Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 01:48 am BST

PDB ID	:	2WFK
Title	:	Calcium bound LipL32
Authors	:	Tung, J.-Y.; Yang, C.-W.; Sun, Y.-J.
Deposited on	:	2009-04-07
Resolution	:	2.30 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

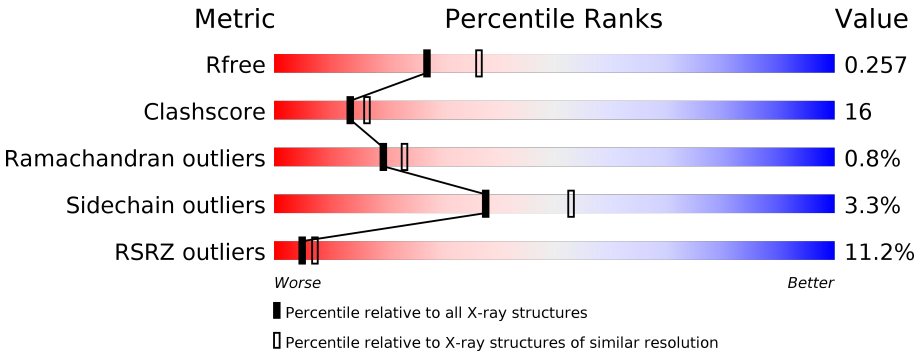
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.30 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}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	259	10% 69% 28% ••
1	B	259	8% 64% 25% • 10%
1	C	259	7% 66% 22% • 10%
1	D	259	11% 61% 27% • 11%
1	E	259	16% 64% 32% • •

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9868 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 LIPL32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	256	Total	C	N	O	Se	0	0	1
			1985	1272	332	376	5			
1	B	233	Total	C	N	O	Se	0	0	1
			1790	1148	295	342	5			
1	C	233	Total	C	N	O	Se	0	0	0
			1802	1155	296	346	5			
1	D	231	Total	C	N	O	Se	0	0	0
			1781	1141	292	343	5			
1	E	255	Total	C	N	O	Se	0	0	1
			1977	1268	331	373	5			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	ASP	-	expression tag	UNP Q6S9S1
A	-4	ARG	-	expression tag	UNP Q6S9S1
A	-3	TRP	-	expression tag	UNP Q6S9S1
A	-2	ILE	-	expression tag	UNP Q6S9S1
A	-1	ARG	-	expression tag	UNP Q6S9S1
A	0	PRO	-	expression tag	UNP Q6S9S1
A	1	ARG	-	expression tag	UNP Q6S9S1
A	249	SER	-	expression tag	UNP Q6S9S1
A	250	ASP	-	expression tag	UNP Q6S9S1
A	251	ALA	-	expression tag	UNP Q6S9S1
A	252	THR	-	expression tag	UNP Q6S9S1
A	253	LYS	-	expression tag	UNP Q6S9S1
B	-5	ASP	-	expression tag	UNP Q6S9S1
B	-4	ARG	-	expression tag	UNP Q6S9S1
B	-3	TRP	-	expression tag	UNP Q6S9S1
B	-2	ILE	-	expression tag	UNP Q6S9S1
B	-1	ARG	-	expression tag	UNP Q6S9S1
B	0	PRO	-	expression tag	UNP Q6S9S1
B	1	ARG	-	expression tag	UNP Q6S9S1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	249	SER	-	expression tag	UNP Q6S9S1
B	250	ASP	-	expression tag	UNP Q6S9S1
B	251	ALA	-	expression tag	UNP Q6S9S1
B	252	THR	-	expression tag	UNP Q6S9S1
B	253	LYS	-	expression tag	UNP Q6S9S1
C	-5	ASP	-	expression tag	UNP Q6S9S1
C	-4	ARG	-	expression tag	UNP Q6S9S1
C	-3	TRP	-	expression tag	UNP Q6S9S1
C	-2	ILE	-	expression tag	UNP Q6S9S1
C	-1	ARG	-	expression tag	UNP Q6S9S1
C	0	PRO	-	expression tag	UNP Q6S9S1
C	1	ARG	-	expression tag	UNP Q6S9S1
C	249	SER	-	expression tag	UNP Q6S9S1
C	250	ASP	-	expression tag	UNP Q6S9S1
C	251	ALA	-	expression tag	UNP Q6S9S1
C	252	THR	-	expression tag	UNP Q6S9S1
C	253	LYS	-	expression tag	UNP Q6S9S1
D	-5	ASP	-	expression tag	UNP Q6S9S1
D	-4	ARG	-	expression tag	UNP Q6S9S1
D	-3	TRP	-	expression tag	UNP Q6S9S1
D	-2	ILE	-	expression tag	UNP Q6S9S1
D	-1	ARG	-	expression tag	UNP Q6S9S1
D	0	PRO	-	expression tag	UNP Q6S9S1
D	1	ARG	-	expression tag	UNP Q6S9S1
D	249	SER	-	expression tag	UNP Q6S9S1
D	250	ASP	-	expression tag	UNP Q6S9S1
D	251	ALA	-	expression tag	UNP Q6S9S1
D	252	THR	-	expression tag	UNP Q6S9S1
D	253	LYS	-	expression tag	UNP Q6S9S1
E	-5	ASP	-	expression tag	UNP Q6S9S1
E	-4	ARG	-	expression tag	UNP Q6S9S1
E	-3	TRP	-	expression tag	UNP Q6S9S1
E	-2	ILE	-	expression tag	UNP Q6S9S1
E	-1	ARG	-	expression tag	UNP Q6S9S1
E	0	PRO	-	expression tag	UNP Q6S9S1
E	1	ARG	-	expression tag	UNP Q6S9S1
E	249	SER	-	expression tag	UNP Q6S9S1
E	250	ASP	-	expression tag	UNP Q6S9S1
E	251	ALA	-	expression tag	UNP Q6S9S1
E	252	THR	-	expression tag	UNP Q6S9S1
E	253	LYS	-	expression tag	UNP Q6S9S1

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

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

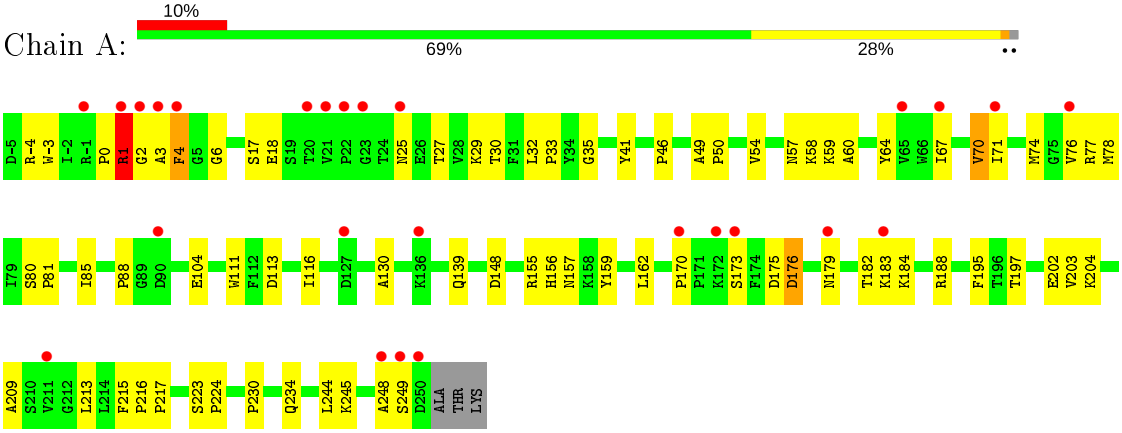
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	137	Total O 137 137	0	0
3	B	155	Total O 155 155	0	0
3	C	109	Total O 109 109	0	0
3	D	77	Total O 77 77	0	0
3	E	50	Total O 50 50	0	0

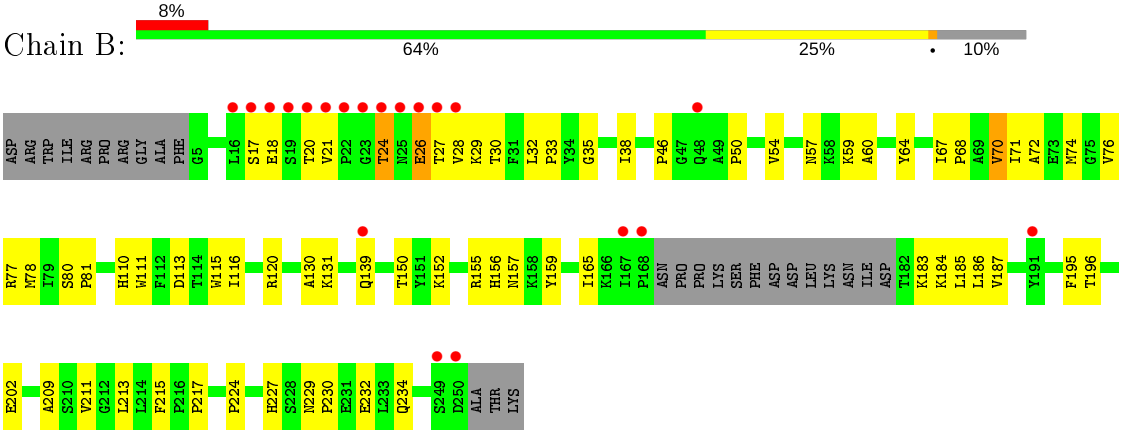
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

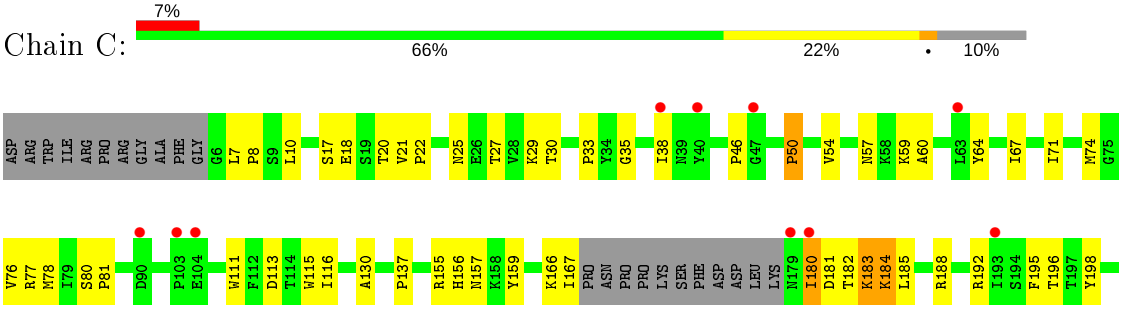
- Molecule 1: LIPL32

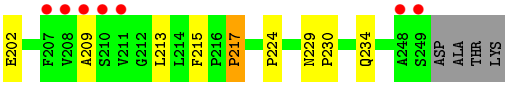


- Molecule 1: LIPL32



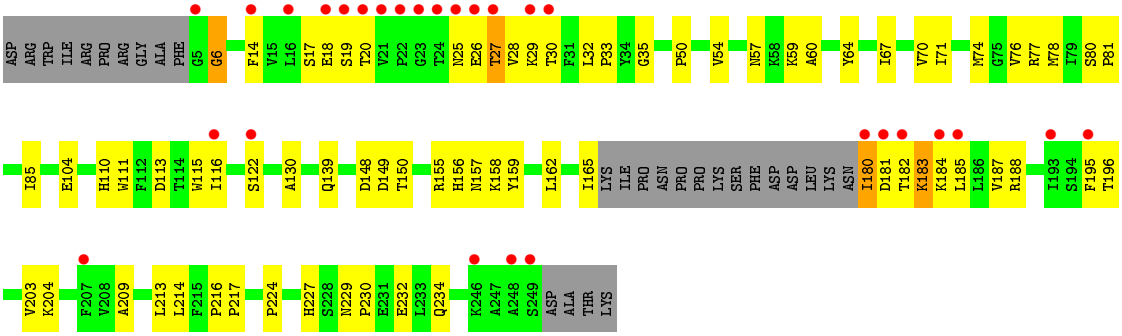
- Molecule 1: LIPL32





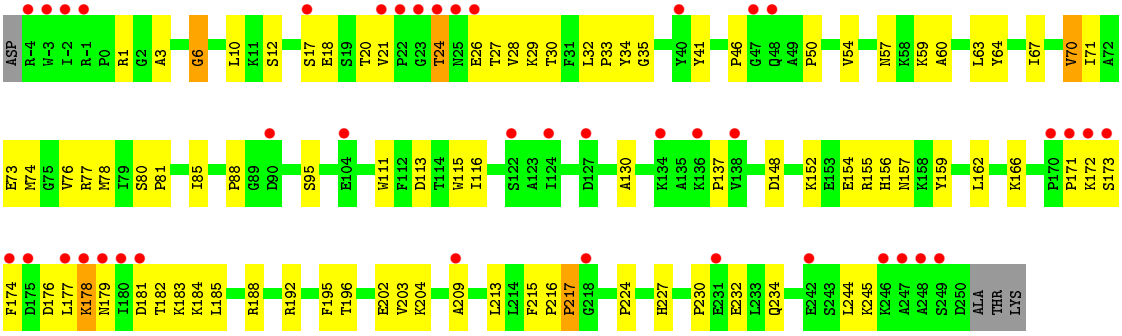
- Molecule 1: LIPL32

Chain D:



- Molecule 1: LIPL32

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	121.91Å 121.91Å 206.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.26 – 2.30 27.26 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.3 (27.26-2.30) 99.6 (27.26-2.30)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.30 (at 2.31Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.219 , 0.262 0.216 , 0.257	Depositor DCC
R_{free} test set	3517 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	44.9	Xtriage
Anisotropy	0.208	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 42.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	9868	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.71% 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, 0.333 respectively for untwinned datasets, and 0.375, 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	0.28	0/2032	0.49	0/2750
1	B	0.28	0/1829	0.48	0/2473
1	C	0.25	0/1840	0.45	0/2487
1	D	0.25	0/1819	0.49	0/2459
1	E	0.27	0/2024	0.49	0/2739
All	All	0.27	0/9544	0.48	0/12908

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	1985	0	1985	52	0
1	B	1790	0	1793	75	0
1	C	1802	0	1804	48	0
1	D	1781	0	1777	76	0
1	E	1977	0	1981	77	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1	0	0	0	0
2	E	1	0	0	0	0
3	A	137	0	0	3	0
3	B	155	0	0	4	0
3	C	109	0	0	4	0
3	D	77	0	0	2	0
3	E	50	0	0	2	0
All	All	9868	0	9340	299	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 16.

All (299) 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:B:185:LEU:HD22	1:B:187:VAL:HG13	1.34	1.05
1:D:183:LYS:HB3	1:E:178:LYS:HA	1.41	1.03
1:B:185:LEU:HD22	1:B:187:VAL:CG1	1.92	0.99
1:E:1:ARG:HG3	1:E:152:LYS:HD3	1.45	0.98
1:B:70:VAL:HG23	1:B:185:LEU:HD21	1.45	0.96
1:E:171:PRO:HG3	1:E:177:LEU:HD21	1.47	0.96
1:B:30:THR:HG23	1:D:25:ASN:HD22	1.34	0.92
1:A:71:ILE:HD11	1:A:224:PRO:HG3	1.49	0.92
1:E:71:ILE:HD11	1:E:224:PRO:HG3	1.53	0.90
1:B:71:ILE:HD11	1:B:224:PRO:HG3	1.55	0.88
1:C:71:ILE:HD11	1:C:224:PRO:HG3	1.55	0.87
1:E:166:LYS:O	1:E:184:LYS:HD2	1.74	0.87
1:D:71:ILE:HD11	1:D:224:PRO:HG3	1.57	0.87
1:A:245:LYS:HE2	1:B:17:SER:HB2	1.59	0.84
1:D:185:LEU:HG	1:D:187:VAL:HG13	1.60	0.84
1:D:139:GLN:HE22	1:D:183:LYS:HG3	1.41	0.83
1:B:20:THR:HB	1:D:150:THR:O	1.81	0.80
1:D:17:SER:HB2	1:E:245:LYS:HE2	1.62	0.80
1:A:0:PRO:O	1:A:1:ARG:HB2	1.80	0.79
1:B:70:VAL:CG2	1:B:185:LEU:HD21	2.13	0.79
1:E:81:PRO:HG3	1:E:111:TRP:HB3	1.65	0.79
1:C:180:ILE:HD11	1:C:185:LEU:HD21	1.64	0.79
1:C:81:PRO:HG3	1:C:111:TRP:HB3	1.65	0.78
1:B:17:SER:HB3	1:B:30:THR:HB	1.65	0.77
1:D:81:PRO:HG3	1:D:111:TRP:HB3	1.66	0.76
1:D:50:PRO:HG3	1:D:59:LYS:HG2	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:139:GLN:NE2	1:B:183:LYS:HB2	2.00	0.75
1:B:50:PRO:HG3	1:B:59:LYS:HG2	1.68	0.75
1:A:50:PRO:HG3	1:A:59:LYS:HG2	1.69	0.75
1:D:165:ILE:HG23	1:D:184:LYS:HD2	1.70	0.74
1:C:7:LEU:HD12	1:C:8:PRO:HD2	1.69	0.74
1:B:30:THR:HG23	1:D:25:ASN:ND2	2.02	0.74
1:E:50:PRO:HG3	1:E:59:LYS:HG2	1.71	0.73
1:E:156:HIS:HD2	1:E:157:ASN:O	1.71	0.73
1:A:156:HIS:HD2	1:A:157:ASN:O	1.72	0.72
1:C:156:HIS:HD2	1:C:157:ASN:O	1.70	0.72
1:A:81:PRO:HG3	1:A:111:TRP:HB3	1.71	0.72
1:E:21:VAL:HG23	1:E:21:VAL:O	1.87	0.72
1:B:156:HIS:HD2	1:B:157:ASN:O	1.73	0.72
1:A:76:VAL:HG12	1:A:116:ILE:HD13	1.70	0.71
1:B:150:THR:O	1:D:20:THR:HB	1.89	0.71
1:D:139:GLN:HE22	1:D:183:LYS:CG	2.02	0.71
1:D:180:ILE:HG12	1:D:180:ILE:O	1.91	0.71
1:D:183:LYS:CB	1:E:178:LYS:HA	2.20	0.71
1:D:156:HIS:HD2	1:D:157:ASN:O	1.74	0.71
1:A:244:LEU:HD21	1:B:32:LEU:HD13	1.72	0.71
1:D:17:SER:HB2	1:E:245:LYS:CE	2.20	0.71
1:C:76:VAL:HG12	1:C:116:ILE:HD13	1.72	0.70
1:B:81:PRO:HG3	1:B:111:TRP:HB3	1.74	0.70
1:B:139:GLN:HE22	1:B:183:LYS:HB2	1.56	0.69
1:A:245:LYS:CE	1:B:17:SER:HB2	2.22	0.69
1:E:174:PHE:HA	1:E:177:LEU:HG	1.74	0.68
1:C:167:ILE:HG23	1:C:180:ILE:HD13	1.76	0.68
1:D:76:VAL:HG12	1:D:116:ILE:HD13	1.75	0.68
1:C:180:ILE:HD11	1:C:185:LEU:CD2	2.22	0.67
1:B:185:LEU:HD23	1:B:185:LEU:C	2.14	0.67
1:E:21:VAL:HG23	1:E:24:THR:OG1	1.94	0.67
1:A:35:GLY:O	1:A:217:PRO:HG3	1.94	0.66
1:B:120:ARG:NH1	1:B:183:LYS:O	2.28	0.66
1:D:17:SER:HB3	1:D:30:THR:HB	1.78	0.66
1:E:64:TYR:CE2	1:E:230:PRO:HG3	2.32	0.65
1:B:185:LEU:HD23	1:B:186:LEU:N	2.12	0.65
1:B:139:GLN:HE22	1:B:183:LYS:CB	2.09	0.64
1:D:130:ALA:H	1:D:234:GLN:NE2	1.95	0.64
1:E:20:THR:HG22	1:E:21:VAL:N	2.11	0.64
1:C:130:ALA:H	1:C:234:GLN:NE2	1.95	0.64
1:C:50:PRO:HG3	1:C:59:LYS:HG2	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:113:ASP:OD1	1:D:159:TYR:HB3	1.98	0.64
1:E:130:ALA:H	1:E:234:GLN:NE2	1.96	0.63
1:C:35:GLY:O	1:C:217:PRO:HG3	1.99	0.63
1:E:76:VAL:HG12	1:E:116:ILE:HD13	1.79	0.63
1:C:113:ASP:OD1	1:C:159:TYR:HB3	1.99	0.63
1:D:17:SER:HB2	1:E:245:LYS:NZ	2.13	0.63
1:E:21:VAL:HG22	1:E:26:GLU:O	1.99	0.63
1:D:32:LEU:HD13	1:E:244:LEU:HD21	1.80	0.62
1:B:186:LEU:HD22	1:B:186:LEU:N	2.12	0.62
1:B:35:GLY:O	1:B:217:PRO:HG3	2.00	0.62
1:D:35:GLY:O	1:D:217:PRO:HG3	1.99	0.62
1:E:70:VAL:HB	3:E:2016:HOH:O	2.00	0.61
1:D:185:LEU:HG	1:D:187:VAL:CG1	2.29	0.61
1:E:20:THR:CG2	1:E:21:VAL:N	2.63	0.61
1:A:179:ASN:CG	1:A:179:ASN:O	2.38	0.61
1:B:21:VAL:HG12	1:B:24:THR:CG2	2.32	0.60
1:E:21:VAL:HG21	1:E:26:GLU:HB2	1.83	0.60
1:E:21:VAL:HG23	1:E:24:THR:HG1	1.66	0.60
1:B:77:ARG:HD2	3:B:2127:HOH:O	2.01	0.60
1:D:64:TYR:CE2	1:D:230:PRO:HG3	2.37	0.60
1:A:77:ARG:HD2	3:A:2125:HOH:O	2.01	0.59
1:B:18:GLU:OE1	1:B:29:LYS:HD3	2.02	0.59
1:E:174:PHE:HD2	1:E:177:LEU:HD11	1.68	0.59
1:E:35:GLY:O	1:E:217:PRO:HG3	2.03	0.58
1:B:130:ALA:H	1:B:234:GLN:NE2	2.00	0.58
1:D:158:LYS:HE3	3:D:2050:HOH:O	2.04	0.58
1:B:26:GLU:HB3	1:D:29:LYS:O	2.04	0.58
1:B:70:VAL:HG23	1:B:185:LEU:CD2	2.25	0.58
1:B:76:VAL:HG12	1:B:116:ILE:HD13	1.84	0.58
1:E:113:ASP:OD1	1:E:159:TYR:HB3	2.04	0.57
1:E:21:VAL:CG2	1:E:24:THR:OG1	2.52	0.57
1:E:1:ARG:CG	1:E:152:LYS:HD3	2.28	0.57
1:B:113:ASP:OD1	1:B:159:TYR:HB3	2.05	0.57
1:B:185:LEU:HD22	1:B:187:VAL:HG12	1.82	0.57
1:B:77:ARG:HG2	1:B:78:MSE:N	2.20	0.57
1:A:64:TYR:CE2	1:A:230:PRO:HG3	2.39	0.57
1:A:113:ASP:OD1	1:A:159:TYR:HB3	2.05	0.56
1:A:33:PRO:HG3	1:C:25:ASN:OD1	2.05	0.56
1:D:183:LYS:HD3	1:D:183:LYS:N	2.20	0.56
1:E:172:LYS:HD3	1:E:176:ASP:OD1	2.05	0.56
1:A:130:ALA:H	1:A:234:GLN:NE2	2.03	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:185:LEU:CD2	1:B:187:VAL:CG1	2.77	0.55
1:A:245:LYS:NZ	1:B:17:SER:HB2	2.22	0.55
1:C:77:ARG:HD2	3:C:2090:HOH:O	2.07	0.54
1:D:14:PHE:CE2	1:D:214:LEU:HD21	2.42	0.54
1:E:21:VAL:CG2	1:E:26:GLU:HB2	2.38	0.54
1:B:152:LYS:HD2	1:D:19:SER:HB3	1.89	0.54
1:B:74:MSE:HE2	1:B:213:LEU:HD21	1.90	0.54
1:A:17:SER:HB3	1:A:30:THR:HB	1.90	0.54
1:E:17:SER:HB3	1:E:30:THR:HB	1.89	0.54
1:B:139:GLN:NE2	1:B:183:LYS:CB	2.69	0.54
1:D:183:LYS:N	1:D:183:LYS:CD	2.71	0.54
1:B:20:THR:CB	1:D:150:THR:O	2.54	0.54
1:C:64:TYR:CE2	1:C:230:PRO:HG3	2.42	0.53
1:E:18:GLU:HA	1:E:28:VAL:O	2.08	0.53
1:C:156:HIS:CD2	1:C:157:ASN:O	2.58	0.53
1:A:139:GLN:HE22	1:A:182:THR:HG23	1.72	0.53
1:B:64:TYR:CE2	1:B:230:PRO:HG3	2.43	0.53
1:D:180:ILE:CG1	1:D:180:ILE:O	2.57	0.53
1:B:150:THR:O	1:D:20:THR:CB	2.54	0.53
1:E:174:PHE:HD2	1:E:177:LEU:CD1	2.21	0.53
1:E:67:ILE:HG23	1:E:71:ILE:HD12	1.91	0.53
1:D:18:GLU:OE1	1:D:29:LYS:HD3	2.09	0.52
1:E:21:VAL:O	1:E:21:VAL:CG2	2.55	0.52
1:B:21:VAL:HG12	1:B:24:THR:HG23	1.92	0.52
1:E:67:ILE:O	1:E:188:ARG:HA	2.10	0.52
1:C:181:ASP:OD2	1:C:183:LYS:HG2	2.09	0.52
1:C:115:TRP:HB3	1:C:196:THR:HG23	1.93	0.51
1:B:185:LEU:CD2	1:B:185:LEU:C	2.78	0.51
1:B:110:HIS:HD2	3:B:2055:HOH:O	1.92	0.51
1:D:67:ILE:HG23	1:D:71:ILE:HD12	1.93	0.51
1:D:67:ILE:O	1:D:188:ARG:HA	2.11	0.51
1:E:156:HIS:CD2	1:E:157:ASN:O	2.58	0.51
1:B:152:LYS:HD2	1:D:19:SER:CB	2.40	0.51
1:C:74:MSE:HE2	1:C:213:LEU:HD21	1.93	0.51
1:E:21:VAL:HG23	1:E:24:THR:CG2	2.41	0.50
1:C:183:LYS:HB3	1:C:183:LYS:NZ	2.27	0.50
1:A:4:PHE:CG	1:C:22:PRO:HB3	2.46	0.50
1:C:67:ILE:HG23	1:C:71:ILE:HD12	1.93	0.50
1:B:80:SER:O	1:B:156:HIS:HE1	1.93	0.50
1:B:81:PRO:HD2	1:B:155:ARG:CZ	2.41	0.50
1:D:77:ARG:HD2	3:D:2070:HOH:O	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:18:GLU:OE1	1:E:29:LYS:HD3	2.11	0.50
1:A:104:GLU:HB2	3:A:2073:HOH:O	2.12	0.50
1:E:77:ARG:HG2	1:E:78:MSE:N	2.26	0.50
1:B:21:VAL:HG12	1:B:24:THR:HG21	1.94	0.50
1:B:195:PHE:CZ	1:B:209:ALA:HB1	2.47	0.49
1:C:17:SER:HB3	1:C:30:THR:HB	1.93	0.49
1:D:115:TRP:HB3	1:D:196:THR:HG23	1.94	0.49
1:B:227:HIS:NE2	1:B:232:GLU:HG2	2.26	0.49
1:D:80:SER:O	1:D:156:HIS:HE1	1.94	0.49
1:D:54:VAL:HG23	1:D:60:ALA:HB2	1.95	0.49
1:D:6:GLY:HA3	1:D:85:ILE:O	2.13	0.49
1:C:7:LEU:HD11	1:C:77:ARG:NH1	2.27	0.49
1:D:185:LEU:CG	1:D:187:VAL:HG13	2.38	0.49
1:E:181:ASP:HB3	1:E:184:LYS:HZ1	1.78	0.49
1:D:18:GLU:CD	1:D:29:LYS:HD3	2.33	0.49
1:E:80:SER:O	1:E:156:HIS:HE1	1.95	0.49
1:D:14:PHE:CE2	1:D:214:LEU:CD2	2.96	0.49
1:D:81:PRO:HD2	1:D:155:ARG:CZ	2.43	0.49
1:C:181:ASP:OD1	1:C:182:THR:N	2.45	0.48
1:B:165:ILE:HG23	1:B:184:LYS:HE2	1.95	0.48
1:A:54:VAL:HG23	1:A:60:ALA:HB2	1.95	0.48
1:B:165:ILE:HG23	1:B:184:LYS:HB3	1.96	0.48
1:C:81:PRO:HD2	1:C:155:ARG:CZ	2.42	0.48
1:E:81:PRO:HD2	1:E:155:ARG:CZ	2.44	0.48
1:B:185:LEU:CD2	1:B:187:VAL:HG12	2.43	0.48
1:B:115:TRP:HB3	1:B:196:THR:HG23	1.96	0.48
1:B:139:GLN:NE2	1:B:183:LYS:HD2	2.29	0.48
1:A:156:HIS:CD2	1:A:157:ASN:O	2.62	0.47
1:A:70:VAL:HG12	1:B:72:ALA:HB2	1.96	0.47
1:D:77:ARG:HG2	1:D:78:MSE:N	2.29	0.47
1:E:174:PHE:CD2	1:E:177:LEU:HD11	2.49	0.47
1:B:32:LEU:HD12	1:B:33:PRO:HD2	1.95	0.47
1:C:80:SER:O	1:C:156:HIS:HE1	1.98	0.47
1:A:18:GLU:OE1	1:A:29:LYS:HD3	2.15	0.47
1:A:25:ASN:OD1	1:C:33:PRO:HG3	2.14	0.47
1:D:74:MSE:HE2	1:D:213:LEU:HD21	1.97	0.47
1:E:73:GLU:HG3	1:E:166:LYS:HB3	1.97	0.47
1:A:67:ILE:O	1:A:188:ARG:HA	2.15	0.47
1:D:20:THR:HG23	1:D:26:GLU:O	2.14	0.47
1:E:6:GLY:HA2	1:E:85:ILE:O	2.14	0.47
1:E:181:ASP:C	1:E:183:LYS:H	2.18	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:20:THR:HG22	1:E:21:VAL:C	2.35	0.47
1:C:77:ARG:HG2	1:C:78:MSE:N	2.30	0.46
1:D:185:LEU:CD2	1:D:187:VAL:CG1	2.93	0.46
1:B:18:GLU:CD	1:B:29:LYS:HD3	2.35	0.46
1:D:181:ASP:OD2	1:D:182:THR:N	2.44	0.46
1:E:174:PHE:HA	1:E:177:LEU:CG	2.45	0.46
1:A:182:THR:C	1:A:184:LYS:H	2.18	0.46
1:E:71:ILE:HD11	1:E:224:PRO:CG	2.38	0.46
1:B:54:VAL:HG23	1:B:60:ALA:HB2	1.96	0.46
1:B:46:PRO:HA	1:B:202:GLU:OE2	2.16	0.46
1:E:74:MSE:HE2	1:E:213:LEU:HD21	1.98	0.46
1:E:227:HIS:NE2	1:E:232:GLU:HG2	2.31	0.46
1:A:2:GLY:O	1:A:3:ALA:C	2.53	0.45
1:B:186:LEU:N	1:B:186:LEU:CD2	2.79	0.45
1:D:156:HIS:CD2	1:D:157:ASN:O	2.63	0.45
1:E:216:PRO:HA	1:E:217:PRO:HD3	1.77	0.45
1:A:173:SER:O	1:A:176:ASP:HB2	2.16	0.45
1:C:166:LYS:O	1:C:184:LYS:HG3	2.16	0.45
1:C:185:LEU:HD11	3:C:2077:HOH:O	2.16	0.45
1:D:216:PRO:HA	1:D:217:PRO:HD3	1.76	0.45
1:D:122:SER:O	1:E:174:PHE:HZ	2.00	0.45
1:E:54:VAL:HG23	1:E:60:ALA:HB2	1.98	0.45
1:A:195:PHE:CZ	1:A:209:ALA:HB1	2.51	0.45
1:A:77:ARG:HG2	1:A:78:MSE:N	2.32	0.45
1:A:248:ALA:O	1:D:25:ASN:OD1	2.34	0.45
1:A:80:SER:O	1:A:156:HIS:HE1	2.00	0.45
1:C:54:VAL:HG23	1:C:60:ALA:HB2	1.99	0.45
1:D:183:LYS:HD3	1:D:183:LYS:H	1.81	0.45
1:D:14:PHE:CD1	1:D:14:PHE:N	2.85	0.45
1:E:32:LEU:HD12	1:E:33:PRO:HD2	1.98	0.45
1:C:195:PHE:CZ	1:C:209:ALA:HB1	2.52	0.45
1:A:183:LYS:HD2	3:A:2114:HOH:O	2.17	0.45
1:C:195:PHE:CE1	1:C:209:ALA:HB1	2.52	0.45
1:A:18:GLU:CD	1:A:29:LYS:HD3	2.38	0.44
1:C:67:ILE:O	1:C:188:ARG:HA	2.17	0.44
1:C:18:GLU:OE1	1:C:29:LYS:HD3	2.17	0.44
1:E:95:SER:HA	3:E:2024:HOH:O	2.16	0.44
1:B:18:GLU:CD	1:D:149:ASP:HB2	2.37	0.44
1:B:131:LYS:HE3	1:C:198:TYR:CE2	2.52	0.44
1:D:19:SER:OG	1:D:28:VAL:CG2	2.65	0.44
1:A:32:LEU:HD12	1:A:33:PRO:HD2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:180:ILE:O	1:C:180:ILE:HG13	2.13	0.44
1:D:14:PHE:N	1:D:14:PHE:HD1	2.16	0.44
1:E:195:PHE:CZ	1:E:209:ALA:HB1	2.53	0.44
1:E:203:VAL:HG13	1:E:204:LYS:N	2.32	0.43
1:A:216:PRO:HA	1:A:217:PRO:HD3	1.77	0.43
1:A:6:GLY:HA3	1:A:85:ILE:O	2.18	0.43
1:D:139:GLN:NE2	1:D:183:LYS:HG3	2.20	0.43
1:D:195:PHE:CZ	1:D:209:ALA:HB1	2.53	0.43
1:B:156:HIS:CD2	1:B:157:ASN:O	2.61	0.43
1:B:195:PHE:CE1	1:B:209:ALA:HB1	2.53	0.43
1:A:46:PRO:HA	1:A:202:GLU:OE2	2.18	0.43
1:D:227:HIS:NE2	1:D:232:GLU:HG2	2.33	0.43
1:E:41:TYR:CG	1:E:88:PRO:HG3	2.54	0.43
1:A:49:ALA:HA	1:A:50:PRO:HD3	1.81	0.43
1:D:229:ASN:HA	1:D:230:PRO:HD3	1.89	0.43
1:E:172:LYS:O	1:E:173:SER:HB2	2.19	0.43
1:E:184:LYS:C	1:E:185:LEU:HD23	2.39	0.42
1:A:74:MSE:HE2	1:A:213:LEU:HD21	2.01	0.42
1:B:229:ASN:HA	1:B:230:PRO:HD3	1.85	0.42
1:A:203:VAL:HG13	1:A:204:LYS:N	2.34	0.42
1:C:18:GLU:CD	1:C:29:LYS:HD3	2.40	0.42
1:C:156:HIS:HB2	3:C:2064:HOH:O	2.18	0.42
1:E:178:LYS:H	1:E:178:LYS:HG2	1.55	0.42
1:E:148:ASP:HA	1:E:162:LEU:CB	2.50	0.42
1:E:71:ILE:HG12	1:E:215:PHE:HB2	2.00	0.42
1:C:46:PRO:HA	1:C:202:GLU:OE2	2.19	0.42
1:C:20:THR:HG22	1:C:21:VAL:N	2.35	0.42
1:D:203:VAL:HG13	1:D:204:LYS:N	2.35	0.42
1:A:71:ILE:HG12	1:A:215:PHE:HB2	2.01	0.41
1:B:67:ILE:HG23	1:B:71:ILE:HD12	2.01	0.41
1:D:80:SER:O	1:D:156:HIS:CE1	2.73	0.41
1:E:115:TRP:HB3	1:E:196:THR:HG23	2.02	0.41
1:A:41:TYR:CG	1:A:88:PRO:HG3	2.56	0.41
1:C:35:GLY:HA3	1:C:215:PHE:O	2.20	0.41
1:B:80:SER:O	1:B:156:HIS:CE1	2.73	0.41
1:C:7:LEU:HD12	1:C:8:PRO:CD	2.44	0.41
1:D:20:THR:HA	1:D:27:THR:HA	2.01	0.41
1:E:174:PHE:HA	1:E:177:LEU:CD1	2.50	0.41
1:A:4:PHE:CD1	1:C:22:PRO:HB3	2.55	0.41
1:D:50:PRO:CG	1:D:59:LYS:HG2	2.45	0.41
1:D:122:SER:HA	1:E:174:PHE:CZ	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:152:LYS:HE2	1:E:154:GLU:OE1	2.21	0.41
1:A:148:ASP:HA	1:A:162:LEU:CB	2.51	0.41
1:C:229:ASN:HA	1:C:230:PRO:HD3	1.91	0.41
1:A:71:ILE:HD11	1:A:224:PRO:CG	2.35	0.41
1:D:32:LEU:HD12	1:D:33:PRO:HD2	2.03	0.41
1:C:137:PRO:HG3	1:C:192:ARG:NH2	2.36	0.41
1:E:12:SER:HA	1:E:34:TYR:CZ	2.56	0.41
1:B:71:ILE:HG12	1:B:215:PHE:HB2	2.03	0.41
1:E:63:LEU:HD23	1:E:63:LEU:HA	1.91	0.41
1:B:183:LYS:HG3	1:B:184:LYS:HG3	2.02	0.40
1:C:38:ILE:HD12	3:C:2034:HOH:O	2.19	0.40
1:A:223:SER:HA	1:A:224:PRO:HD3	1.92	0.40
1:B:120:ARG:HD3	3:B:2119:HOH:O	2.20	0.40
1:B:38:ILE:HG22	1:B:211:VAL:HB	2.03	0.40
1:D:148:ASP:HA	1:D:162:LEU:CB	2.52	0.40
1:A:58:LYS:HE2	1:A:197:THR:O	2.21	0.40
1:A:81:PRO:HD2	1:A:155:ARG:CZ	2.52	0.40
1:B:68:PRO:HD2	3:B:2132:HOH:O	2.21	0.40
1:D:104:GLU:OE2	1:D:110:HIS:HE1	2.03	0.40
1:E:46:PRO:HA	1:E:202:GLU:OE2	2.21	0.40
1:E:185:LEU:N	1:E:185:LEU:HD23	2.36	0.40
1:E:18:GLU:CD	1:E:29:LYS:HD3	2.41	0.40
1:A:-3:TRP:CE3	1:A:35:GLY:HA2	2.56	0.40
1:B:21:VAL:CG1	1:B:24:THR:HG21	2.51	0.40
1:D:195:PHE:CE1	1:D:209:ALA:HB1	2.57	0.40
1:D:14:PHE:CD2	1:D:214:LEU:HD21	2.57	0.40
1:E:137:PRO:HG3	1:E:192:ARG:NH2	2.37	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	254/259 (98%)	233 (92%)	18 (7%)	3 (1%)	13	14
1	B	229/259 (88%)	217 (95%)	11 (5%)	1 (0%)	34	42
1	C	229/259 (88%)	221 (96%)	8 (4%)	0	100	100
1	D	227/259 (88%)	214 (94%)	11 (5%)	2 (1%)	17	20
1	E	253/259 (98%)	234 (92%)	16 (6%)	3 (1%)	13	14
All	All	1192/1295 (92%)	1119 (94%)	64 (5%)	9 (1%)	19	23

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1	ARG
1	E	6	GLY
1	A	4	PHE
1	D	6	GLY
1	E	3	ALA
1	A	70	VAL
1	D	70	VAL
1	B	70	VAL
1	E	70	VAL

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	215/213 (101%)	207 (96%)	8 (4%)	34	48
1	B	194/213 (91%)	189 (97%)	5 (3%)	46	63
1	C	196/213 (92%)	188 (96%)	8 (4%)	30	43
1	D	193/213 (91%)	189 (98%)	4 (2%)	53	70
1	E	214/213 (100%)	206 (96%)	8 (4%)	34	48
All	All	1012/1065 (95%)	979 (97%)	33 (3%)	38	53

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-4	ARG
1	A	1	ARG
1	A	27	THR
1	A	57	ASN
1	A	170	PRO
1	A	175	ASP
1	A	176	ASP
1	A	249	SER
1	B	24	THR
1	B	26	GLU
1	B	27	THR
1	B	28	VAL
1	B	57	ASN
1	C	10	LEU
1	C	27	THR
1	C	50	PRO
1	C	57	ASN
1	C	180	ILE
1	C	183	LYS
1	C	184	LYS
1	C	217	PRO
1	D	27	THR
1	D	57	ASN
1	D	180	ILE
1	D	183	LYS
1	E	10	LEU
1	E	24	THR
1	E	27	THR
1	E	57	ASN
1	E	178	LYS
1	E	179	ASN
1	E	182	THR
1	E	217	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	ASN
1	A	110	HIS
1	A	139	GLN
1	A	156	HIS
1	A	234	GLN
1	A	236	GLN

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Mol	Chain	Res	Type
1	B	57	ASN
1	B	110	HIS
1	B	139	GLN
1	B	156	HIS
1	B	234	GLN
1	B	236	GLN
1	C	57	ASN
1	C	110	HIS
1	C	156	HIS
1	C	234	GLN
1	C	236	GLN
1	D	25	ASN
1	D	57	ASN
1	D	110	HIS
1	D	139	GLN
1	D	156	HIS
1	D	234	GLN
1	D	236	GLN
1	E	57	ASN
1	E	110	HIS
1	E	156	HIS
1	E	234	GLN
1	E	236	GLN

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 5 ligands modelled in this entry, 5 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	251/259 (96%)	0.57	26 (10%) 6 9	32, 47, 60, 65	0
1	B	228/259 (88%)	0.63	20 (8%) 10 13	31, 44, 62, 68	0
1	C	228/259 (88%)	0.45	17 (7%) 14 19	37, 47, 58, 65	0
1	D	226/259 (87%)	0.78	28 (12%) 4 5	34, 52, 63, 69	0
1	E	250/259 (96%)	0.87	41 (16%) 1 2	41, 55, 62, 66	0
All	All	1183/1295 (91%)	0.66	132 (11%) 5 7	31, 49, 62, 69	0

All (132) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	23	GLY	7.5
1	D	27	THR	7.1
1	E	248	ALA	7.1
1	B	24	THR	7.0
1	D	25	ASN	6.3
1	D	180	ILE	6.3
1	A	2	GLY	6.3
1	A	23	GLY	6.1
1	E	23	GLY	5.9
1	B	167	ILE	5.9
1	B	21	VAL	5.9
1	D	19	SER	5.9
1	A	3	ALA	5.7
1	D	18	GLU	5.5
1	D	24	THR	5.4
1	A	4	PHE	5.3
1	C	90	ASP	5.2
1	D	23	GLY	5.1
1	D	182	THR	4.8
1	B	26	GLU	4.8

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Mol	Chain	Res	Type	RSRZ
1	D	181	ASP	4.8
1	B	18	GLU	4.6
1	B	22	PRO	4.6
1	D	22	PRO	4.6
1	E	21	VAL	4.5
1	A	22	PRO	4.5
1	D	5	GLY	4.5
1	B	250	ASP	4.2
1	E	249	SER	4.1
1	A	172	LYS	4.0
1	E	22	PRO	3.9
1	E	174	PHE	3.9
1	E	104	GLU	3.8
1	B	25	ASN	3.8
1	E	247	ALA	3.8
1	A	20	THR	3.7
1	A	248	ALA	3.7
1	D	30	THR	3.6
1	D	16	LEU	3.6
1	E	-4	ARG	3.6
1	B	27	THR	3.6
1	E	90	ASP	3.5
1	D	26	GLU	3.5
1	A	1	ARG	3.5
1	A	90	ASP	3.4
1	E	175	ASP	3.4
1	E	178	LYS	3.3
1	E	25	ASN	3.3
1	A	136	LYS	3.2
1	A	170	PRO	3.2
1	D	184	LYS	3.2
1	E	172	LYS	3.1
1	D	249	SER	3.1
1	C	179	ASN	3.1
1	E	-3	TRP	3.1
1	E	24	THR	3.0
1	D	14	PHE	3.0
1	E	122	SER	2.9
1	B	19	SER	2.9
1	E	242	GLU	2.9
1	C	180	ILE	2.9
1	A	249	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	168	PRO	2.9
1	B	28	VAL	2.8
1	D	248	ALA	2.8
1	C	249	SER	2.8
1	E	17	SER	2.8
1	C	210	SER	2.8
1	E	177	LEU	2.8
1	C	211	VAL	2.7
1	A	250	ASP	2.7
1	E	48	GLN	2.7
1	D	21	VAL	2.7
1	E	246	LYS	2.7
1	C	63	LEU	2.7
1	D	185	LEU	2.6
1	E	136	LYS	2.6
1	E	179	ASN	2.6
1	E	26	GLU	2.6
1	D	246	LYS	2.6
1	D	195	PHE	2.5
1	E	47	GLY	2.5
1	E	173	SER	2.5
1	A	71	ILE	2.5
1	A	21	VAL	2.5
1	D	207	PHE	2.5
1	D	20	THR	2.5
1	A	67	ILE	2.5
1	A	127	ASP	2.5
1	E	231	GLU	2.4
1	C	40	TYR	2.4
1	B	16	LEU	2.4
1	E	181	ASP	2.4
1	E	209	ALA	2.4
1	A	65	VAL	2.4
1	E	170	PRO	2.4
1	B	20	THR	2.4
1	D	193	ILE	2.4
1	E	127	ASP	2.4
1	E	218	GLY	2.4
1	E	134	LYS	2.4
1	E	40	TYR	2.3
1	E	171	PRO	2.3
1	A	-1	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	209	ALA	2.3
1	A	173	SER	2.3
1	E	138	VAL	2.3
1	D	122	SER	2.3
1	B	191	TYR	2.3
1	E	-1	ARG	2.3
1	C	207	PHE	2.3
1	E	124	ILE	2.3
1	A	179	ASN	2.2
1	C	38	ILE	2.2
1	A	211	VAL	2.2
1	C	103	PRO	2.2
1	A	76	VAL	2.2
1	C	47	GLY	2.2
1	C	193	ILE	2.2
1	C	208	VAL	2.2
1	E	180	ILE	2.2
1	B	249	SER	2.2
1	C	248	ALA	2.2
1	C	104	GLU	2.1
1	D	116	ILE	2.1
1	B	139	GLN	2.1
1	B	17	SER	2.1
1	A	183	LYS	2.1
1	D	29	LYS	2.1
1	B	48	GLN	2.0
1	A	25	ASN	2.0
1	E	-2	ILE	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. 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	B-factors(Å^2)	Q<0.9
2	CA	C	1250	1/1	0.98	0.25	45,45,45,45	0
2	CA	A	1250	1/1	0.99	0.23	41,41,41,41	0
2	CA	B	1250	1/1	0.99	0.17	42,42,42,42	0
2	CA	D	1250	1/1	0.99	0.24	54,54,54,54	0
2	CA	E	1250	1/1	1.00	0.17	54,54,54,54	0

6.5 Other polymers (i)

There are no such residues in this entry.