:87:GLY:O	2:J:88:GLU:C	2.51	0.49
1:C:180:ARG:NH2	2:J:40:LYS:HD2	2.28	0.49
1:B:210:ILE:HD12	1:B:210:ILE:N	2.28	0.49
1:A:185:GLN:OE1	1:A:256:PHE:HB3	2.13	0.49
2:H:32:ASP:O	2:H:65:ALA:HA	2.13	0.49
2:J:35:LEU:C	2:J:35:LEU:HD23	2.32	0.48
1:A:142:VAL:HG11	1:A:165:ALA:HB2	1.94	0.48
2:H:14:ILE:HD12	2:H:55:ILE:HG21	1.96	0.48
2:I:18:PRO:CB	2:I:86:LEU:HD21	2.41	0.48
2:H:69:ASP:O	2:H:70:GLU:C	2.51	0.48
1:B:144:VAL:HG22	1:B:153:ILE:HD11	1.94	0.48
1:A:210:ILE:HD12	1:A:210:ILE:N	2.28	0.48
1:A:185:GLN:HG2	1:A:187:ASP:O	2.13	0.48
1:B:136:ARG:NH2	1:B:184:TYR:CD2	2.81	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:210:ILE:N	1:C:210:ILE:HD12	2.28	0.48
2:J:19:ALA:HB3	2:J:47:ILE:HD11	1.95	0.48
1:B:176:ILE:HG12	1:B:226:THR:HG22	1.95	0.48
1:B:305:ILE:O	2:J:56:ALA:HB2	2.14	0.48
1:B:171:ARG:NH1	1:B:278:GLU:OE2	2.47	0.48
2:J:40:LYS:HB2	2:J:40:LYS:HE3	1.70	0.47
1:A:136:ARG:HG2	2:H:40:LYS:NZ	2.28	0.47
2:I:78:GLU:O	2:I:81:MET:HB2	2.14	0.47
1:B:142:VAL:HG11	1:B:165:ALA:HB2	1.97	0.47
1:A:136:ARG:HG2	2:H:40:LYS:HZ1	1.79	0.47
2:H:47:ILE:HG12	2:H:51:MET:CE	2.43	0.47
1:A:163:GLU:N	1:A:163:GLU:OE2	2.43	0.47
1:B:234:LEU:HD23	1:B:265:VAL:HG23	1.96	0.47
1:A:267:VAL:HG22	1:A:273:LEU:HD11	1.96	0.47
1:A:152:LEU:HB3	1:A:231:ILE:HD12	1.97	0.47
1:A:176:ILE:CD1	1:A:223:ARG:HB3	2.44	0.47
1:C:176:ILE:HG12	1:C:226:THR:HG22	1.96	0.47
1:C:200:SER:O	1:C:201:HIS:HB2	2.15	0.47
1:C:255:ILE:HD12	1:C:255:ILE:N	2.30	0.47
1:B:185:GLN:NE2	1:B:256:PHE:O	2.48	0.46
1:C:185:GLN:HE21	1:C:258:VAL:HG23	1.80	0.46
1:C:184:TYR:HA	1:C:256:PHE:CE1	2.49	0.46
1:B:163:GLU:OE2	1:B:163:GLU:N	2.45	0.46
1:A:198:ILE:HD11	1:C:301:LEU:HD13	1.97	0.46
1:A:152:LEU:HD23	1:A:231:ILE:HD12	1.98	0.46
1:B:200:SER:O	1:B:201:HIS:HB2	2.16	0.46
1:C:163:GLU:N	1:C:163:GLU:OE2	2.46	0.46
1:C:185:GLN:NE2	1:C:258:VAL:HG23	2.31	0.46
1:B:267:VAL:HG22	1:B:273:LEU:HD11	1.98	0.46
1:B:159:VAL:CG2	1:B:267:VAL:HG21	2.46	0.46
1:C:186:GLN:O	1:C:187:ASP:HB3	2.16	0.45
2:J:63:ILE:CG2	2:J:77:LEU:HD13	2.41	0.45
1:B:185:GLN:HE21	1:B:258:VAL:CG1	2.27	0.45
2:I:47:ILE:HG12	2:I:51:MET:CE	2.46	0.45
2:I:6:PHE:HB2	2:I:61:ILE:HD11	1.98	0.45
1:A:198:ILE:HD12	1:C:304:LEU:HD22	1.97	0.45
1:B:171:ARG:HH11	1:B:278:GLU:CD	2.19	0.45
2:J:43:ASN:C	2:J:43:ASN:ND2	2.70	0.45
1:A:178:ASP:HB2	1:A:203:LEU:HD23	1.98	0.45
1:B:231:ILE:HD12	1:B:260:VAL:HB	1.98	0.45
1:A:308:ASN:HA	1:A:308:ASN:HD22	1.61	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:191:ILE:CD1	1:C:258:VAL:HG21	2.47	0.44
1:A:185:GLN:HG3	1:A:191:ILE:CD1	2.47	0.44
1:A:308:ASN:C	1:A:310:GLU:N	2.70	0.44
1:C:267:VAL:HG22	1:C:273:LEU:HD11	1.99	0.44
1:B:191:ILE:CG2	1:B:228:ILE:HD12	2.47	0.44
1:C:191:ILE:HG21	1:C:228:ILE:HD12	1.98	0.44
1:B:232:VAL:HG11	1:B:277:ILE:HG13	1.98	0.44
1:B:184:TYR:HA	1:B:256:PHE:HE2	1.83	0.44
1:A:200:SER:O	1:A:201:HIS:HB2	2.17	0.44
1:B:263:ILE:HD12	1:B:265:VAL:HG13	2.00	0.44
1:B:145:ASP:HB2	1:B:176:ILE:HD11	1.99	0.43
1:B:179:ASP:OD2	2:I:46:SER:OG	2.34	0.43
2:I:5:THR:HG22	2:I:6:PHE:N	2.32	0.43
2:J:19:ALA:CB	2:J:47:ILE:HD11	2.48	0.43
2:H:18:PRO:HB3	2:H:86:LEU:HD21	2.00	0.43
2:I:7:LYS:HE2	2:I:58:GLY:HA2	2.01	0.43
1:B:275:ILE:HG23	1:C:170:GLN:OE1	2.19	0.43
2:I:69:ASP:O	2:I:70:GLU:C	2.57	0.43
1:B:180:ARG:HH21	2:I:40:LYS:CE	2.31	0.43
1:B:191:ILE:HG22	1:B:228:ILE:HD12	1.99	0.43
2:J:43:ASN:HD22	2:J:44:LEU:N	2.16	0.43
1:A:252:THR:CG2	1:A:253:GLN:N	2.82	0.42
1:A:144:VAL:HG22	1:A:153:ILE:HD11	2.01	0.42
1:C:145:ASP:HB2	1:C:176:ILE:HD11	2.02	0.42
1:B:178:ASP:HB2	1:B:203:LEU:HD23	2.01	0.42
1:A:176:ILE:CD1	1:A:223:ARG:O	2.55	0.42
2:H:5:THR:CG2	2:H:6:PHE:N	2.82	0.42
2:I:35:LEU:HD23	2:I:36:GLU:N	2.34	0.42
2:H:61:ILE:HD13	2:H:61:ILE:N	2.16	0.42
2:H:34:ASN:HD22	2:H:41:THR:HG21	1.80	0.42
2:J:18:PRO:CB	2:J:86:LEU:HD21	2.47	0.42
1:A:146:ILE:HD12	1:A:151:VAL:HG21	2.02	0.42
2:J:29:TYR:HB3	2:J:69:ASP:CB	2.50	0.42
2:I:47:ILE:HG12	2:I:51:MET:HE2	2.02	0.42
2:J:47:ILE:O	2:J:47:ILE:HG13	2.20	0.42
1:C:153:ILE:HD13	1:C:232:VAL:HB	2.02	0.41
1:A:138:SER:HB3	1:A:182:ASP:OD1	2.20	0.41
1:C:203:LEU:CB	1:C:211:ILE:HD11	2.50	0.41
1:A:159:VAL:CG2	1:A:267:VAL:HG21	2.50	0.41
1:C:171:ARG:CZ	1:C:275:ILE:CD1	2.99	0.41
1:A:177:ALA:HB2	1:A:195:ALA:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:136:ARG:CG	1:B:136:ARG:NH2	2.83	0.41
1:C:191:ILE:HD13	1:C:258:VAL:HB	2.02	0.41
2:J:69:ASP:O	2:J:72:ASP:N	2.54	0.41
1:A:277:ILE:N	1:A:277:ILE:CD1	2.84	0.41
2:J:88:GLU:HG2	2:J:88:GLU:O	2.20	0.41
1:C:186:GLN:O	1:C:186:GLN:HG2	2.21	0.41
2:H:34:ASN:ND2	2:H:41:THR:HG22	2.32	0.41
1:A:256:PHE:O	1:A:258:VAL:HG12	2.21	0.40
1:A:176:ILE:HD11	1:A:223:ARG:HB3	2.02	0.40
1:C:145:ASP:CG	1:C:174:ARG:NH1	2.74	0.40
2:I:10:ALA:HB2	2:I:86:LEU:HA	2.03	0.40
1:C:165:ALA:O	1:C:169:VAL:HG13	2.21	0.40
1:C:232:VAL:HG11	1:C:277:ILE:HG13	2.02	0.40
1:B:185:GLN:NE2	1:B:258:VAL:HG12	2.34	0.40
2:H:47:ILE:HG12	2:H:51:MET:HE2	2.01	0.40
1:B:277:ILE:N	1:B:277:ILE:CD1	2.85	0.40
1:C:304:LEU:O	1:C:307:HIS:HB3	2.21	0.40
2:H:4:LYS:HE2	2:H:78:GLU:OE1	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	163/205 (80%)	155 (95%)	8 (5%)	0	100	100
1	B	162/205 (79%)	152 (94%)	10 (6%)	0	100	100
1	C	164/205 (80%)	154 (94%)	10 (6%)	0	100	100
2	H	84/100 (84%)	79 (94%)	3 (4%)	2 (2%)	7	25
2	I	85/100 (85%)	70 (82%)	13 (15%)	2 (2%)	7	25
2	J	86/100 (86%)	77 (90%)	7 (8%)	2 (2%)	8	26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	744/915 (81%)	687 (92%)	51 (7%)	6 (1%)	24 58

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	70	GLU
2	J	70	GLU
2	H	16	ALA
2	I	16	ALA
2	J	16	ALA
2	I	12	SER

5.3.2 Protein sidechains (i)

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	137/174 (79%)	130 (95%)	7 (5%)	29 63
1	B	134/174 (77%)	127 (95%)	7 (5%)	29 62
1	C	136/174 (78%)	130 (96%)	6 (4%)	35 69
2	H	66/79 (84%)	63 (96%)	3 (4%)	34 68
2	I	66/79 (84%)	61 (92%)	5 (8%)	16 42
2	J	65/79 (82%)	57 (88%)	8 (12%)	6 18
All	All	604/759 (80%)	568 (94%)	36 (6%)	24 56

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	143	LEU
1	A	169	VAL
1	A	174	ARG
1	A	232	VAL
1	A	257	ASP
1	A	258	VAL

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Mol	Chain	Res	Type
1	A	308	ASN
1	B	143	LEU
1	B	169	VAL
1	B	174	ARG
1	B	255	ILE
1	B	256	PHE
1	B	258	VAL
1	B	263	ILE
1	C	143	LEU
1	C	169	VAL
1	C	174	ARG
1	C	189	GLN
1	C	211	ILE
1	C	252	THR
2	H	36	GLU
2	H	44	LEU
2	H	61	ILE
2	I	9	THR
2	I	12	SER
2	I	32	ASP
2	I	33	VAL
2	I	61	ILE
2	J	11	ASP
2	J	22	LEU
2	J	23	VAL
2	J	32	ASP
2	J	38	ASN
2	J	41	THR
2	J	43	ASN
2	J	72	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	283	ASN
1	A	300	ASN
1	A	308	ASN
1	B	185	GLN
1	B	251	GLN
1	B	300	ASN
1	B	302	ASN
1	B	307	HIS

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Mol	Chain	Res	Type
1	B	308	ASN
1	C	185	GLN
1	C	300	ASN
2	H	34	ASN
2	H	38	ASN
2	I	15	HIS
2	J	34	ASN
2	J	43	ASN

5.3.3 RNA

There are no RNA molecules 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

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

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

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, 95^{th} 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	167/205 (81%)	-0.32	5 (2%) 54 41	26, 44, 80, 93	0
1	B	166/205 (80%)	-0.30	7 (4%) 40 28	0, 45, 76, 97	0
1	C	168/205 (81%)	-0.39	2 (1%) 81 73	28, 43, 71, 94	0
2	H	86/100 (86%)	-0.15	0 100 100	27, 58, 75, 84	0
2	I	87/100 (87%)	-0.18	0 100 100	34, 56, 77, 86	0
2	J	88/100 (88%)	-0.04	3 (3%) 49 36	43, 58, 78, 95	0
All	All	762/915 (83%)	-0.26	17 (2%) 65 54	0, 49, 77, 97	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	238	THR	4.6
1	A	238	THR	3.5
1	B	249	GLY	3.4
1	A	240	ASP	3.2
1	B	239	PRO	3.0
2	J	88	GLU	2.8
1	A	257	ASP	2.8
1	A	239	PRO	2.7
1	C	240	ASP	2.6
1	B	307	HIS	2.4
2	J	11	ASP	2.3
1	B	237	TRP	2.3
1	A	288	SER	2.3
2	J	60	GLU	2.1
1	B	251	GLN	2.1
1	C	134	ALA	2.1
1	B	189	GLN	2.0

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

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

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, 95^{th} 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	CA	B	402	1/1	0.87	0.18	-	69,69,69,69	0
3	CA	C	403	1/1	0.93	0.12	-	54,54,54,54	0
3	CA	A	401	1/1	0.92	0.13	-	57,57,57,57	0

6.5 Other polymers (i)

There are no such residues in this entry.