



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 4, 2016 – 04:48 AM EDT

PDB ID : 5KLG
Title : Structure of CavAb(W195Y) in complex with Br-dihydropyridine derivative UK-59811
Authors : Tang, L.; Gamal EL-Din, T.M.; Swanson, T.M.; Pryde, D.C.; Scheuer, T.; Zheng, N.; Catterall, W.A.
Deposited on : 2016-06-24
Resolution : 3.30 Å(reported)

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

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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027939
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) : rb-20027939

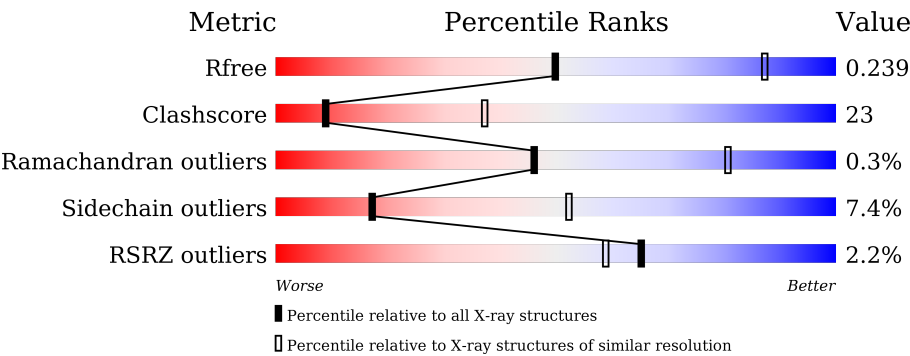
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)

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

Mol	Chain	Length	Quality of chain
1	A	285	<div><div>2%</div><div><div></div><div>41%</div><div>31%</div><div>5%</div><div>23%</div></div></div>
1	B	285	<div><div>%</div><div><div></div><div>50%</div><div>26%</div><div>•</div><div>23%</div></div></div>
1	C	285	<div><div>2%</div><div><div></div><div>40%</div><div>34%</div><div>•</div><div>23%</div></div></div>
1	D	285	<div><div>2%</div><div><div></div><div>45%</div><div>30%</div><div>•</div><div>23%</div></div></div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	6UC	C	1303	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7400 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 Ion transport protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	219	Total	C	N	O	S	0	0	0
			1798	1225	268	295	10			
1	B	219	Total	C	N	O	S	0	0	0
			1798	1225	268	295	10			
1	C	219	Total	C	N	O	S	0	0	0
			1798	1225	268	295	10			
1	D	219	Total	C	N	O	S	0	0	0
			1798	1225	268	295	10			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	983	MET	-	initiating methionine	UNP A8EVM5
A	984	ASP	-	expression tag	UNP A8EVM5
A	985	TYR	-	expression tag	UNP A8EVM5
A	986	LYS	-	expression tag	UNP A8EVM5
A	987	ASP	-	expression tag	UNP A8EVM5
A	988	ASP	-	expression tag	UNP A8EVM5
A	989	ASP	-	expression tag	UNP A8EVM5
A	990	ASP	-	expression tag	UNP A8EVM5
A	991	LYS	-	expression tag	UNP A8EVM5
A	992	GLY	-	expression tag	UNP A8EVM5
A	993	SER	-	expression tag	UNP A8EVM5
A	994	LEU	-	expression tag	UNP A8EVM5
A	995	VAL	-	expression tag	UNP A8EVM5
A	996	PRO	-	expression tag	UNP A8EVM5
A	997	ARG	-	expression tag	UNP A8EVM5
A	998	GLY	-	expression tag	UNP A8EVM5
A	999	SER	-	expression tag	UNP A8EVM5
A	1000	HIS	-	expression tag	UNP A8EVM5
A	1177	ASP	GLU	conflict	UNP A8EVM5
A	1178	ASP	SER	conflict	UNP A8EVM5
A	1181	ASN	MET	conflict	UNP A8EVM5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1195	TYR	TRP	conflict	UNP A8EVM5
B	983	MET	-	initiating methionine	UNP A8EVM5
B	984	ASP	-	expression tag	UNP A8EVM5
B	985	TYR	-	expression tag	UNP A8EVM5
B	986	LYS	-	expression tag	UNP A8EVM5
B	987	ASP	-	expression tag	UNP A8EVM5
B	988	ASP	-	expression tag	UNP A8EVM5
B	989	ASP	-	expression tag	UNP A8EVM5
B	990	ASP	-	expression tag	UNP A8EVM5
B	991	LYS	-	expression tag	UNP A8EVM5
B	992	GLY	-	expression tag	UNP A8EVM5
B	993	SER	-	expression tag	UNP A8EVM5
B	994	LEU	-	expression tag	UNP A8EVM5
B	995	VAL	-	expression tag	UNP A8EVM5
B	996	PRO	-	expression tag	UNP A8EVM5
B	997	ARG	-	expression tag	UNP A8EVM5
B	998	GLY	-	expression tag	UNP A8EVM5
B	999	SER	-	expression tag	UNP A8EVM5
B	1000	HIS	-	expression tag	UNP A8EVM5
B	1177	ASP	GLU	conflict	UNP A8EVM5
B	1178	ASP	SER	conflict	UNP A8EVM5
B	1181	ASN	MET	conflict	UNP A8EVM5
B	1195	TYR	TRP	conflict	UNP A8EVM5
C	983	MET	-	initiating methionine	UNP A8EVM5
C	984	ASP	-	expression tag	UNP A8EVM5
C	985	TYR	-	expression tag	UNP A8EVM5
C	986	LYS	-	expression tag	UNP A8EVM5
C	987	ASP	-	expression tag	UNP A8EVM5
C	988	ASP	-	expression tag	UNP A8EVM5
C	989	ASP	-	expression tag	UNP A8EVM5
C	990	ASP	-	expression tag	UNP A8EVM5
C	991	LYS	-	expression tag	UNP A8EVM5
C	992	GLY	-	expression tag	UNP A8EVM5
C	993	SER	-	expression tag	UNP A8EVM5
C	994	LEU	-	expression tag	UNP A8EVM5
C	995	VAL	-	expression tag	UNP A8EVM5
C	996	PRO	-	expression tag	UNP A8EVM5
C	997	ARG	-	expression tag	UNP A8EVM5
C	998	GLY	-	expression tag	UNP A8EVM5
C	999	SER	-	expression tag	UNP A8EVM5
C	1000	HIS	-	expression tag	UNP A8EVM5
C	1177	ASP	GLU	conflict	UNP A8EVM5

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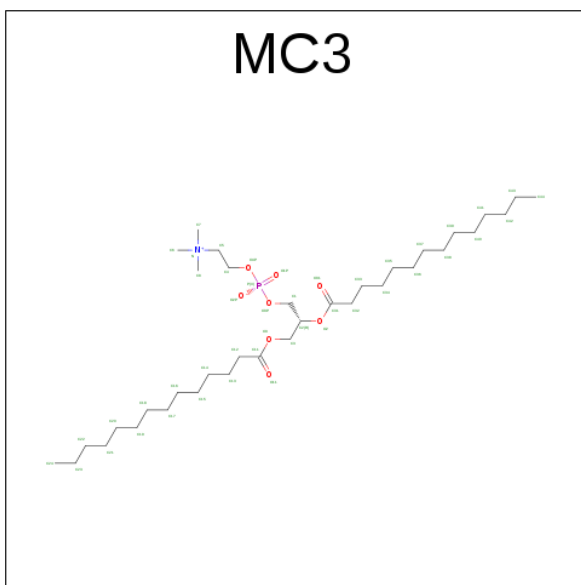
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Chain	Residue	Modelled	Actual	Comment	Reference
C	1178	ASP	SER	conflict	UNP A8EVM5
C	1181	ASN	MET	conflict	UNP A8EVM5
C	1195	TYR	TRP	conflict	UNP A8EVM5
D	983	MET	-	initiating methionine	UNP A8EVM5
D	984	ASP	-	expression tag	UNP A8EVM5
D	985	TYR	-	expression tag	UNP A8EVM5
D	986	LYS	-	expression tag	UNP A8EVM5
D	987	ASP	-	expression tag	UNP A8EVM5
D	988	ASP	-	expression tag	UNP A8EVM5
D	989	ASP	-	expression tag	UNP A8EVM5
D	990	ASP	-	expression tag	UNP A8EVM5
D	991	LYS	-	expression tag	UNP A8EVM5
D	992	GLY	-	expression tag	UNP A8EVM5
D	993	SER	-	expression tag	UNP A8EVM5
D	994	LEU	-	expression tag	UNP A8EVM5
D	995	VAL	-	expression tag	UNP A8EVM5
D	996	PRO	-	expression tag	UNP A8EVM5
D	997	ARG	-	expression tag	UNP A8EVM5
D	998	GLY	-	expression tag	UNP A8EVM5
D	999	SER	-	expression tag	UNP A8EVM5
D	1000	HIS	-	expression tag	UNP A8EVM5
D	1177	ASP	GLU	conflict	UNP A8EVM5
D	1178	ASP	SER	conflict	UNP A8EVM5
D	1181	ASN	MET	conflict	UNP A8EVM5
D	1195	TYR	TRP	conflict	UNP A8EVM5

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

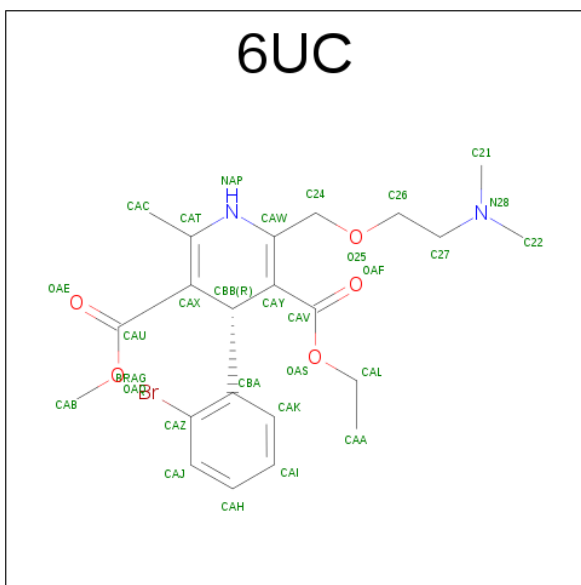
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Ca 1 1	0	0
2	D	1	Total Ca 1 1	0	0

- Molecule 3 is 1,2-DIMYRISTOYL-RAC-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: MC3) (formula: C₃₆H₇₂NO₈P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			21	13	7	1		
3	A	1	Total	C	O	P	0	0
			10	3	6	1		
3	A	1	Total	C	O	P	0	0
			10	3	6	1		
3	A	1	Total	C	O	P	0	0
			10	3	6	1		
3	B	1	Total	C	O	P	0	0
			21	13	7	1		
3	B	1	Total	C	O	P	0	0
			10	3	6	1		
3	C	1	Total	C	O	P	0	0
			10	3	6	1		
3	C	1	Total	C	O	P	0	0
			10	3	6	1		
3	D	1	Total	C	O	P	0	0
			21	13	7	1		
3	D	1	Total	C	O	P	0	0
			10	3	6	1		
3	D	1	Total	C	O	P	0	0
			10	3	6	1		

- Molecule 4 is O3-ethyl O5-methyl (4R)-4-(2-bromophenyl)-2-[2-(dimethylamino)ethoxymethyl]-6-methyl-1,4-dihydropyridine-3,5-dicarboxylate (three-letter code: 6UC) (formula: C₂₂H₂₉BrN₂O₅).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	C	1	Total 30	Br 1	C 22	N 2	O 5	0	0
4	D	1	Total 30	Br 1	C 22	N 2	O 5	0	0

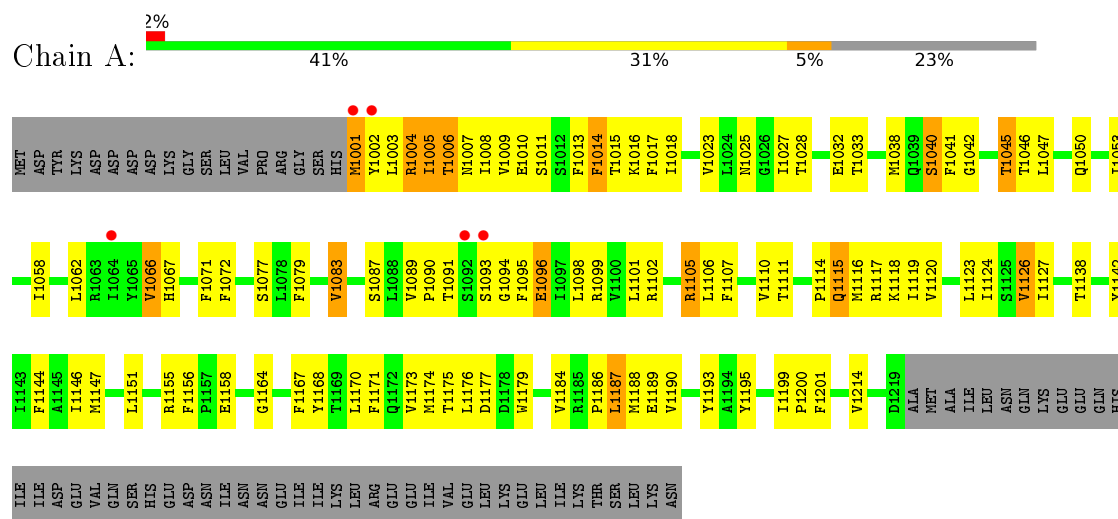
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	2	Total O 2 2	0	0
5	B	1	Total O 1 1	0	0

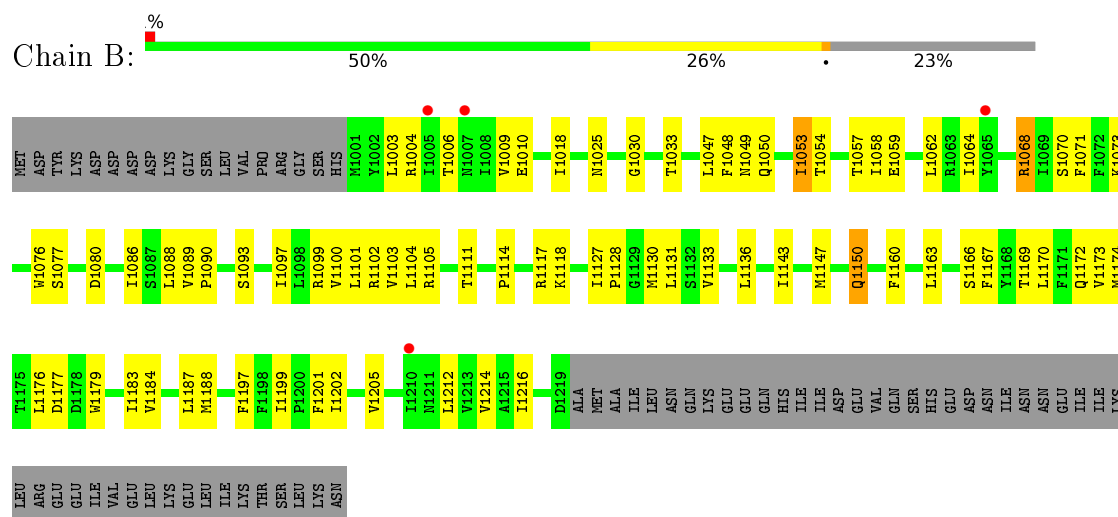
3 Residue-property plots [i](#)

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.

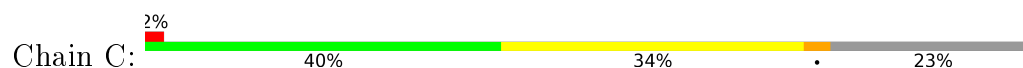
• Molecule 1: Ion transport protein

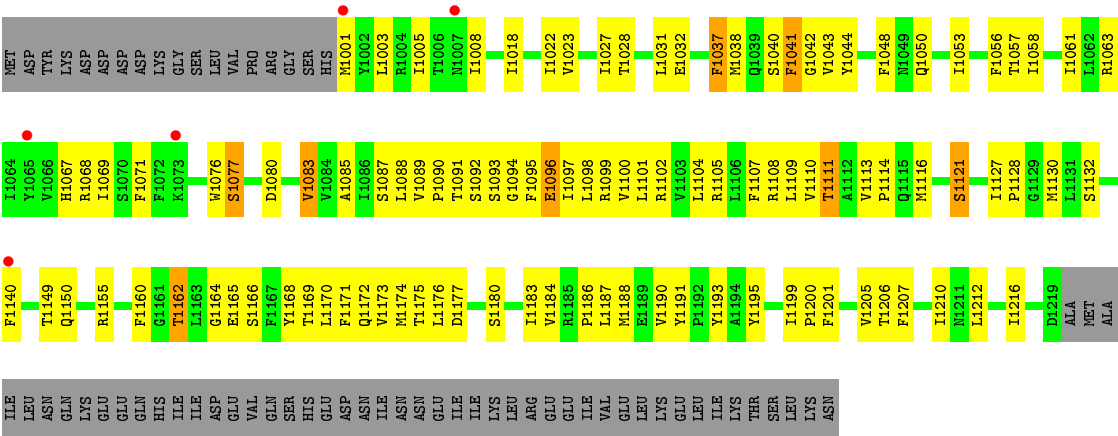


• Molecule 1: Ion transport protein

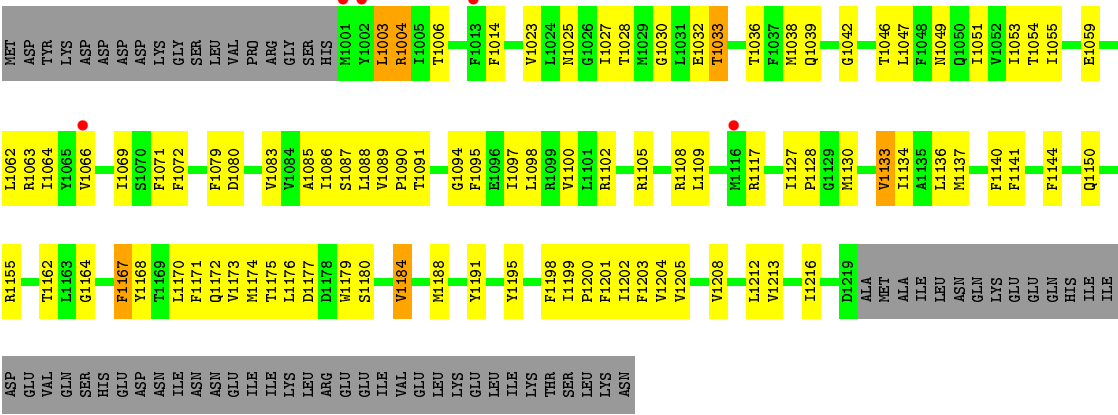


• Molecule 1: Ion transport protein





● Molecule 1: Ion transport protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 2 21	Depositor
Cell constants a, b, c, α , β , γ	125.92Å 126.03Å 192.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.94 – 3.30 29.94 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.94-3.30) 99.6 (29.94-3.30)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.34 (at 3.31Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1839)	Depositor
R, R_{free}	0.279 , 0.303 0.223 , 0.239	Depositor DCC
R_{free} test set	2348 reflections (5.04%)	DCC
Wilson B-factor (Å ²)	90.3	Xtriage
Anisotropy	0.423	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 69.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.450 for k,h,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	7400	wwPDB-VP
Average B, all atoms (Å ²)	109.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.35% 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: CA, MC3, 6UC

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	0.68	0/1848	0.88	0/2515
1	B	0.67	0/1848	0.85	0/2515
1	C	0.68	0/1848	0.85	0/2515
1	D	0.67	0/1848	0.88	0/2515
All	All	0.67	0/7392	0.87	0/10060

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1798	0	1868	109	0
1	B	1798	0	1868	72	0
1	C	1798	0	1868	108	0
1	D	1798	0	1868	81	0
2	A	1	0	0	0	0
2	D	1	0	0	0	0
3	A	51	0	34	5	0
3	B	31	0	24	0	0
3	C	20	0	10	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	41	0	29	1	0
4	C	30	0	0	0	0
4	D	30	0	0	3	0
5	A	2	0	0	0	0
5	B	1	0	0	0	0
All	All	7400	0	7569	349	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 23.

All (349) 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)
1:A:1003:LEU:HB2	1:A:1006:THR:CB	1.72	1.17
1:C:1090:PRO:HG2	1:C:1093:SER:HB3	1.10	1.10
1:A:1003:LEU:CB	1:A:1006:THR:OG1	2.01	1.09
1:B:1089:VAL:HG13	1:B:1090:PRO:HD2	1.37	1.06
1:A:1009:VAL:HA	1:A:1014:PHE:CE2	1.92	1.04
1:A:1003:LEU:HB2	1:A:1006:THR:OG1	1.55	1.03
1:A:1003:LEU:HB2	1:A:1006:THR:HB	1.39	0.98
1:C:1160:PHE:CZ	1:C:1169:THR:HG21	2.01	0.95
1:C:1090:PRO:HG2	1:C:1093:SER:CB	1.98	0.94
1:A:1009:VAL:HA	1:A:1014:PHE:CD2	2.04	0.92
1:D:1130:MET:HG2	1:D:1212:LEU:HD11	1.49	0.92
1:A:1003:LEU:CB	1:A:1006:THR:CB	2.50	0.88
1:A:1001:MET:HB2	1:A:1003:LEU:O	1.76	0.85
1:C:1162:THR:HG22	1:C:1165:GLU:H	1.41	0.84
1:B:1128:PRO:HA	1:B:1131:LEU:HD12	1.62	0.82
1:B:1025:ASN:HD21	1:B:1105:ARG:HH11	1.26	0.82
1:C:1100:VAL:HG12	1:D:1150:GLN:OE1	1.80	0.82
1:B:1025:ASN:ND2	1:B:1105:ARG:HD2	1.96	0.81
1:C:1090:PRO:CG	1:C:1093:SER:HB3	2.03	0.81
1:C:1096:GLU:C	1:C:1097:ILE:HD12	2.01	0.81
1:C:1085:ALA:O	1:C:1088:LEU:HB2	1.82	0.80
1:D:1130:MET:O	1:D:1133:VAL:HG23	1.81	0.79
1:A:1014:PHE:O	1:A:1017:PHE:HB3	1.83	0.79
1:A:1089:VAL:CG1	1:A:1090:PRO:HD2	2.13	0.78
1:B:1166:SER:O	1:B:1170:LEU:HD23	1.84	0.78
1:C:1107:PHE:O	1:C:1110:VAL:HG12	1.85	0.76
1:A:1071:PHE:CZ	1:A:1077:SER:HB2	2.21	0.76
1:A:1090:PRO:HG2	1:A:1093:SER:OG	1.86	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1170:LEU:HD12	1:B:1201:PHE:CE2	2.22	0.75
1:A:1005:ILE:N	1:A:1005:ILE:HD12	2.03	0.73
1:A:1124:ILE:HG13	1:A:1127:ILE:HD12	1.71	0.73
1:B:1183:ILE:O	1:B:1187:LEU:HD23	1.89	0.73
1:A:1001:MET:HA	1:A:1002:TYR:HB2	1.71	0.73
1:B:1053:ILE:HD13	1:B:1088:LEU:HD13	1.70	0.72
1:A:1003:LEU:CB	1:A:1006:THR:HB	2.15	0.72
1:A:1089:VAL:HG12	1:A:1090:PRO:HD2	1.71	0.72
1:A:1171:PHE:HB2	3:A:1302:MC3:H131	1.72	0.71
1:C:1177:ASP:OD2	1:D:1180:SER:HB3	1.91	0.71
1:A:1005:ILE:H	1:A:1005:ILE:HD12	1.55	0.71
1:A:1067:HIS:HB2	1:A:1071:PHE:HB2	1.73	0.71
1:B:1089:VAL:CG1	1:B:1090:PRO:HD2	2.19	0.70
1:A:1003:LEU:HB3	1:A:1006:THR:OG1	1.89	0.70
3:D:1304:MC3:O3P	3:D:1304:MC3:O3	2.09	0.70
1:A:1119:ILE:HD11	1:C:1132:SER:HB2	1.75	0.69
1:A:1087:SER:OG	1:A:1105:ARG:NH1	2.25	0.69
1:A:1050:GLN:HA	1:A:1053:ILE:HG22	1.75	0.69
1:D:1085:ALA:O	1:D:1088:LEU:HB2	1.92	0.68
1:B:1053:ILE:O	1:B:1057:THR:N	2.26	0.68
1:D:1173:VAL:O	1:D:1176:LEU:HD23	1.94	0.68
1:B:1025:ASN:ND2	1:B:1105:ARG:HH11	1.91	0.67
1:C:1089:VAL:CG1	1:C:1090:PRO:HD2	2.24	0.67
1:B:1133:VAL:HG11	1:B:1212:LEU:HD12	1.75	0.67
1:D:1213:VAL:HA	1:D:1216:ILE:HD12	1.77	0.67
1:A:1189:GLU:OE1	1:A:1189:GLU:HA	1.95	0.67
1:D:1170:LEU:HD22	1:D:1201:PHE:CE2	2.29	0.67
1:B:1173:VAL:O	1:B:1176:LEU:HD23	1.95	0.67
1:A:1001:MET:CA	1:A:1002:TYR:HB2	2.24	0.66
1:C:1097:ILE:O	1:C:1100:VAL:HG22	1.95	0.66
1:A:1005:ILE:O	1:A:1007:ASN:N	2.29	0.66
1:C:1174:MET:HG3	1:C:1205:VAL:CG1	2.25	0.66
1:C:1067:HIS:HB2	1:C:1071:PHE:HB2	1.77	0.66
1:C:1193:TYR:HA	1:C:1195:TYR:CE2	2.30	0.66
1:C:1089:VAL:O	1:C:1102:ARG:NH2	2.27	0.66
1:A:1090:PRO:HG2	1:A:1093:SER:CB	2.26	0.65
1:D:1080:ASP:OD1	1:D:1108:ARG:HD2	1.96	0.65
1:A:1008:ILE:HG22	1:A:1009:VAL:N	2.11	0.65
1:B:1025:ASN:HD21	1:B:1105:ARG:HD2	1.62	0.65
1:C:1063:ARG:HH22	1:C:1077:SER:HB3	1.62	0.65
1:C:1050:GLN:HA	1:C:1053:ILE:HG22	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1030:GLY:O	1:D:1033:THR:HB	1.97	0.65
1:C:1028:THR:O	1:C:1032:GLU:HG3	1.98	0.64
1:C:1171:PHE:CE2	1:C:1175:THR:CG2	2.80	0.64
1:A:1001:MET:HA	1:A:1002:TYR:CB	2.26	0.64
1:A:1005:ILE:HG22	1:A:1008:ILE:HD12	1.79	0.64
1:C:1089:VAL:HG12	1:C:1090:PRO:HD2	1.80	0.64
1:C:1096:GLU:O	1:C:1097:ILE:HD12	1.97	0.64
1:B:1053:ILE:HD12	1:B:1053:ILE:C	2.17	0.64
1:A:1005:ILE:CG2	1:A:1008:ILE:HD12	2.28	0.63
1:B:1089:VAL:HG13	1:B:1090:PRO:CD	2.23	0.63
1:A:1008:ILE:O	1:A:1009:VAL:HB	1.99	0.63
1:A:1098:LEU:HD23	1:A:1101:LEU:HD12	1.81	0.62
1:A:1170:LEU:HD22	1:A:1201:PHE:CZ	2.34	0.62
1:D:1133:VAL:O	1:D:1136:LEU:HB3	1.99	0.62
1:D:1086:ILE:O	1:D:1089:VAL:HG22	1.99	0.61
1:A:1001:MET:CE	1:A:1004:ARG:HG2	2.31	0.61
1:D:1137:MET:SD	1:D:1208:VAL:HG11	2.40	0.61
1:B:1179:TRP:CE3	1:B:1184:VAL:HG21	2.36	0.61
1:B:1160:PHE:CZ	1:B:1169:THR:HG21	2.34	0.61
1:C:1027:ILE:O	1:C:1031:LEU:HG	2.01	0.61
1:C:1172:GLN:HG3	1:C:1177:ASP:HB3	1.83	0.61
1:A:1071:PHE:HD2	1:A:1072:PHE:CD1	2.19	0.60
1:A:1015:THR:O	1:A:1018:ILE:N	2.34	0.60
1:C:1098:LEU:HA	1:C:1101:LEU:HB2	1.81	0.60
1:B:1174:MET:HG3	1:B:1205:VAL:HG21	1.84	0.60
1:B:1179:TRP:CZ3	1:B:1184:VAL:HG21	2.36	0.60
1:B:1176:LEU:HD13	1:D:1175:THR:HB	1.82	0.60
1:C:1040:SER:HB3	1:C:1041:PHE:CE2	2.37	0.60
1:C:1171:PHE:O	1:C:1175:THR:HG23	2.01	0.60
1:C:1173:VAL:O	1:C:1176:LEU:N	2.31	0.59
1:D:1179:TRP:O	1:D:1184:VAL:HG23	2.01	0.59
1:B:1018:ILE:HG13	1:B:1059:GLU:CD	2.24	0.58
1:A:1171:PHE:O	1:A:1175:THR:HG23	2.02	0.58
1:C:1174:MET:HG3	1:C:1205:VAL:HG11	1.86	0.57
1:D:1134:ILE:CD1	1:D:1134:ILE:H	2.17	0.57
1:A:1096:GLU:HB3	1:A:1099:ARG:HE	1.67	0.57
1:C:1155:ARG:HD2	1:C:1190:VAL:HG11	1.85	0.57
1:A:1005:ILE:O	1:A:1008:ILE:N	2.37	0.57
1:C:1113:VAL:HG23	1:C:1116:MET:HG2	1.87	0.57
1:B:1199:ILE:HD12	1:D:1171:PHE:CE2	2.41	0.56
1:A:1001:MET:HE2	1:A:1004:ARG:HG2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1008:ILE:HG22	1:A:1009:VAL:H	1.71	0.55
1:C:1109:LEU:O	1:C:1113:VAL:HG22	2.07	0.55
1:C:1040:SER:CB	1:C:1041:PHE:CE2	2.89	0.55
1:A:1005:ILE:O	1:A:1006:THR:C	2.45	0.55
1:A:1116:MET:N	1:A:1116:MET:SD	2.79	0.55
1:A:1214:VAL:HG11	1:B:1216:ILE:HG22	1.88	0.55
1:D:1086:ILE:O	1:D:1089:VAL:HG13	2.07	0.55
1:A:1001:MET:HA	1:A:1003:LEU:N	2.22	0.55
1:B:1070:SER:HA	1:B:1073:LYS:HG2	1.88	0.55
1:C:1193:TYR:HA	1:C:1195:TYR:HE2	1.71	0.55
1:D:1047:LEU:O	1:D:1051:ILE:HG12	2.06	0.55
1:A:1001:MET:HA	1:A:1002:TYR:C	2.27	0.54
1:D:1130:MET:O	1:D:1134:ILE:HD13	2.08	0.54
1:C:1110:VAL:HG23	1:C:1116:MET:HB3	1.89	0.54
1:B:1199:ILE:HD13	1:B:1202:ILE:HD12	1.90	0.54
1:C:1038:MET:O	1:C:1042:GLY:N	2.39	0.54
1:D:1025:ASN:OD1	1:D:1105:ARG:HD2	2.07	0.54
1:A:1177:ASP:OD2	1:C:1180:SER:OG	2.26	0.54
1:B:1076:TRP:HB3	1:B:1111:THR:HB	1.90	0.54
1:D:1051:ILE:O	1:D:1055:ILE:HG13	2.07	0.54
1:B:1199:ILE:HD12	1:D:1171:PHE:CD2	2.43	0.54
1:A:1167:PHE:HB3	3:A:1302:MC3:H122	1.89	0.53
1:B:1054:THR:O	1:B:1057:THR:HB	2.07	0.53
1:D:1174:MET:HG3	1:D:1205:VAL:HB	1.90	0.53
1:B:1025:ASN:HD21	1:B:1105:ARG:NH1	2.02	0.53
1:A:1179:TRP:N	1:B:1177:ASP:OD1	2.41	0.53
1:B:1114:PRO:O	1:B:1118:LYS:N	2.41	0.53
1:C:1097:ILE:N	1:C:1097:ILE:HD12	2.19	0.53
1:D:1036:THR:O	1:D:1039:GLN:HG2	2.09	0.53
1:D:1201:PHE:O	1:D:1205:VAL:HG13	2.09	0.53
1:A:1184:VAL:O	1:A:1188:MET:HG3	2.08	0.53
1:A:1066:VAL:HG22	1:A:1067:HIS:ND1	2.24	0.53
1:B:1076:TRP:HE3	1:B:1111:THR:HG22	1.73	0.53
1:A:1110:VAL:HA	1:A:1116:MET:HB2	1.91	0.53
1:C:1050:GLN:O	1:C:1053:ILE:HG22	2.09	0.53
1:A:1089:VAL:HG13	1:A:1090:PRO:HD2	1.87	0.53
1:D:1086:ILE:HG13	1:D:1087:SER:N	2.24	0.52
1:B:1099:ARG:O	1:B:1102:ARG:HG3	2.09	0.52
1:B:1170:LEU:HD12	1:B:1201:PHE:CZ	2.43	0.52
1:C:1108:ARG:O	1:C:1111:THR:HG22	2.09	0.52
1:A:1193:TYR:HA	1:A:1195:TYR:CE2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1041:PHE:N	1:C:1041:PHE:CD2	2.78	0.52
1:D:1134:ILE:HD12	1:D:1134:ILE:N	2.23	0.52
1:B:1166:SER:O	1:B:1170:LEU:CD2	2.55	0.52
1:B:1071:PHE:CE1	1:B:1077:SER:HB2	2.45	0.51
1:B:1174:MET:HG3	1:B:1205:VAL:CG2	2.41	0.51
1:C:1040:SER:C	1:C:1041:PHE:CD2	2.84	0.51
1:A:1025:ASN:OD1	1:A:1105:ARG:NH2	2.44	0.51
1:C:1160:PHE:CZ	1:C:1169:THR:CG2	2.84	0.51
1:A:1146:ILE:HG12	1:B:1033:THR:HG21	1.92	0.50
1:D:1097:ILE:HG13	1:D:1098:LEU:N	2.26	0.50
1:D:1141:PHE:HB3	1:D:1167:PHE:CE2	2.46	0.50
1:D:1184:VAL:O	1:D:1188:MET:HG3	2.10	0.50
1:D:1003:LEU:N	1:D:1003:LEU:HD12	2.26	0.50
1:C:1018:ILE:HG23	1:C:1056:PHE:CE1	2.45	0.50
1:C:1053:ILE:HD11	1:C:1087:SER:HB3	1.94	0.50
1:A:1105:ARG:HG2	1:A:1106:LEU:HD23	1.94	0.50
1:D:1091:THR:HA	1:D:1102:ARG:NH2	2.27	0.50
1:D:1170:LEU:HD22	1:D:1201:PHE:CZ	2.46	0.50
1:B:1163:LEU:HB2	1:D:1033:THR:HG21	1.92	0.50
1:C:1089:VAL:HG13	1:C:1090:PRO:HD2	1.93	0.50
1:D:1133:VAL:O	1:D:1136:LEU:N	2.45	0.50
1:C:1094:GLY:O	1:C:1095:PHE:CD2	2.65	0.50
1:C:1183:ILE:C	1:C:1186:PRO:HD2	2.32	0.49
1:C:1108:ARG:HA	1:C:1111:THR:HB	1.94	0.49
1:D:1144:PHE:CD2	1:D:1201:PHE:HD2	2.30	0.49
1:C:1169:THR:O	1:C:1173:VAL:HG23	2.12	0.49
1:A:1032:GLU:HG2	1:A:1038:MET:HE3	1.95	0.49
1:C:1100:VAL:HG23	1:C:1101:LEU:N	2.26	0.49
1:A:1003:LEU:CA	1:A:1006:THR:OG1	2.58	0.49
1:B:1184:VAL:O	1:B:1187:LEU:HB2	2.12	0.49
1:C:1068:ARG:HG3	1:C:1069:ILE:HG23	1.94	0.49
1:B:1053:ILE:CD1	1:B:1088:LEU:HD13	2.42	0.49
1:B:1114:PRO:HA	1:B:1117:ARG:HB2	1.94	0.49
1:A:1170:LEU:HD22	1:A:1201:PHE:CE1	2.48	0.48
1:D:1134:ILE:HD12	1:D:1134:ILE:H	1.78	0.48
1:D:1201:PHE:CE1	1:D:1205:VAL:HG11	2.47	0.48
1:C:1097:ILE:CD1	1:C:1097:ILE:N	2.75	0.48
1:A:1079:PHE:O	1:A:1083:VAL:HB	2.13	0.48
1:B:1064:ILE:O	1:B:1068:ARG:N	2.36	0.48
1:D:1063:ARG:HA	1:D:1066:VAL:HG22	1.94	0.48
1:A:1033:THR:HG23	1:C:1149:THR:HG21	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1005:ILE:HA	1:C:1008:ILE:HD12	1.95	0.48
1:D:1014:PHE:CE1	1:D:1059:GLU:HG3	2.48	0.48
1:D:1162:THR:HG22	1:D:1164:GLY:H	1.77	0.48
1:B:1089:VAL:CG1	1:B:1090:PRO:CD	2.88	0.47
1:C:1068:ARG:HG3	1:C:1069:ILE:N	2.30	0.47
1:A:1008:ILE:CG2	1:A:1009:VAL:N	2.78	0.47
1:B:1053:ILE:HD12	1:B:1057:THR:OG1	2.14	0.47
1:C:1031:LEU:HB3	1:C:1037:PHE:CZ	2.49	0.47
1:C:1083:VAL:CG1	1:C:1105:ARG:HA	2.45	0.47
1:C:1113:VAL:CG2	1:C:1116:MET:HG2	2.45	0.47
1:A:1013:PHE:C	1:A:1013:PHE:CD2	2.86	0.47
1:C:1001:MET:HG2	1:C:1005:ILE:HG13	1.97	0.47
1:C:1023:VAL:O	1:C:1027:ILE:HG13	2.15	0.47
1:D:1032:GLU:HA	1:D:1038:MET:HE3	1.96	0.47
1:D:1109:LEU:HD12	1:D:1109:LEU:HA	1.73	0.47
1:D:1195:TYR:CE1	4:D:1305:6UC:NAP	2.83	0.47
1:B:1184:VAL:O	1:B:1188:MET:HG3	2.15	0.47
1:C:1022:ILE:HG13	1:C:1056:PHE:CZ	2.50	0.47
1:C:1207:PHE:HA	1:C:1210:ILE:HD12	1.96	0.47
1:C:1168:TYR:CD1	1:C:1168:TYR:C	2.86	0.47
1:D:1134:ILE:CD1	1:D:1134:ILE:N	2.77	0.47
1:B:1086:ILE:O	1:B:1102:ARG:NH1	2.48	0.46
1:D:1174:MET:C	1:D:1176:LEU:H	2.19	0.46
1:D:1171:PHE:O	1:D:1175:THR:HG23	2.16	0.46
1:C:1130:MET:HG2	1:C:1212:LEU:HD11	1.97	0.46
1:A:1071:PHE:HD2	1:A:1072:PHE:CE1	2.32	0.46
1:B:1179:TRP:HE3	1:B:1184:VAL:CG2	2.29	0.46
1:C:1038:MET:HE2	1:C:1042:GLY:HA2	1.97	0.46
1:C:1050:GLN:O	1:C:1050:GLN:HG3	2.16	0.46
1:C:1170:LEU:HD22	1:C:1201:PHE:CZ	2.51	0.46
1:A:1144:PHE:CD2	1:A:1201:PHE:HD2	2.33	0.46
1:A:1040:SER:O	1:A:1041:PHE:CD2	2.69	0.46
1:A:1009:VAL:CA	1:A:1014:PHE:CD2	2.88	0.46
1:C:1040:SER:HB2	1:C:1041:PHE:CE2	2.51	0.46
1:A:1058:ILE:O	1:A:1062:LEU:HG	2.16	0.46
1:A:1123:LEU:O	1:A:1126:VAL:HG23	2.16	0.46
1:A:1155:ARG:HD3	1:A:1190:VAL:HG11	1.98	0.46
1:D:1188:MET:HA	1:D:1191:TYR:O	2.16	0.46
1:D:1198:PHE:O	1:D:1202:ILE:HG13	2.16	0.46
1:A:1115:GLN:O	1:A:1118:LYS:HB2	2.16	0.45
1:A:1003:LEU:HG	1:A:1003:LEU:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1079:PHE:CZ	1:A:1083:VAL:HG21	2.51	0.45
1:C:1080:ASP:OD1	1:C:1111:THR:HG21	2.15	0.45
1:D:1064:ILE:HG12	1:D:1071:PHE:CD2	2.51	0.45
1:D:1085:ALA:HA	1:D:1088:LEU:HD12	1.98	0.45
1:C:1188:MET:HA	1:C:1191:TYR:O	2.16	0.45
1:D:1094:GLY:O	1:D:1095:PHE:CG	2.70	0.45
1:A:1067:HIS:CB	1:A:1071:PHE:HB2	2.45	0.45
1:A:1091:THR:OG1	1:A:1102:ARG:NH1	2.39	0.45
1:B:1058:ILE:O	1:B:1062:LEU:HG	2.17	0.45
1:C:1089:VAL:HG12	1:C:1090:PRO:CD	2.46	0.45
1:C:1162:THR:HG22	1:C:1165:GLU:N	2.21	0.45
1:A:1168:TYR:CE2	1:C:1188:MET:HE1	2.52	0.45
1:A:1147:MET:HG2	1:B:1103:VAL:HG11	1.99	0.45
1:C:1058:ILE:HA	1:C:1061:ILE:HD12	1.98	0.45
1:D:1062:LEU:O	1:D:1066:VAL:HG13	2.17	0.45
1:A:1110:VAL:HG11	1:A:1120:VAL:HG21	1.99	0.44
1:C:1083:VAL:HG11	1:C:1105:ARG:HA	1.99	0.44
1:C:1166:SER:O	1:C:1170:LEU:HG	2.17	0.44
1:C:1003:LEU:HA	1:C:1003:LEU:HD23	1.64	0.44
1:A:1011:SER:OG	1:A:1014:PHE:HB3	2.18	0.44
1:C:1089:VAL:CG1	1:C:1090:PRO:CD	2.94	0.44
1:D:1053:ILE:HG13	1:D:1054:THR:N	2.32	0.44
1:C:1050:GLN:CA	1:C:1053:ILE:HG22	2.47	0.44
1:C:1184:VAL:O	1:C:1188:MET:HG3	2.17	0.44
1:B:1143:ILE:O	1:B:1147:MET:HG3	2.17	0.44
1:A:1107:PHE:HZ	1:C:1140:PHE:CD1	2.35	0.44
1:D:1094:GLY:O	1:D:1095:PHE:CD2	2.71	0.44
1:D:1127:ILE:HB	1:D:1128:PRO:HD3	1.99	0.44
1:C:1050:GLN:HA	1:C:1053:ILE:CG2	2.46	0.44
1:B:1077:SER:HA	1:B:1080:ASP:HB2	2.00	0.43
1:A:1025:ASN:OD1	1:A:1105:ARG:NE	2.50	0.43
1:A:1050:GLN:O	1:A:1053:ILE:HG22	2.17	0.43
1:C:1057:THR:O	1:C:1061:ILE:HG13	2.18	0.43
1:D:1003:LEU:O	1:D:1006:THR:HG22	2.17	0.43
1:C:1087:SER:HB3	1:C:1105:ARG:HH21	1.83	0.43
1:C:1171:PHE:C	1:C:1171:PHE:CD2	2.91	0.43
1:C:1199:ILE:HB	1:C:1200:PRO:HD3	2.00	0.43
1:D:1213:VAL:O	1:D:1216:ILE:HB	2.17	0.43
1:C:1206:THR:O	1:C:1210:ILE:HG13	2.19	0.43
1:A:1171:PHE:O	1:A:1174:MET:HB3	2.18	0.43
1:B:1188:MET:HE2	1:D:1168:TYR:CE2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1005:ILE:HG22	1:A:1008:ILE:HB	2.01	0.43
1:A:1199:ILE:HB	1:A:1200:PRO:HD3	2.00	0.43
1:B:1199:ILE:HA	1:B:1199:ILE:HD13	1.79	0.43
1:C:1038:MET:O	1:C:1042:GLY:CA	2.66	0.43
1:D:1079:PHE:CE2	1:D:1083:VAL:HG21	2.54	0.43
1:A:1164:GLY:CA	3:A:1302:MC3:H12	2.48	0.43
1:A:1164:GLY:HA3	3:A:1302:MC3:H12	2.00	0.43
1:B:1127:ILE:HB	1:B:1128:PRO:HD3	2.00	0.43
1:D:1003:LEU:HD12	1:D:1004:ARG:H	1.83	0.43
1:B:1169:THR:O	1:B:1172:GLN:HB3	2.19	0.42
1:C:1080:ASP:HB3	1:C:1108:ARG:HH12	1.84	0.42
1:C:1076:TRP:HZ2	1:C:1121:SER:HG	1.65	0.42
1:D:1097:ILE:CG1	1:D:1098:LEU:N	2.82	0.42
1:C:1171:PHE:CE2	1:C:1175:THR:HG21	2.52	0.42
1:A:1102:ARG:O	1:A:1105:ARG:HD2	2.19	0.42
1:A:1199:ILE:HA	1:A:1199:ILE:HD13	1.65	0.42
1:C:1001:MET:HG2	1:C:1001:MET:O	2.20	0.42
1:B:1150:GLN:OE1	1:D:1100:VAL:HG13	2.18	0.42
1:A:1123:LEU:HD12	1:A:1124:ILE:N	2.35	0.42
1:B:1133:VAL:O	1:B:1136:LEU:HB3	2.20	0.42
1:C:1053:ILE:HD12	1:C:1053:ILE:HA	1.86	0.42
1:D:1071:PHE:HD2	1:D:1072:PHE:CD1	2.37	0.42
1:D:1200:PRO:O	1:D:1201:PHE:C	2.58	0.42
1:B:1214:VAL:HG11	1:D:1216:ILE:HG22	2.02	0.42
1:C:1109:LEU:HA	1:C:1109:LEU:HD12	1.89	0.42
1:C:1130:MET:CE	1:C:1216:ILE:HD11	2.50	0.42
1:D:1137:MET:O	1:D:1140:PHE:N	2.53	0.42
1:D:1130:MET:SD	1:D:1216:ILE:HD11	2.59	0.42
1:B:1077:SER:O	1:B:1080:ASP:HB2	2.19	0.42
1:C:1088:LEU:HA	1:C:1088:LEU:HD23	1.82	0.42
1:D:1086:ILE:HG13	1:D:1087:SER:H	1.82	0.42
1:D:1195:TYR:CZ	4:D:1305:6UC:NAP	2.87	0.42
1:A:1047:LEU:HD12	1:A:1050:GLN:OE1	2.20	0.42
1:B:1179:TRP:CE3	1:B:1184:VAL:CG2	3.00	0.42
1:D:1023:VAL:O	1:D:1027:ILE:HG13	2.20	0.42
1:C:1087:SER:HA	1:C:1102:ARG:HG2	2.01	0.41
1:D:1083:VAL:CG1	1:D:1105:ARG:HA	2.50	0.41
1:B:1188:MET:CE	1:D:1168:TYR:CE2	3.03	0.41
1:A:1071:PHE:CE1	1:A:1077:SER:HB2	2.55	0.41
1:A:1142:TYR:OH	1:B:1030:GLY:HA3	2.20	0.41
1:A:1146:ILE:HG23	1:B:1033:THR:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1028:THR:HG21	1:C:1048:PHE:CD2	2.55	0.41
1:C:1164:GLY:HA3	4:D:1305:6UC:BRAG	2.75	0.41
1:A:1001:MET:SD	1:A:1001:MET:O	2.79	0.41
1:A:1138:THR:HA	3:A:1302:MC3:H181	2.02	0.41
1:A:1156:PHE:CZ	1:A:1187:LEU:HA	2.55	0.41
1:B:1009:VAL:O	1:B:1010:GLU:HB2	2.20	0.41
1:D:1038:MET:HE2	1:D:1042:GLY:HA2	2.02	0.41
1:D:1137:MET:O	1:D:1141:PHE:N	2.41	0.41
1:D:1172:GLN:NE2	1:D:1177:ASP:O	2.48	0.41
1:A:1114:PRO:O	1:A:1118:LYS:HG2	2.20	0.41
1:A:1173:VAL:O	1:A:1176:LEU:HD23	2.20	0.41
1:A:1155:ARG:CD	1:A:1190:VAL:HG11	2.51	0.41
1:D:1174:MET:C	1:D:1176:LEU:N	2.73	0.41
1:C:1113:VAL:HA	1:C:1114:PRO:HD3	1.87	0.41
1:B:1169:THR:O	1:B:1173:VAL:HG23	2.20	0.41
1:C:1038:MET:O	1:C:1042:GLY:HA3	2.21	0.41
1:C:1091:THR:OG1	1:C:1092:SER:N	2.54	0.41
1:D:1172:GLN:HG3	1:D:1177:ASP:HB3	2.02	0.41
1:B:1049:ASN:O	1:B:1053:ILE:HG23	2.21	0.41
1:C:1127:ILE:HB	1:C:1128:PRO:HD3	2.03	0.41
1:B:1050:GLN:O	1:B:1053:ILE:HG13	2.21	0.40
1:C:1174:MET:C	1:C:1176:LEU:H	2.25	0.40
1:A:1023:VAL:O	1:A:1027:ILE:HG13	2.21	0.40
1:A:1151:LEU:HG	1:B:1100:VAL:HG11	2.03	0.40
1:B:1101:LEU:O	1:B:1104:LEU:HB2	2.21	0.40
1:C:1104:LEU:HA	1:C:1104:LEU:HD23	1.86	0.40
1:A:1186:PRO:O	1:A:1187:LEU:C	2.59	0.40
1:B:1054:THR:O	1:B:1058:ILE:N	2.44	0.40
1:D:1071:PHE:HD2	1:D:1072:PHE:CE1	2.39	0.40
1:D:1140:PHE:CZ	1:D:1204:VAL:HG11	2.56	0.40
1:A:1042:GLY:O	1:A:1045:THR:HG22	2.21	0.40
1:A:1114:PRO:O	1:A:1118:LYS:N	2.54	0.40
1:A:1158:GLU:H	1:A:1158:GLU:HG2	1.54	0.40
1:C:1067:HIS:HB3	1:C:1071:PHE:N	2.36	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	217/285 (76%)	204 (94%)	11 (5%)	2 (1%)	21	60
1	B	217/285 (76%)	211 (97%)	6 (3%)	0	100	100
1	C	217/285 (76%)	211 (97%)	6 (3%)	0	100	100
1	D	217/285 (76%)	206 (95%)	10 (5%)	1 (0%)	34	71
All	All	868/1140 (76%)	832 (96%)	33 (4%)	3 (0%)	46	81

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1006	THR
1	A	1094	GLY
1	D	1090	PRO

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	202/264 (76%)	182 (90%)	20 (10%)	10	37
1	B	202/264 (76%)	189 (94%)	13 (6%)	22	60
1	C	202/264 (76%)	189 (94%)	13 (6%)	22	60
1	D	202/264 (76%)	188 (93%)	14 (7%)	19	57
All	All	808/1056 (76%)	748 (93%)	60 (7%)	17	52

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1001	MET
1	A	1004	ARG
1	A	1005	ILE
1	A	1010	GLU
1	A	1014	PHE
1	A	1016	LYS
1	A	1028	THR
1	A	1040	SER
1	A	1045	THR
1	A	1046	THR
1	A	1066	VAL
1	A	1083	VAL
1	A	1095	PHE
1	A	1096	GLU
1	A	1105	ARG
1	A	1111	THR
1	A	1115	GLN
1	A	1117	ARG
1	A	1126	VAL
1	A	1187	LEU
1	B	1003	LEU
1	B	1004	ARG
1	B	1006	THR
1	B	1047	LEU
1	B	1048	PHE
1	B	1053	ILE
1	B	1068	ARG
1	B	1093	SER
1	B	1097	ILE
1	B	1130	MET
1	B	1150	GLN
1	B	1167	PHE
1	B	1197	PHE
1	C	1037	PHE
1	C	1041	PHE
1	C	1043	VAL
1	C	1044	TYR
1	C	1077	SER
1	C	1083	VAL
1	C	1096	GLU
1	C	1099	ARG
1	C	1111	THR
1	C	1121	SER

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Mol	Chain	Res	Type
1	C	1150	GLN
1	C	1162	THR
1	C	1187	LEU
1	D	1003	LEU
1	D	1004	ARG
1	D	1028	THR
1	D	1033	THR
1	D	1046	THR
1	D	1049	ASN
1	D	1069	ILE
1	D	1117	ARG
1	D	1133	VAL
1	D	1155	ARG
1	D	1167	PHE
1	D	1184	VAL
1	D	1199	ILE
1	D	1203	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1025	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 2 are monoatomic - leaving 13 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
3	MC3	A	1302	-	20,20,45	1.17	2 (10%)	21,24,53	0.92	1 (4%)
3	MC3	A	1303	-	9,9,45	1.09	1 (11%)	11,12,53	0.92	0
3	MC3	A	1304	-	9,9,45	1.07	1 (11%)	11,12,53	1.25	1 (9%)
3	MC3	A	1305	-	9,9,45	0.97	1 (11%)	11,12,53	0.86	0
3	MC3	B	1301	-	20,20,45	1.24	2 (10%)	21,24,53	1.10	1 (4%)
3	MC3	B	1302	-	9,9,45	1.20	1 (11%)	11,12,53	1.64	1 (9%)
3	MC3	C	1301	-	9,9,45	1.06	1 (11%)	11,12,53	1.01	1 (9%)
3	MC3	C	1302	-	9,9,45	1.13	1 (11%)	11,12,53	1.06	0
4	6UC	C	1303	-	31,31,31	3.37	10 (32%)	38,42,42	3.24	12 (31%)
3	MC3	D	1302	-	20,20,45	1.22	2 (10%)	21,24,53	0.96	1 (4%)
3	MC3	D	1303	-	9,9,45	1.16	1 (11%)	11,12,53	0.64	0
3	MC3	D	1304	-	9,9,45	0.99	1 (11%)	11,12,53	1.21	1 (9%)
4	6UC	D	1305	-	31,31,31	3.84	11 (35%)	38,42,42	4.91	25 (65%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MC3	A	1302	-	-	0/22/22/49	0/0/0/0
3	MC3	A	1303	-	-	0/8/8/49	0/0/0/0
3	MC3	A	1304	-	-	0/8/8/49	0/0/0/0
3	MC3	A	1305	-	-	0/8/8/49	0/0/0/0
3	MC3	B	1301	-	-	0/22/22/49	0/0/0/0
3	MC3	B	1302	-	-	0/8/8/49	0/0/0/0
3	MC3	C	1301	-	-	0/8/8/49	0/0/0/0
3	MC3	C	1302	-	-	0/8/8/49	0/0/0/0
4	6UC	C	1303	-	-	2/24/44/44	0/2/2/2
3	MC3	D	1302	-	-	0/22/22/49	0/0/0/0
3	MC3	D	1303	-	-	0/8/8/49	0/0/0/0
3	MC3	D	1304	-	-	0/8/8/49	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	6UC	D	1305	-	-	0/24/44/44	0/2/2/2

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1302	MC3	O3-C3	-2.36	1.40	1.45
4	C	1303	6UC	C24-CAW	-2.35	1.45	1.50
3	D	1302	MC3	P-O4P	2.07	1.67	1.59
3	A	1305	MC3	P-O3P	2.17	1.66	1.60
4	C	1303	6UC	BRAG-CAZ	2.33	1.95	1.89
3	B	1301	MC3	P-O4P	2.38	1.68	1.59
4	D	1305	6UC	CBB-CAY	2.42	1.57	1.52
3	A	1303	MC3	P-O3P	2.45	1.67	1.60
3	D	1303	MC3	P-O3P	2.48	1.67	1.60
3	D	1304	MC3	P-O3P	2.56	1.67	1.60
3	A	1304	MC3	P-O3P	2.58	1.67	1.60
3	C	1301	MC3	P-O3P	2.60	1.67	1.60
3	C	1302	MC3	P-O3P	2.70	1.67	1.60
4	D	1305	6UC	CAI-CAK	2.75	1.44	1.38
3	B	1302	MC3	P-O3P	2.78	1.68	1.60
3	A	1302	MC3	O3-C11	3.10	1.42	1.33
4	C	1303	6UC	CAC-CAT	3.11	1.56	1.50
3	D	1302	MC3	O3-C11	3.23	1.42	1.33
4	D	1305	6UC	CAK-CBA	3.31	1.44	1.39
3	B	1301	MC3	O3-C11	3.41	1.43	1.33
4	D	1305	6UC	CBA-CAZ	3.44	1.43	1.39
4	D	1305	6UC	OAQ-CAU	4.12	1.43	1.33
4	C	1303	6UC	OAQ-CAU	4.19	1.43	1.33
4	C	1303	6UC	CAV-CAY	4.20	1.56	1.47
4	C	1303	6UC	CBA-CBB	4.23	1.59	1.53
4	D	1305	6UC	CAT-NAP	4.48	1.46	1.38
4	C	1303	6UC	OAS-CAV	4.62	1.43	1.33
4	D	1305	6UC	CAV-CAY	5.29	1.58	1.47
4	D	1305	6UC	OAS-CAV	5.30	1.45	1.33
4	C	1303	6UC	CAT-NAP	5.81	1.49	1.38
4	D	1305	6UC	CAW-NAP	8.15	1.51	1.37
4	C	1303	6UC	CAU-CAX	8.94	1.66	1.47
4	D	1305	6UC	CAU-CAX	9.58	1.67	1.47
4	C	1303	6UC	CAW-NAP	11.11	1.56	1.37
4	D	1305	6UC	CBA-CBB	11.75	1.71	1.53

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1305	6UC	CAT-NAP-CAW	-20.37	103.14	122.35
4	C	1303	6UC	CAT-NAP-CAW	-14.07	109.08	122.35
4	D	1305	6UC	CAY-CAW-NAP	-10.72	108.73	120.58
4	D	1305	6UC	CAK-CBA-CAZ	-6.33	108.03	116.88
4	D	1305	6UC	BRAG-CAZ-CAJ	-5.59	106.75	117.82
4	C	1303	6UC	CAC-CAT-CAX	-5.10	119.78	127.67
4	D	1305	6UC	OAE-CAU-CAX	-4.75	114.64	125.19
4	C	1303	6UC	CAY-CAW-NAP	-4.34	115.78	120.58
4	D	1305	6UC	CBB-CAY-CAW	-4.33	116.42	121.53
4	D	1305	6UC	CAC-CAT-CAX	-4.27	121.06	127.67
4	D	1305	6UC	CBB-CAX-CAT	-4.08	112.68	120.99
4	D	1305	6UC	CAX-CAT-NAP	-3.62	114.00	119.28
4	D	1305	6UC	OAS-CAV-OAF	-3.50	116.71	123.29
4	D	1305	6UC	CAI-CAH-CAJ	-3.45	115.42	120.20
4	C	1303	6UC	C26-C27-N28	-3.34	105.52	114.73
4	C	1303	6UC	OAE-CAU-CAX	-3.33	117.81	125.19
4	C	1303	6UC	OAF-CAV-CAY	-3.02	118.48	125.19
4	C	1303	6UC	CAJ-CAZ-CBA	-2.63	118.91	121.99
4	D	1305	6UC	CAV-CAY-CAW	-2.61	116.51	121.13
4	D	1305	6UC	CAU-CAX-CAT	-2.45	116.01	122.46
4	D	1305	6UC	OAF-CAV-CAY	-2.22	120.28	125.19
4	D	1305	6UC	C26-C27-N28	-2.03	109.11	114.73
3	A	1302	MC3	O2-C2-C1	2.11	117.22	109.32
3	C	1301	MC3	O4P-P-O3P	2.24	110.78	105.33
3	D	1304	MC3	O4P-P-O3P	2.39	111.16	105.33
4	D	1305	6UC	CAB-OAQ-CAU	2.47	120.70	115.89
4	D	1305	6UC	BRAG-CAZ-CBA	2.56	126.76	120.89
4	D	1305	6UC	CBB-CAX-CAU	2.57	124.62	116.94
3	D	1302	MC3	O3-C11-C12	2.68	120.10	111.85
4	D	1305	6UC	CBB-CAY-CAV	2.69	124.97	116.94
3	A	1304	MC3	O4P-P-O3P	3.02	112.67	105.33
4	C	1303	6UC	C24-O25-C26	3.06	119.92	113.14
4	D	1305	6UC	CAL-OAS-CAV	3.19	122.12	116.54
3	B	1301	MC3	O3-C11-C12	3.61	122.95	111.85
4	C	1303	6UC	CAL-OAS-CAV	3.77	123.12	116.54
4	D	1305	6UC	CAJ-CAZ-CBA	3.86	126.49	121.99
4	D	1305	6UC	CAI-CAK-CBA	3.96	126.15	121.02
4	C	1303	6UC	C21-N28-C22	4.14	120.61	109.71
4	C	1303	6UC	OAS-CAV-CAY	4.57	121.43	112.44
4	D	1305	6UC	CBA-CBB-CAY	4.81	123.95	110.73
3	B	1302	MC3	O4P-P-O3P	4.86	117.17	105.33
4	C	1303	6UC	OAQ-CAU-CAX	5.08	122.37	112.29
4	D	1305	6UC	OAS-CAV-CAY	5.37	123.00	112.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1305	6UC	OAQ-CAU-CAX	6.52	125.22	112.29

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	1303	6UC	CAL-OAS-CAV-CAY
4	C	1303	6UC	CAL-OAS-CAV-OAF

There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1302	MC3	5	0
3	D	1304	MC3	1	0
4	D	1305	6UC	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, 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	219/285 (76%)	0.21	5 (2%) 64 57	41, 110, 185, 244	0
1	B	219/285 (76%)	0.18	4 (1%) 71 65	40, 109, 186, 243	0
1	C	219/285 (76%)	0.18	5 (2%) 64 57	43, 104, 172, 199	0
1	D	219/285 (76%)	0.17	5 (2%) 64 57	40, 105, 168, 248	0
All	All	876/1140 (76%)	0.19	19 (2%) 65 59	40, 109, 180, 248	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1065	TYR	4.4
1	D	1001	MET	4.3
1	A	1002	TYR	3.8
1	C	1007	ASN	3.6
1	B	1007	ASN	3.5
1	C	1001	MET	3.1
1	A	1064	ILE	3.1
1	D	1002	TYR	2.9
1	D	1066	VAL	2.8
1	B	1005	ILE	2.7
1	C	1073	LYS	2.6
1	A	1092	SER	2.3
1	D	1013	PHE	2.2
1	B	1210	ILE	2.2
1	A	1093	SER	2.2
1	C	1065	TYR	2.1
1	C	1140	PHE	2.1
1	A	1001	MET	2.0
1	D	1116	MET	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	6UC	C	1303	30/30	0.77	0.45	2.55	74,141,170,181	0
4	6UC	D	1305	30/30	0.87	0.35	1.38	81,106,116,119	0
3	MC3	D	1302	21/46	0.93	0.29	0.96	68,74,84,88	0
3	MC3	B	1301	21/46	0.93	0.29	0.71	59,76,84,88	0
3	MC3	A	1303	10/46	0.82	0.24	0.67	60,90,110,112	0
3	MC3	A	1302	21/46	0.91	0.27	0.60	66,74,131,131	0
2	CA	D	1301	1/1	0.80	0.23	-0.16	83,83,83,83	0
3	MC3	C	1301	10/46	0.89	0.19	-0.70	75,113,119,122	0
3	MC3	D	1304	10/46	0.80	0.23	-0.71	77,99,129,129	0
3	MC3	B	1302	10/46	0.94	0.23	-0.97	69,81,101,104	0
3	MC3	A	1304	10/46	0.89	0.17	-1.12	107,129,147,149	0
3	MC3	C	1302	10/46	0.82	0.19	-1.81	106,127,145,148	0
2	CA	A	1301	1/1	0.98	0.13	-8.28	41,41,41,41	0
3	MC3	A	1305	10/46	0.87	0.26	-	93,107,116,120	0
3	MC3	D	1303	10/46	0.86	0.23	-	60,98,116,118	0

6.5 Other polymers [i](#)

There are no such residues in this entry.