Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 08:30 PM GMT

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
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:

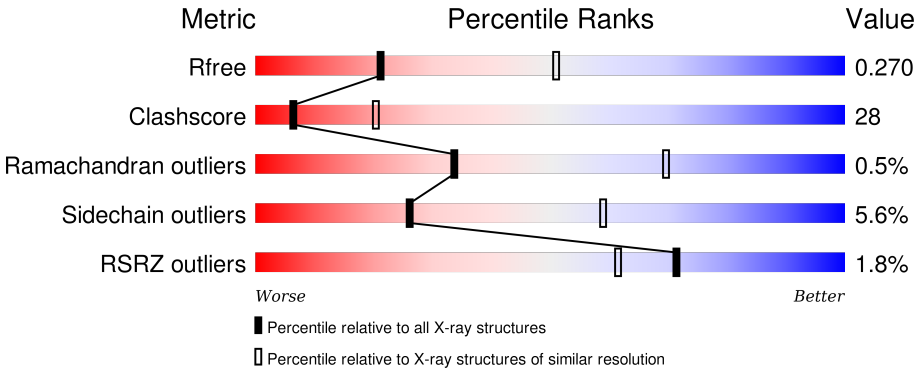
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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	5% 53% 30% • 14%
1	B	205	% 54% 29% • 14%
1	C	205	% 52% 30% • 15%
2	H	100	47% 35% • • 13%
2	I	100	48% 33% 5% • 13%

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Mol	Chain	Length	Quality of chain
2	J	100	59% 26% 13%

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

2 Entry composition (i)

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

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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	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

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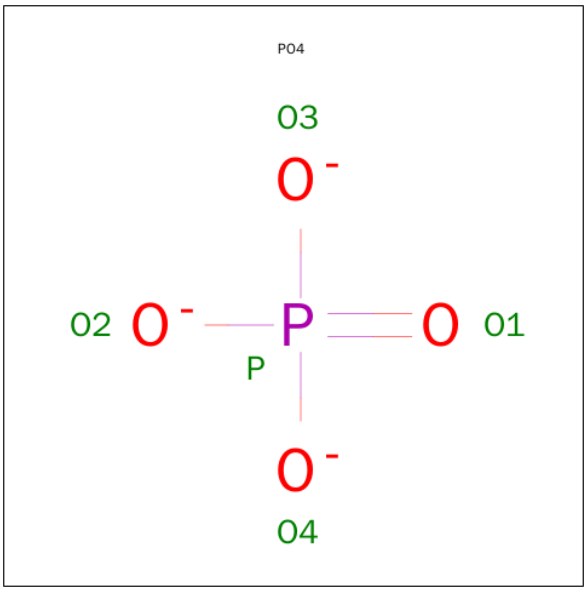
Chain	Residue	Modelled	Actual	Comment	Reference
H	46	SEP	SER	MODIFIED RESIDUE	UNP P08877
H	85	ARG	GLY	ENGINEERED	UNP P08877
I	-11	MET	-	EXPRESSION TAG	UNP P08877
I	-10	ARG	-	EXPRESSION TAG	UNP P08877
I	-9	GLY	-	EXPRESSION TAG	UNP P08877
I	-8	SER	-	EXPRESSION TAG	UNP P08877
I	-7	HIS	-	EXPRESSION TAG	UNP 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	46	SEP	SER	MODIFIED RESIDUE	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	46	SEP	SER	MODIFIED RESIDUE	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 PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- Molecule 5 is water.

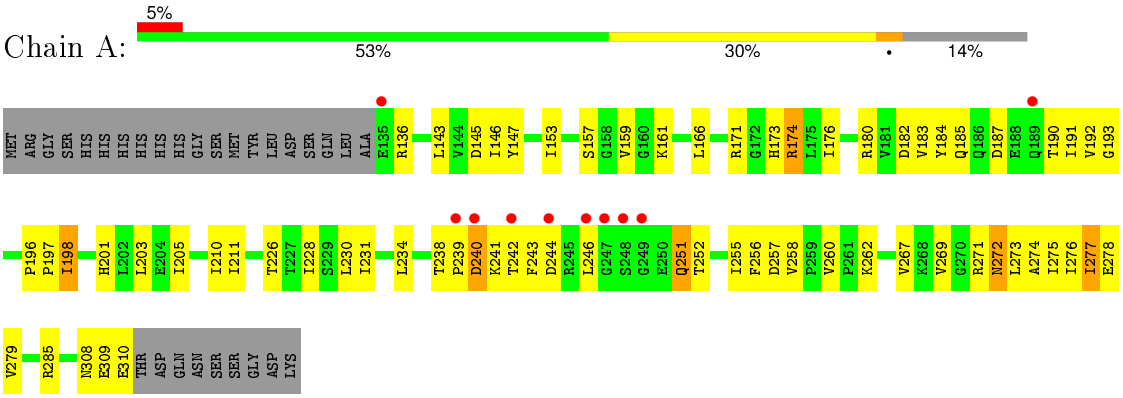
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	39	Total O 39 39	0	0
5	B	48	Total O 48 48	0	0
5	C	40	Total O 40 40	0	0
5	H	14	Total O 14 14	0	0
5	I	14	Total O 14 14	0	0
5	J	16	Total O 16 16	0	0

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.

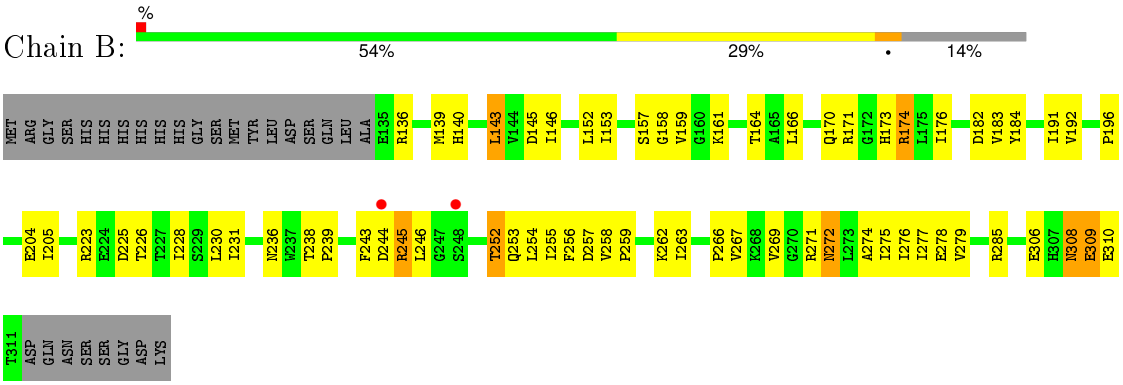
- Molecule 1: HprK protein

Chain A:



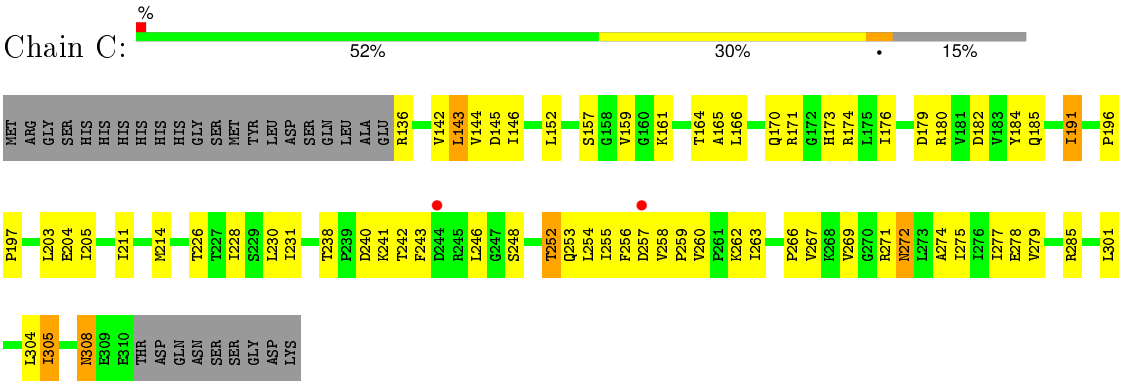
- Molecule 1: HprK protein

Chain B:



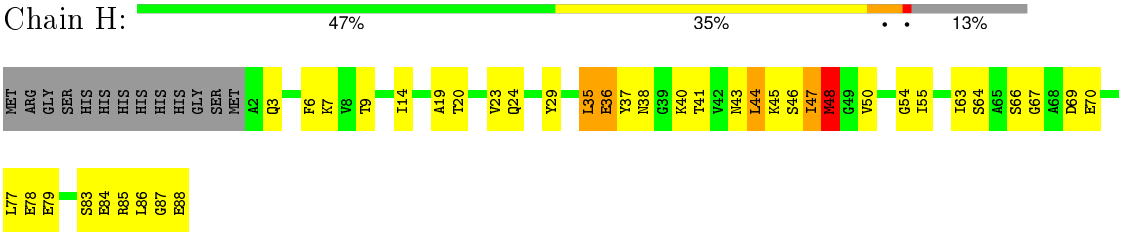
- Molecule 1: HprK protein

Chain C:



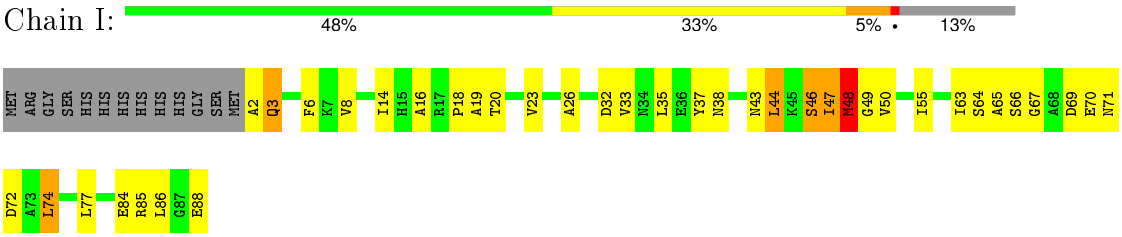
• Molecule 2: PHOSPHOCARRIER PROTEIN HPR

Chain H:



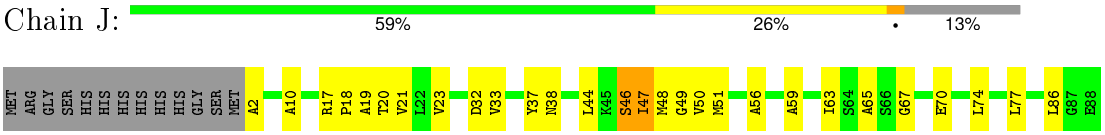
• Molecule 2: PHOSPHOCARRIER PROTEIN HPR

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	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
$< I/\sigma(I) >$ [1]	9.31 (at 2.79Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.200 , 0.257 0.225 , 0.270	Depositor DCC
R_{free} test set	1133 reflections (4.83%)	DCC
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
Estimated twinning fraction	0.053 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 23472 reflections	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.*

[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: 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(^{o})	Ideal(^{o})
1	C	285	ARG	NE-CZ-NH1	-18.84	110.88	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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

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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:C:143:LEU:HD21	1:C:228:ILE:HD12	1.50	0.92
1:A:191:ILE:HD11	1:A:258:VAL:HB	1.51	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
2:I:67:GLY:H	2:I:70:GLU:HG3	1.46	0.80
1:B:279:VAL:HG21	1:C:166:LEU:HD21	1.64	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

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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:35:LEU:HG	2:H:63:ILE:CD1	2.18	0.74
2:H:9:THR:HG23	2:H:87:GLY:HA2	1.70	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
2:H:47:ILE:HG23	2:H:48:MET:N	2.04	0.71
1:B:272:ASN:C	1:B:272:ASN:HD22	1.93	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:B:176:ILE:HG13	1:B:226:THR:HG22	1.75	0.68
1:A:279:VAL:HG21	1:B:166:LEU:HD21	1.73	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:B:176:ILE:HD12	1:B:225:ASP:CA	2.25	0.66
1:A:176:ILE:HG12	1:A:226:THR:HG22	1.76	0.66
2:H:37:TYR:CE1	2:H:55:ILE:HA	2.31	0.66
1:C:305:ILE:HD11	2:H:54:GLY:HA2	1.77	0.66
1:B:254:LEU:O	1:B:255:ILE:HD13	1.95	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
2:I:35:LEU:HG	2:I:63:ILE:CD1	2.27	0.65
1:C:152:LEU:HB3	1:C:231:ILE:HD13	1.78	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

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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
2:J:19:ALA:O	2:J:23:VAL:HG13	2.04	0.58
1:C:238:THR:HG22	1:C:240:ASP:H	1.69	0.58
1:C:191:ILE:HD13	1:C:255:ILE:HB	1.86	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
2:I:44:LEU:CD1	2:I:63:ILE:HD12	2.33	0.58
1:A:269:VAL:HG12	1:B:269:VAL:HG12	1.86	0.58
1:B:166:LEU:HD22	1:B:205:ILE:HD13	1.85	0.58
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:B:191:ILE:CG2	1:B:228:ILE:HD12	2.33	0.57
1:A:191:ILE:CD1	1:A:255:ILE:HB	2.34	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
1:B:146:ILE:HD13	1:B:173:HIS:CG	2.39	0.57
2:J:32:ASP:O	2:J:65:ALA:HA	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:47:ILE:CG2	2:H:48:MET:N	2.67	0.57
1:B:164:THR:HG21	1:B:277:ILE:HD12	1.85	0.57
1:C:301:LEU:CD1	1:C:305:ILE:HD11	2.35	0.57
1:A:166:LEU:HD22	1:A:205:ILE:HD13	1.87	0.57
1:A:159:VAL:CG2	1:A:267:VAL:HG21	2.35	0.57
2:H:44:LEU:HD12	2:H:63:ILE:HD12	1.86	0.57
2:I:35:LEU:HG	2:I:63:ILE:HD13	1.86	0.57
1:B:256:PHE:O	1:B:257:ASP:HB2	2.03	0.57
1:C:301:LEU:HD12	1:C:305:ILE:CD1	2.36	0.56
2:I:66:SER:HA	2:I:70:GLU:HG2	1.87	0.56
1:C:252:THR:HG21	1:C:259:PRO:HB3	1.87	0.56
1:A:146:ILE:HD13	1:A:173:HIS:CG	2.40	0.56
2:J:2:ALA:HB1	2:J:74:LEU:CD2	2.34	0.56
1:B:252:THR:HG23	1:B:253:GLN:N	2.20	0.56
2:I:16:ALA:O	2:I:20:THR:HG23	2.06	0.56
1:C:243:PHE:CZ	1:C:266:PRO:HB3	2.40	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:C:305:ILE:N	1:C:305:ILE:CD1	2.71	0.54
1:B:136:ARG:HG3	1:B:136:ARG:HH11	1.72	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
2:J:19:ALA:HB1	2:J:47:ILE:HD11	1.91	0.53
1:C:262:LYS:C	1:C:263:ILE:HD12	2.29	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
2:J:47:ILE:HD12	2:J:50:VAL:HB	1.92	0.52
1:B:271:ARG:HH11	1:B:271:ARG:HG2	1.75	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
2:H:66:SER:HA	2:H:70:GLU:OE2	2.10	0.51
1:B:245:ARG:NH2	2:J:46:SEP:HA	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:47:ILE:HG23	2:J:48:MET:N	2.25	0.51
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
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
2:I:47:ILE:CD1	2:I:50:VAL:HB	2.38	0.51
2:H:19:ALA:HB1	2:H:47:ILE:CD1	2.32	0.51
1:C:253:GLN:O	1:C:255:ILE:HD12	2.11	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:I:35:LEU:HB2	2:I:44:LEU:HG	1.93	0.50
2:H:36:GLU:HA	2:H:40:LYS:O	2.11	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:N	1:B:153:ILE:HD12	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:C:185:GLN:NE2	1:C:258:VAL:HG23	2.26	0.49
1:B:191:ILE:HD13	1:B:258:VAL:CB	2.42	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
2:H:35:LEU:HG	2:H:63:ILE:HD13	1.94	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
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
2:I:33:VAL:HG21	2:I:77:LEU:HD11	1.95	0.48
1:A:251:GLN:HG3	1:A:262:LYS:O	2.13	0.48
1:A:228:ILE:HD12	1:A:228:ILE:H	1.79	0.48
2:H:23:VAL:HG11	2:H:47:ILE:CD1	2.40	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:SER:HA	4:A:501:PO4:O1	2.13	0.48
1:B:256:PHE:O	1:B:257:ASP:CB	2.61	0.48
1:A:210:ILE:HD11	2:H:48:MET:SD	2.53	0.48
1:C:228:ILE:N	1:C:228:ILE:HD13	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: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
1:A:182:ASP:OD2	1:A:196:PRO:HG3	2.13	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
2:H:23:VAL:HG12	2:H:50:VAL:HG21	1.97	0.47
1:B:176:ILE:CD1	1:B:223:ARG:HB3	2.45	0.47
1:B:309:GLU:HB3	2:J:56:ALA:CB	2.42	0.46
1:A:275:ILE:HG23	1:B:170:GLN:OE1	2.15	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: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
1:B:236:ASN:HA	1:B:267:VAL:HB	1.98	0.46
2:J:18:PRO:HA	2:J:21:VAL:HG12	1.97	0.46
2:I:23:VAL:HG11	2:I:47:ILE:CD1	2.31	0.46
1:C:144:VAL:HG11	1:C:146:ILE:HD11	1.98	0.46
1:A:256:PHE:O	1:A:257:ASP:HB2	2.16	0.46
2:H:43:ASN:OD1	2:H:45:LYS:HB2	2.16	0.46
1:B:204:GLU:HB2	2:I:48:MET:CG	2.46	0.45
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:145:ASP:CG	1:B:174:ARG:HH11	2.20	0.45
1:C:145:ASP:C	1:C:145:ASP:OD2	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

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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:C:272:ASN:CG	1:C:275:ILE:HG12	2.37	0.45
1:A:145:ASP:CG	1:A:174:ARG:NH1	2.70	0.45
2:I:47:ILE:C	2:I:49:GLY:H	2.19	0.45
2:H:67:GLY:H	2:H:70:GLU:CG	2.30	0.45
2:J:47:ILE:HG13	2:J:51:MET:HE2	1.99	0.45
2:I:71:ASN:ND2	5:I:101:HOH:O	2.50	0.45
1:B:243:PHE:CE2	1:B:266:PRO:HB3	2.52	0.45
1:B:139:MET:SD	1:B:255:ILE:HD12	2.57	0.45
2:H:29:TYR:O	2:H:45:LYS:NZ	2.37	0.44
1:B:182:ASP:OD2	1:B:196:PRO:HG3	2.16	0.44
2:H:47:ILE:CD1	2:H:50:VAL:HB	2.38	0.44
1:B:272:ASN:HD21	1:B:274:ALA:HB3	1.83	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
2:I:18:PRO:HB3	2:I:86:LEU:HD21	1.98	0.44
1:C:142:VAL:HG11	1:C:165:ALA:HB2	2.00	0.44
2:I:6:PHE:HD1	2:I:88:GLU:HA	1.82	0.44
1:A:272:ASN:ND2	1:A:272:ASN:C	2.65	0.44
2:J:37:TYR:O	2:J:38:ASN:HB2	2.18	0.44
1:A:201:HIS:HD2	5:A:526:HOH:O	2.01	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:C:301:LEU:HD12	1:C:305:ILE:HD13	2.00	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
2:J:47:ILE:C	2:J:49:GLY:N	2.68	0.43
1:B:191:ILE:HG21	1:B:228:ILE:HD12	2.00	0.43
1:C:308:ASN:HA	1:C:308:ASN:HD22	1.56	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:B:272:ASN:CG	1:B:275:ILE:HG12	2.39	0.42
1:A:147:TYR:CE2	1:A:173:HIS:HE1	2.36	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:244:ASP:C	1:A:246:LEU:H	2.22	0.42
1:B:176:ILE:HD12	1:B:225:ASP:N	2.33	0.42
1:A:276:ILE:HD12	1:B:205:ILE:HG21	2.00	0.42
1:C:242:THR:C	1:C:243:PHE:CD1	2.93	0.42
2:J:33:VAL:HG22	2:J:65:ALA:HB2	2.01	0.42
2:I:37:TYR:CZ	2:I:38:ASN:ND2	2.87	0.42
2:H:69:ASP:O	2:H:70:GLU:C	2.58	0.42
1:A:171:ARG:HH11	1:A:278:GLU:CD	2.23	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: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
1:A:275:ILE:O	1:A:279:VAL:HG23	2.20	0.42
1:A:203:LEU:HB2	1:A:211:ILE:HD11	2.02	0.42
1:A:211:ILE:C	1:A:211:ILE:HD12	2.40	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
2:I:33:VAL:HA	2:I:64:SER:O	2.20	0.41
2:H:44:LEU:HD11	2:H:63:ILE:HD12	2.01	0.41
1:C:196:PRO:O	1:C:197:PRO:C	2.58	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
2:H:63:ILE:HG21	2:H:77:LEU:HD13	2.03	0.41
1:C:185:GLN:HE21	1:C:258:VAL:CG2	2.34	0.41
1:A:240:ASP:O	1:A:241:LYS:C	2.58	0.41
1:A:196:PRO:O	1:A:197:PRO:C	2.59	0.41
1:B:238:THR:CG2	1:B:239:PRO:HD2	2.51	0.41
1:B:269:VAL:HG12	1:C:269:VAL:CG1	2.49	0.41
1:C:179:ASP:CG	2:J:46:SEP:O3P	2.58	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:A:210:ILE:HD12	2:H:48:MET:SD	2.61	0.41
1:C:146:ILE:HD13	1:C:173:HIS:CG	2.56	0.41
1:B:161:LYS:N	4:B:502:PO4:O3	2.53	0.41
2:I:66:SER:HA	2:I:70:GLU:CG	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:243:PHE:CE2	1:C:266:PRO:HB3	2.56	0.40
1:B:245:ARG:C	1:B:246:LEU:HD12	2.42	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:C:211:ILE:HD12	1:C:211:ILE:C	2.41	0.40
1:B:183:VAL:HA	1:B:192:VAL:O	2.22	0.40
1:B:230:LEU:HD12	1:B:231:ILE:H	1.86	0.40
1:B:191:ILE:CD1	1:B:258:VAL:HB	2.51	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
1:A:242:THR:CG2	1:A:243:PHE:N	2.85	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	174/205 (85%)	160 (92%)	13 (8%)	1 (1%)	30	65
1	B	175/205 (85%)	165 (94%)	9 (5%)	1 (1%)	30	65
1	C	173/205 (84%)	162 (94%)	11 (6%)	0	100	100
2	H	84/100 (84%)	73 (87%)	10 (12%)	1 (1%)	16	47
2	I	84/100 (84%)	70 (83%)	13 (16%)	1 (1%)	16	47
2	J	84/100 (84%)	76 (90%)	8 (10%)	0	100	100
All	All	774/915 (85%)	706 (91%)	64 (8%)	4 (0%)	34	69

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	239	PRO

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

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	143/174 (82%)	134 (94%)	9 (6%)	22	53
1	B	142/174 (82%)	135 (95%)	7 (5%)	31	65
1	C	143/174 (82%)	134 (94%)	9 (6%)	22	53
2	H	61/78 (78%)	57 (93%)	4 (7%)	21	51
2	I	61/78 (78%)	57 (93%)	4 (7%)	21	51
2	J	62/78 (80%)	61 (98%)	1 (2%)	70	93
All	All	612/756 (81%)	578 (94%)	34 (6%)	26	59

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

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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

Some 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

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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	3,2	8,9,10	0.73	0	8,12,14	1.96	2 (25%)
2	SEP	I	46	3,2	8,9,10	0.71	0	8,12,14	2.28	4 (50%)
2	SEP	J	46	3,2	8,9,10	0.65	0	8,12,14	3.02	3 (37%)

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	3,2	-	0/6/8/10	0/0/0/0
2	SEP	I	46	3,2	-	0/6/8/10	0/0/0/0
2	SEP	J	46	3,2	-	0/6/8/10	0/0/0/0

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	46	SEP	OG-P-O1P	-3.65	97.84	107.14
2	J	46	SEP	OG-P-O1P	-2.83	99.94	107.14
2	I	46	SEP	OG-P-O1P	-2.54	100.69	107.14
2	I	46	SEP	O2P-P-OG	-2.01	100.78	106.56
2	H	46	SEP	O3P-P-O2P	2.34	116.30	107.38
2	J	46	SEP	O3P-P-O2P	2.34	116.31	107.38
2	I	46	SEP	O3P-P-O2P	2.36	116.37	107.38
2	I	46	SEP	OG-CB-CA	3.78	111.50	108.27
2	J	46	SEP	OG-CB-CA	6.63	113.93	108.27

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

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

5.5 Carbohydrates (i)

There are no carbohydrates 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	1.14	0	6,6,6	0.27	0
4	PO4	B	502	-	4,4,4	1.25	0	6,6,6	0.27	0
4	PO4	C	503	3	4,4,4	1.20	0	6,6,6	0.27	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PO4	A	501	-	-	0/0/0/0	0/0/0/0
4	PO4	B	502	-	-	0/0/0/0	0/0/0/0
4	PO4	C	503	3	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 9 short contacts:

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

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	176/205 (85%)	-0.14	10 (5%) 27 17	25, 48, 80, 97	0
1	B	177/205 (86%)	-0.32	2 (1%) 82 74	27, 45, 75, 89	0
1	C	175/205 (85%)	-0.42	2 (1%) 82 74	27, 45, 79, 94	0
2	H	86/100 (86%)	-0.30	0 100 100	38, 56, 77, 88	0
2	I	86/100 (86%)	-0.30	0 100 100	44, 57, 76, 95	0
2	J	86/100 (86%)	-0.24	0 100 100	38, 53, 71, 79	0
All	All	786/915 (85%)	-0.29	14 (1%) 71 61	25, 50, 78, 97	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	242	THR	4.0
1	A	248	SER	3.9
1	A	244	ASP	3.6
1	A	249	GLY	3.4
1	A	247	GLY	3.4
1	B	244	ASP	3.1
1	B	248	SER	3.1
1	A	239	PRO	3.0
1	A	240	ASP	2.9
1	A	135	GLU	2.8
1	A	189	GLN	2.6
1	A	246	LEU	2.5
1	C	244	ASP	2.4
1	C	257	ASP	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. 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
2	SEP	J	46	10/11	0.90	0.22	-	53,57,59,59	4
2	SEP	I	46	10/11	0.91	0.23	-	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 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
4	PO4	A	501	5/5	0.90	0.34	4.94	96,96,97,98	0
4	PO4	C	503	5/5	0.97	0.23	2.94	43,44,47,48	5
4	PO4	B	502	5/5	0.96	0.20	1.52	39,41,42,43	5
3	CA	B	402	1/1	0.94	0.17	0.04	48,48,48,48	0
3	CA	A	401	1/1	0.85	0.17	-0.84	57,57,57,57	0
3	CA	C	403	1/1	0.95	0.09	-1.37	45,45,45,45	0

6.5 Other polymers (i)

There are no such residues in this entry.