Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 04:27 pm BST

PDB ID	:	5VYW
Title	:	Crystal structure of Lactococcus lactis pyruvate carboxylase
Authors	:	Choi, P.H.; Tong, L.
Deposited on	:	2017-05-26
Resolution	:	3.10 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:

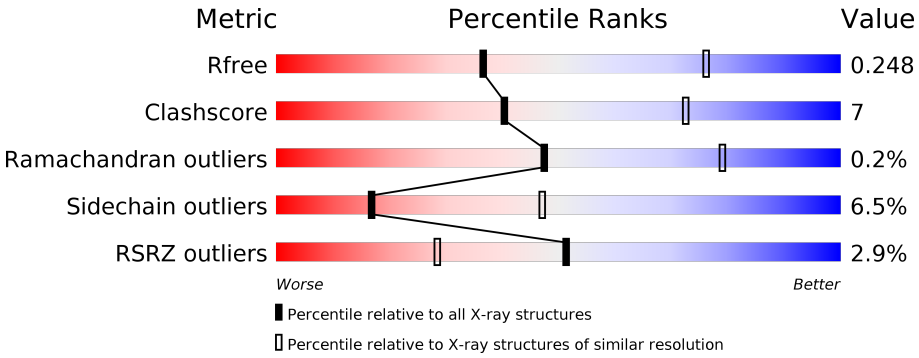
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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	1143	69% 16% • 14%
1	B	1143	4% 69% 15% • 14%
1	C	1143	5% 69% 15% • 14%
1	D	1143	% 72% 17% • 8%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 31425 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 Pyruvate carboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	981	Total	C	N	O	S	0	0	0
			7743	4918	1334	1463	28			
1	B	979	Total	C	N	O	S	0	0	0
			7729	4907	1335	1459	28			
1	C	978	Total	C	N	O	S	0	0	0
			7731	4908	1337	1458	28			
1	D	1046	Total	C	N	O	S	0	0	0
			8202	5206	1413	1552	31			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	VAL	-	expression tag	UNP A0A089XIW4
A	-4	PRO	-	expression tag	UNP A0A089XIW4
A	-3	ARG	-	expression tag	UNP A0A089XIW4
A	-2	GLY	-	expression tag	UNP A0A089XIW4
A	-1	SER	-	expression tag	UNP A0A089XIW4
A	0	HIS	-	expression tag	UNP A0A089XIW4
A	1055	ALA	THR	conflict	UNP A0A089XIW4
B	-5	VAL	-	expression tag	UNP A0A089XIW4
B	-4	PRO	-	expression tag	UNP A0A089XIW4
B	-3	ARG	-	expression tag	UNP A0A089XIW4
B	-2	GLY	-	expression tag	UNP A0A089XIW4
B	-1	SER	-	expression tag	UNP A0A089XIW4
B	0	HIS	-	expression tag	UNP A0A089XIW4
B	1055	ALA	THR	conflict	UNP A0A089XIW4
C	-5	VAL	-	expression tag	UNP A0A089XIW4
C	-4	PRO	-	expression tag	UNP A0A089XIW4
C	-3	ARG	-	expression tag	UNP A0A089XIW4
C	-2	GLY	-	expression tag	UNP A0A089XIW4
C	-1	SER	-	expression tag	UNP A0A089XIW4
C	0	HIS	-	expression tag	UNP A0A089XIW4
C	1055	ALA	THR	conflict	UNP A0A089XIW4

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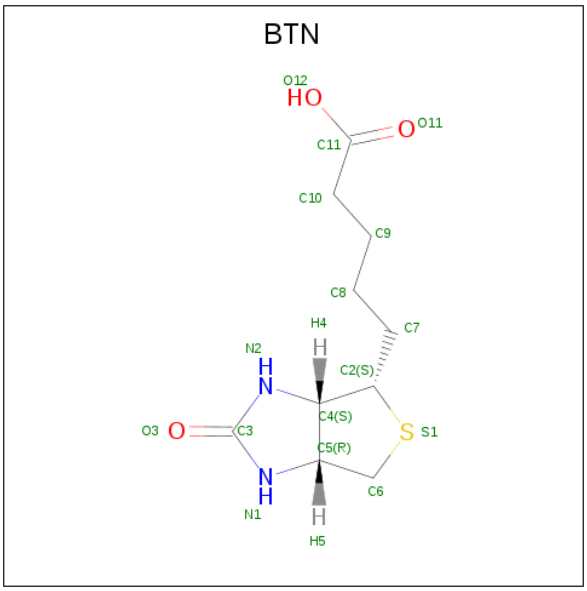
Chain	Residue	Modelled	Actual	Comment	Reference
D	-5	VAL	-	expression tag	UNP A0A089XIW4
D	-4	PRO	-	expression tag	UNP A0A089XIW4
D	-3	ARG	-	expression tag	UNP A0A089XIW4
D	-2	GLY	-	expression tag	UNP A0A089XIW4
D	-1	SER	-	expression tag	UNP A0A089XIW4
D	0	HIS	-	expression tag	UNP A0A089XIW4
D	1055	ALA	THR	conflict	UNP A0A089XIW4

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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

- Molecule 3 is BIOTIN (three-letter code: BTN) (formula: $C_{10}H_{16}N_2O_3S$).



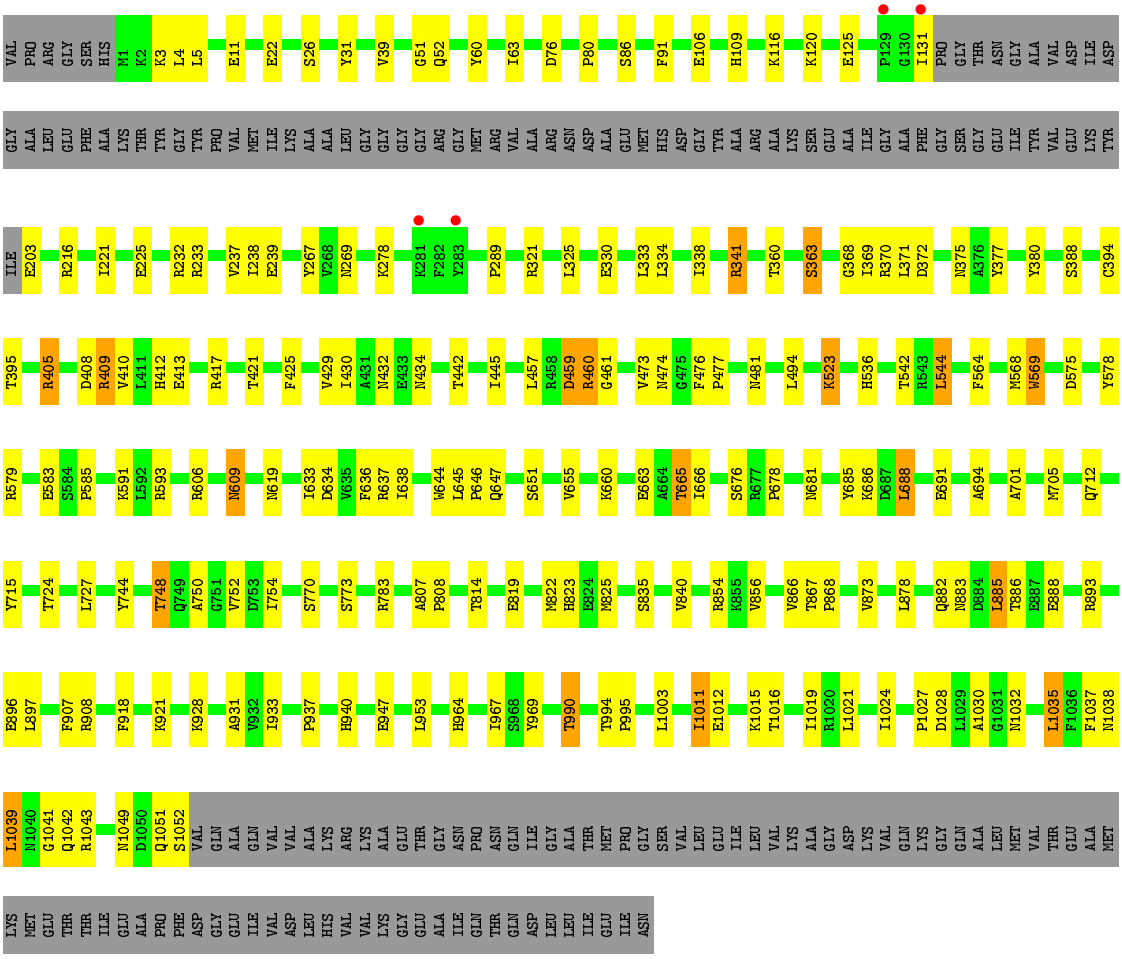
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O S 16 10 2 3 1	0	0

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 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.

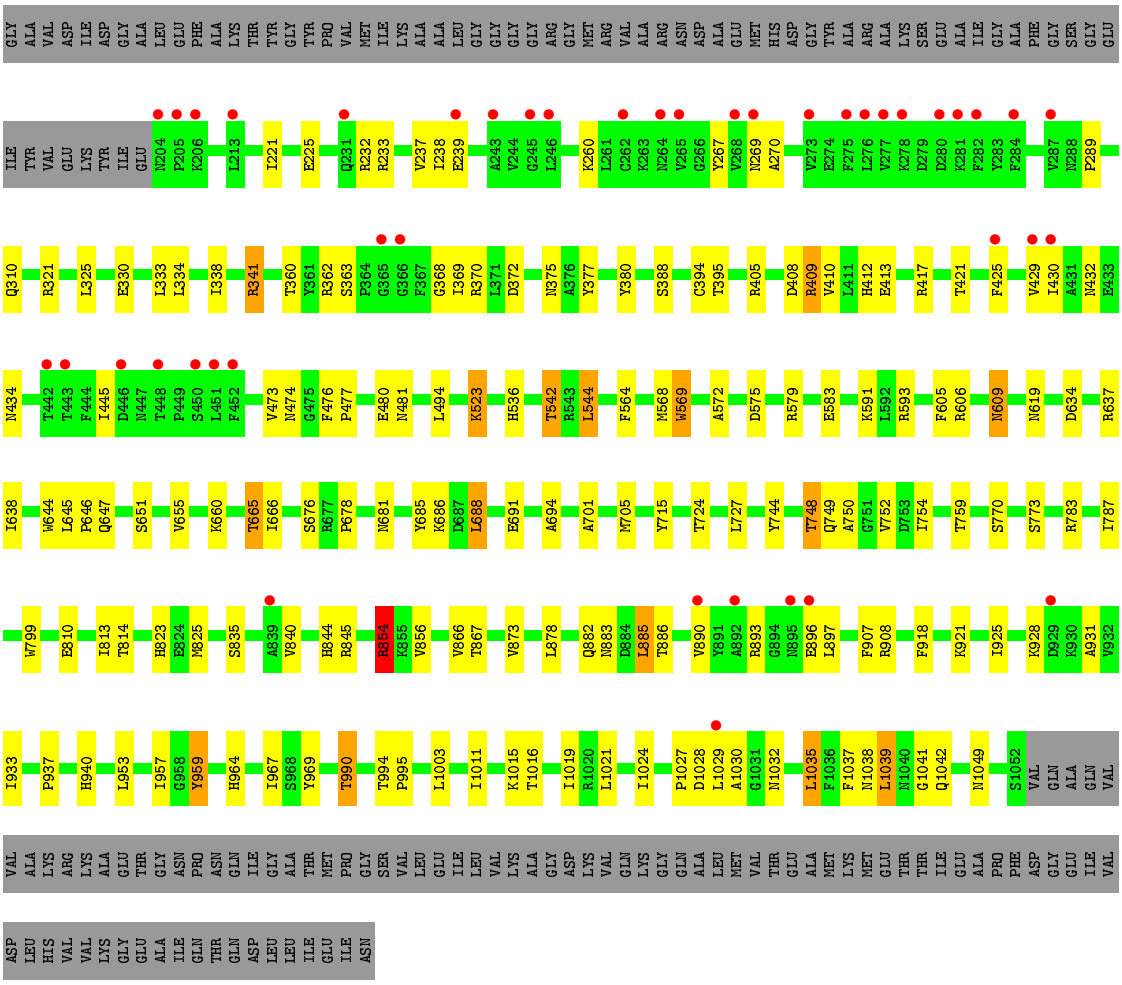
- Molecule 1: Pyruvate carboxylase

Chain A:



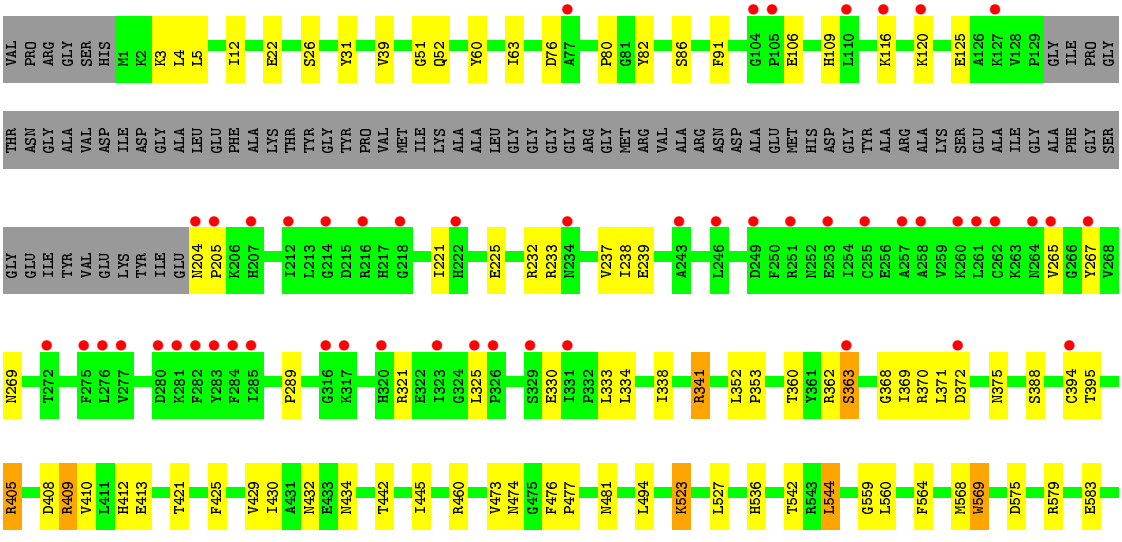
- Molecule 1: Pyruvate carboxylase

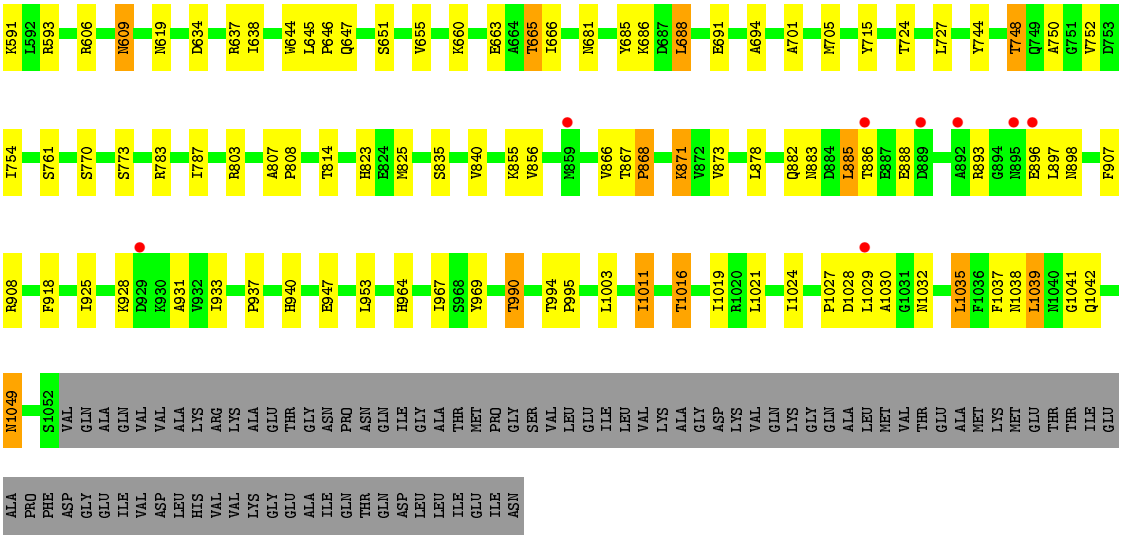
Chain B:



• Molecule 1: Pyruvate carboxylase

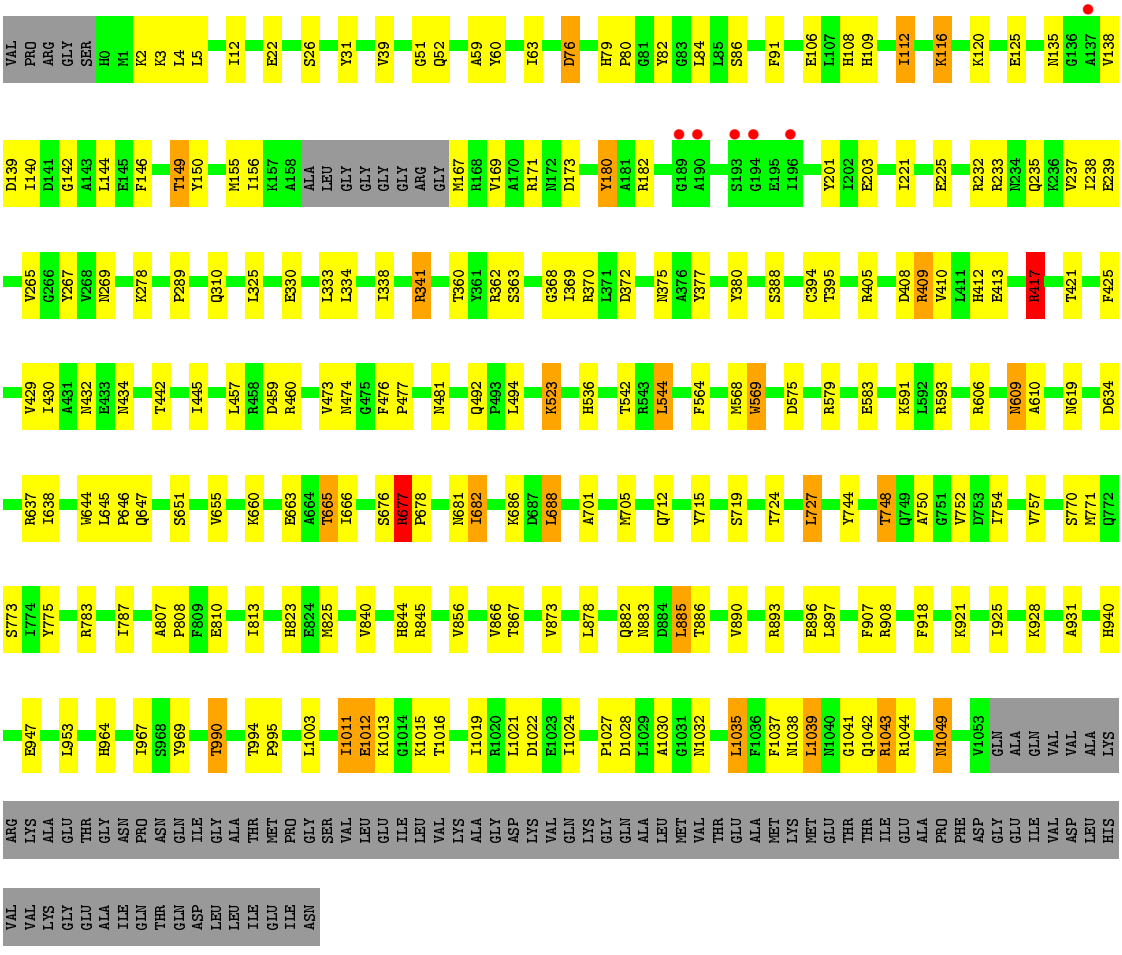
Chain C:





• Molecule 1: Pyruvate carboxylase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 1 2	Depositor
Cell constants a, b, c, α, β, γ	139.66Å 139.66Å 610.49Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.75 – 3.10 49.70 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.75-3.10) 99.7 (49.70-3.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.03 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.200 , 0.248 0.203 , 0.248	Depositor DCC
R_{free} test set	6206 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	77.3	Xtriage
Anisotropy	0.024	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 46.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.049 for -h,-k,l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	31425	wwPDB-VP
Average B, all atoms (Å^2)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.41% 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: MN, BTN

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	0/7899	0.82	5/10693 (0.0%)
1	B	0.65	0/7885	0.79	3/10673 (0.0%)
1	C	0.64	0/7887	0.79	1/10675 (0.0%)
1	D	0.69	0/8367	0.83	7/11329 (0.1%)
All	All	0.66	0/32038	0.81	16/43370 (0.0%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	677	ARG	NE-CZ-NH2	11.19	125.90	120.30
1	B	854	ARG	NE-CZ-NH2	6.94	123.77	120.30
1	A	1043	ARG	NE-CZ-NH2	-6.93	116.83	120.30
1	B	405	ARG	NE-CZ-NH2	6.49	123.55	120.30
1	D	417	ARG	NE-CZ-NH2	6.17	123.38	120.30
1	A	459	ASP	CB-CG-OD2	5.92	123.63	118.30
1	A	1043	ARG	NE-CZ-NH1	5.83	123.22	120.30
1	A	321	ARG	NE-CZ-NH1	5.65	123.12	120.30
1	D	677	ARG	NE-CZ-NH1	-5.46	117.57	120.30
1	B	321	ARG	NE-CZ-NH1	5.45	123.03	120.30
1	C	405	ARG	NE-CZ-NH2	5.42	123.01	120.30
1	A	405	ARG	NE-CZ-NH2	5.38	122.99	120.30
1	D	459	ASP	CB-CG-OD1	5.27	123.05	118.30
1	D	677	ARG	CG-CD-NE	5.12	122.54	111.80
1	D	459	ASP	CB-CG-OD2	-5.09	113.72	118.30
1	D	727	LEU	CA-CB-CG	5.07	126.95	115.30

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	7743	0	7699	110	0
1	B	7729	0	7684	112	0
1	C	7731	0	7692	106	0
1	D	8202	0	8122	134	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	16	0	15	0	0
All	All	31425	0	31212	448	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 7.

All (448) 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:116:LYS:O	1:A:120:LYS:HG2	1.62	0.98
1:A:819:GLU:HG2	1:A:822:MET:HE3	1.51	0.90
1:D:682:ILE:H	1:D:682:ILE:HD12	1.38	0.86
1:C:523:LYS:HA	1:C:523:LYS:HE3	1.57	0.86
1:A:523:LYS:HA	1:A:523:LYS:HE3	1.60	0.83
1:B:523:LYS:HA	1:B:523:LYS:HE3	1.59	0.82
1:D:140:ILE:O	1:D:144:LEU:HD12	1.79	0.82
1:D:523:LYS:HA	1:D:523:LYS:HE3	1.61	0.82
1:B:883:ASN:HB2	1:B:885:LEU:HD21	1.64	0.80
1:B:22:GLU:O	1:C:405:ARG:HD3	1.83	0.78
1:A:883:ASN:HB2	1:A:885:LEU:HD21	1.65	0.78
1:C:883:ASN:HB2	1:C:885:LEU:HD21	1.66	0.78
1:D:883:ASN:HB2	1:D:885:LEU:HD21	1.65	0.77
1:A:239:GLU:OE2	1:A:341:ARG:NH2	2.20	0.75
1:D:744:TYR:O	1:D:748:THR:HG23	1.88	0.73
1:B:744:TYR:O	1:B:748:THR:HG23	1.89	0.73
1:C:239:GLU:OE2	1:C:341:ARG:NH2	2.22	0.73
1:D:665:THR:HB	1:D:701:ALA:HB3	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:239:GLU:OE2	1:D:341:ARG:NH2	2.23	0.72
1:A:744:TYR:O	1:A:748:THR:HG23	1.90	0.71
1:B:823:HIS:HD2	1:B:825:MET:H	1.37	0.71
1:A:116:LYS:O	1:A:120:LYS:CG	2.38	0.71
1:B:665:THR:HB	1:B:701:ALA:HB3	1.71	0.71
1:D:712:GLN:HA	1:D:712:GLN:NE2	2.05	0.71
1:B:239:GLU:OE2	1:B:341:ARG:NH2	2.22	0.71
1:C:744:TYR:O	1:C:748:THR:HG23	1.92	0.70
1:C:823:HIS:HD2	1:C:825:MET:H	1.36	0.70
1:B:686:LYS:HD2	1:B:724:THR:OG1	1.93	0.69
1:A:665:THR:HB	1:A:701:ALA:HB3	1.74	0.69
1:A:819:GLU:HG2	1:A:822:MET:CE	2.23	0.69
1:D:823:HIS:HD2	1:D:825:MET:H	1.40	0.69
1:A:405:ARG:HD3	1:D:22:GLU:O	1.93	0.69
1:D:686:LYS:HD2	1:D:724:THR:OG1	1.93	0.69
1:A:686:LYS:HD2	1:A:724:THR:OG1	1.92	0.68
1:C:686:LYS:HD2	1:C:724:THR:OG1	1.92	0.68
1:B:409:ARG:NH1	1:B:413:GLU:OE1	2.28	0.67
1:A:409:ARG:NH1	1:A:413:GLU:OE1	2.27	0.67
1:D:682:ILE:CD1	1:D:682:ILE:H	2.05	0.67
1:C:665:THR:HB	1:C:701:ALA:HB3	1.75	0.66
1:D:409:ARG:NH1	1:D:413:GLU:OE1	2.27	0.66
1:D:897:LEU:O	1:D:928:LYS:NZ	2.28	0.66
1:C:460:ARG:HD2	1:C:1011:ILE:HG21	1.78	0.66
1:A:823:HIS:HD2	1:A:825:MET:H	1.42	0.66
1:B:957:ILE:HD12	1:B:959:TYR:CE2	2.31	0.66
1:B:897:LEU:O	1:B:928:LYS:NZ	2.29	0.65
1:A:203:GLU:O	1:A:278:LYS:NZ	2.24	0.64
1:C:897:LEU:O	1:C:928:LYS:NZ	2.30	0.64
1:A:897:LEU:O	1:A:928:LYS:NZ	2.31	0.63
1:C:583:GLU:OE2	1:C:990:THR:HG23	1.97	0.63
1:B:583:GLU:OE2	1:B:990:THR:HG23	1.99	0.63
1:C:409:ARG:NH1	1:C:413:GLU:OE1	2.31	0.63
1:B:883:ASN:HB2	1:B:885:LEU:CD2	2.28	0.62
1:D:682:ILE:N	1:D:682:ILE:HD12	2.10	0.62
1:A:840:VAL:HG11	1:A:882:GLN:NE2	2.15	0.62
1:B:744:TYR:O	1:B:748:THR:CG2	2.47	0.62
1:C:883:ASN:HB2	1:C:885:LEU:CD2	2.29	0.62
1:D:744:TYR:O	1:D:748:THR:CG2	2.47	0.61
1:C:369:ILE:HD12	1:C:410:VAL:HG21	1.82	0.61
1:D:360:THR:HG21	1:D:417:ARG:NH2	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1027:PRO:HA	1:B:1032:ASN:O	2.01	0.61
1:D:840:VAL:HG11	1:D:882:GLN:NE2	2.16	0.61
1:A:744:TYR:O	1:A:748:THR:CG2	2.49	0.61
1:D:203:GLU:O	1:D:278:LYS:NZ	2.28	0.61
1:D:460:ARG:HD2	1:D:1011:ILE:HG21	1.81	0.61
1:D:883:ASN:HB2	1:D:885:LEU:CD2	2.30	0.61
1:C:523:LYS:HE3	1:C:523:LYS:CA	2.30	0.61
1:A:883:ASN:HB2	1:A:885:LEU:CD2	2.30	0.61
1:B:1021:LEU:HD13	1:B:1037:PHE:CE1	2.35	0.60
1:C:1021:LEU:HD13	1:C:1037:PHE:CE1	2.36	0.60
1:C:840:VAL:HG11	1:C:882:GLN:NE2	2.16	0.60
1:C:744:TYR:O	1:C:748:THR:CG2	2.50	0.60
1:A:460:ARG:HD2	1:A:1011:ILE:HG21	1.82	0.60
1:D:1027:PRO:HA	1:D:1032:ASN:O	2.02	0.59
1:A:583:GLU:OE2	1:A:990:THR:HG23	2.01	0.59
1:D:583:GLU:OE2	1:D:990:THR:HG23	2.03	0.59
1:A:408:ASP:O	1:A:412:HIS:HD2	1.85	0.59
1:A:593:ARG:O	1:A:593:ARG:HD3	2.02	0.59
1:A:1021:LEU:HD13	1:A:1037:PHE:CE1	2.36	0.59
1:D:1021:LEU:HD13	1:D:1037:PHE:CE1	2.37	0.59
1:A:523:LYS:CA	1:A:523:LYS:HE3	2.33	0.59
1:A:883:ASN:O	1:A:885:LEU:HD23	2.03	0.58
1:D:146:PHE:O	1:D:149:THR:O	2.20	0.58
1:C:883:ASN:O	1:C:885:LEU:HD23	2.04	0.58
1:C:908:ARG:NH1	1:C:931:ALA:O	2.36	0.58
1:B:883:ASN:O	1:B:885:LEU:HD23	2.02	0.58
1:B:523:LYS:CA	1:B:523:LYS:HE3	2.31	0.58
1:C:593:ARG:HD3	1:C:593:ARG:O	2.03	0.58
1:D:748:THR:HA	1:D:752:VAL:HG12	1.85	0.58
1:A:908:ARG:NH1	1:A:931:ALA:O	2.36	0.57
1:B:221:ILE:HD11	1:B:325:LEU:HD13	1.85	0.57
1:B:908:ARG:NH1	1:B:931:ALA:O	2.38	0.57
1:C:1027:PRO:HA	1:C:1032:ASN:O	2.03	0.57
1:D:473:VAL:HG12	1:D:474:ASN:ND2	2.19	0.57
1:D:523:LYS:CA	1:D:523:LYS:HE3	2.33	0.57
1:B:840:VAL:HG11	1:B:882:GLN:NE2	2.19	0.57
1:D:180:TYR:CD2	1:D:180:TYR:O	2.58	0.57
1:D:369:ILE:HD12	1:D:410:VAL:HG21	1.86	0.57
1:D:840:VAL:HG12	1:D:840:VAL:O	2.05	0.57
1:A:369:ILE:HD12	1:A:410:VAL:HG21	1.85	0.57
1:A:3:LYS:HG3	1:A:26:SER:HB3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:953:LEU:HD13	1:C:969:TYR:CD2	2.40	0.57
1:A:1041:GLY:O	1:D:377:TYR:CE1	2.57	0.57
1:A:638:ILE:O	1:A:665:THR:HG23	2.05	0.57
1:B:369:ILE:HD12	1:B:410:VAL:HG21	1.86	0.57
1:C:638:ILE:O	1:C:665:THR:HG23	2.05	0.57
1:D:883:ASN:O	1:D:885:LEU:HD23	2.04	0.57
1:A:1027:PRO:HA	1:A:1032:ASN:O	2.04	0.56
1:B:473:VAL:HG12	1:B:474:ASN:ND2	2.20	0.56
1:B:854:ARG:HG2	1:B:854:ARG:HH21	1.68	0.56
1:B:840:VAL:HG12	1:B:840:VAL:O	2.05	0.56
1:D:221:ILE:HD11	1:D:325:LEU:HD13	1.85	0.56
1:A:221:ILE:HD11	1:A:325:LEU:HD13	1.86	0.56
1:A:840:VAL:O	1:A:840:VAL:HG12	2.05	0.56
1:B:638:ILE:O	1:B:665:THR:HG23	2.05	0.56
1:D:108:HIS:O	1:D:112:ILE:CG2	2.54	0.56
1:A:473:VAL:HG12	1:A:474:ASN:ND2	2.21	0.56
1:C:221:ILE:HD11	1:C:325:LEU:HD13	1.87	0.56
1:B:593:ARG:HD3	1:B:593:ARG:O	2.05	0.56
1:D:593:ARG:O	1:D:593:ARG:HD3	2.06	0.56
1:C:840:VAL:O	1:C:840:VAL:HG12	2.06	0.55
1:D:155:MET:HE2	1:D:169:VAL:HG22	1.88	0.55
1:C:473:VAL:HG12	1:C:474:ASN:ND2	2.22	0.55
1:B:408:ASP:O	1:B:412:HIS:HD2	1.90	0.55
1:D:1019:ILE:HG12	1:D:1039:LEU:HD12	1.89	0.55
1:D:140:ILE:O	1:D:144:LEU:CD1	2.52	0.55
1:A:1012:GLU:OE1	1:A:1015:LYS:CE	2.54	0.55
1:C:1038:ASN:HD21	1:C:1041:GLY:HA2	1.72	0.55
1:C:748:THR:HA	1:C:752:VAL:HG12	1.89	0.55
1:A:334:LEU:HD22	1:D:334:LEU:HD22	1.89	0.55
1:D:408:ASP:O	1:D:412:HIS:HD2	1.90	0.55
1:A:22:GLU:HG3	1:D:409:ARG:HD3	1.89	0.54
1:D:1022:ASP:OD2	1:D:1043:ARG:NH1	2.40	0.54
1:A:575:ASP:OD2	1:A:579:ARG:NH1	2.41	0.54
1:D:476:PHE:CD1	1:D:477:PRO:HD2	2.43	0.54
1:A:748:THR:HA	1:A:752:VAL:HG12	1.90	0.54
1:A:953:LEU:HD13	1:A:969:TYR:CD2	2.43	0.54
1:D:377:TYR:CE1	1:D:380:TYR:HB2	2.43	0.54
1:A:1019:ILE:HG12	1:A:1039:LEU:HD12	1.90	0.53
1:D:908:ARG:NH1	1:D:931:ALA:O	2.40	0.53
1:D:953:LEU:HD13	1:D:969:TYR:CD2	2.42	0.53
1:B:748:THR:HA	1:B:752:VAL:HG12	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:575:ASP:OD2	1:C:579:ARG:NH1	2.41	0.53
1:D:138:VAL:HG12	1:D:139:ASP:O	2.09	0.53
1:C:116:LYS:O	1:C:120:LYS:HG3	2.09	0.53
1:A:1038:ASN:HD21	1:A:1041:GLY:HA2	1.74	0.53
1:A:377:TYR:CE1	1:A:380:TYR:HB2	2.44	0.53
1:B:575:ASP:OD2	1:B:579:ARG:NH1	2.41	0.53
1:D:1012:GLU:HG3	1:D:1015:LYS:HB2	1.90	0.53
1:D:39:VAL:H	1:D:375:ASN:ND2	2.07	0.53
1:D:568:MET:SD	1:D:569:TRP:HB2	2.49	0.53
1:D:575:ASP:OD2	1:D:579:ARG:NH1	2.42	0.53
1:A:370:ARG:HB3	1:A:394:CYS:HB2	1.92	0.52
1:B:370:ARG:HB3	1:B:394:CYS:HB2	1.91	0.52
1:B:953:LEU:HD13	1:B:969:TYR:CD2	2.44	0.52
1:B:334:LEU:HD22	1:C:334:LEU:HD22	1.91	0.52
1:A:360:THR:HG23	1:A:1042:GLN:NE2	2.24	0.52
1:C:609:ASN:N	1:C:609:ASN:OD1	2.43	0.52
1:D:106:GLU:H	1:D:109:HIS:HD2	1.57	0.52
1:A:666:ILE:HG12	1:A:688:LEU:HD13	1.92	0.52
1:D:116:LYS:O	1:D:120:LYS:HG3	2.10	0.52
1:A:4:LEU:HD23	1:A:5:LEU:N	2.25	0.52
1:C:1019:ILE:HG12	1:C:1039:LEU:HD12	1.91	0.52
1:B:609:ASN:OD1	1:B:609:ASN:N	2.42	0.51
1:C:408:ASP:O	1:C:412:HIS:HD2	1.93	0.51
1:D:568:MET:C	1:D:568:MET:SD	2.88	0.51
1:B:1038:ASN:HD21	1:B:1041:GLY:HA2	1.74	0.51
1:C:360:THR:HG23	1:C:1042:GLN:NE2	2.25	0.51
1:A:106:GLU:H	1:A:109:HIS:HD2	1.57	0.51
1:B:1019:ILE:HG12	1:B:1039:LEU:HD12	1.93	0.51
1:D:108:HIS:O	1:D:112:ILE:HG23	2.10	0.51
1:B:813:ILE:HD11	1:D:810:GLU:HG2	1.91	0.51
1:D:638:ILE:O	1:D:665:THR:HG23	2.11	0.51
1:B:666:ILE:HG12	1:B:688:LEU:HD13	1.91	0.51
1:B:377:TYR:CE1	1:C:1041:GLY:O	2.63	0.51
1:B:409:ARG:HD3	1:C:22:GLU:HG3	1.92	0.51
1:A:609:ASN:N	1:A:609:ASN:OD1	2.44	0.50
1:A:237:VAL:HG12	1:A:238:ILE:HG13	1.93	0.50
1:C:370:ARG:HB3	1:C:394:CYS:HB2	1.93	0.50
1:B:360:THR:HG23	1:B:1042:GLN:NE2	2.26	0.50
1:B:80:PRO:HB2	1:B:86:SER:HA	1.92	0.50
1:D:370:ARG:HB3	1:D:394:CYS:HB2	1.92	0.50
1:D:476:PHE:CG	1:D:477:PRO:HD2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:715:TYR:CD1	1:D:750:ALA:HB2	2.46	0.50
1:A:476:PHE:CD1	1:A:477:PRO:HD2	2.47	0.50
1:C:237:VAL:HG12	1:C:238:ILE:HG13	1.94	0.50
1:D:666:ILE:HG12	1:D:688:LEU:HD13	1.93	0.50
1:D:712:GLN:CA	1:D:712:GLN:NE2	2.70	0.50
1:D:1038:ASN:HD21	1:D:1041:GLY:HA2	1.77	0.50
1:A:203:GLU:HB2	1:A:278:LYS:HE2	1.93	0.50
1:B:377:TYR:CE1	1:B:380:TYR:HB2	2.47	0.50
1:D:1043:ARG:HG3	1:D:1044:ARG:N	2.27	0.50
1:A:1012:GLU:OE1	1:A:1015:LYS:HE2	2.12	0.50
1:D:4:LEU:HD23	1:D:5:LEU:N	2.27	0.50
1:A:432:ASN:HD22	1:A:434:ASN:H	1.60	0.49
1:D:237:VAL:HG12	1:D:238:ILE:HG13	1.94	0.49
1:C:476:PHE:CD1	1:C:477:PRO:HD2	2.47	0.49
1:C:80:PRO:HB2	1:C:86:SER:HA	1.94	0.49
1:D:156:ILE:O	1:D:167:MET:HA	2.12	0.49
1:C:964:HIS:HA	1:C:967:ILE:HG22	1.94	0.49
1:C:666:ILE:HG12	1:C:688:LEU:HD13	1.94	0.49
1:B:4:LEU:HD23	1:B:5:LEU:N	2.27	0.49
1:B:715:TYR:CD1	1:B:750:ALA:HB2	2.47	0.49
1:A:644:TRP:CE2	1:A:646:PRO:HG2	2.47	0.49
1:C:568:MET:C	1:C:568:MET:SD	2.91	0.49
1:C:4:LEU:HD23	1:C:5:LEU:N	2.27	0.49
1:C:994:THR:N	1:C:995:PRO:CD	2.75	0.49
1:A:907:PHE:HA	1:A:918:PHE:CE2	2.48	0.49
1:B:237:VAL:HG12	1:B:238:ILE:HG13	1.94	0.48
1:B:568:MET:C	1:B:568:MET:SD	2.92	0.48
1:C:368:GLY:O	1:C:395:THR:HA	2.14	0.48
1:A:638:ILE:O	1:A:665:THR:CG2	2.62	0.48
1:D:536:HIS:CG	1:D:544:LEU:HB2	2.47	0.48
1:C:106:GLU:H	1:C:109:HIS:HD2	1.62	0.48
1:D:432:ASN:HD22	1:D:434:ASN:H	1.61	0.48
1:D:609:ASN:N	1:D:609:ASN:OD1	2.47	0.48
1:A:432:ASN:ND2	1:A:434:ASN:H	2.10	0.48
1:B:39:VAL:H	1:B:375:ASN:ND2	2.11	0.48
1:D:360:THR:HG23	1:D:1042:GLN:NE2	2.28	0.48
1:B:810:GLU:HG2	1:D:813:ILE:HD11	1.94	0.48
1:C:715:TYR:CD1	1:C:750:ALA:HB2	2.48	0.48
1:B:644:TRP:CE2	1:B:646:PRO:HG2	2.49	0.48
1:B:823:HIS:CD2	1:B:825:MET:H	2.26	0.48
1:A:947:GLU:HA	1:A:947:GLU:OE1	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:432:ASN:ND2	1:D:434:ASN:H	2.11	0.47
1:D:994:THR:N	1:D:995:PRO:CD	2.77	0.47
1:B:368:GLY:O	1:B:395:THR:HA	2.14	0.47
1:B:408:ASP:HA	1:B:430:ILE:HD11	1.96	0.47
1:C:644:TRP:CE2	1:C:646:PRO:HG2	2.49	0.47
1:C:666:ILE:HG21	1:C:685:TYR:HD1	1.79	0.47
1:A:564:PHE:CD2	1:A:754:ILE:HD13	2.50	0.47
1:A:39:VAL:H	1:A:375:ASN:ND2	2.12	0.47
1:A:867:THR:O	1:A:867:THR:HG23	2.15	0.47
1:B:638:ILE:O	1:B:665:THR:CG2	2.61	0.47
1:D:947:GLU:HA	1:D:947:GLU:OE1	2.15	0.47
1:A:474:ASN:ND2	1:A:1051:GLN:HG3	2.30	0.47
1:B:866:VAL:HG22	1:B:867:THR:N	2.30	0.47
1:C:536:HIS:CG	1:C:544:LEU:HB2	2.49	0.47
1:A:953:LEU:HD13	1:A:969:TYR:CG	2.50	0.47
1:B:476:PHE:CD1	1:B:477:PRO:HD2	2.50	0.47
1:C:637:ARG:HG2	1:C:665:THR:HG21	1.97	0.47
1:A:476:PHE:CG	1:A:477:PRO:HD2	2.50	0.47
1:C:267:TYR:OH	1:C:289:PRO:HA	2.14	0.47
1:D:362:ARG:NH1	1:D:1042:GLN:HG3	2.30	0.47
1:B:106:GLU:H	1:B:109:HIS:HD2	1.62	0.47
1:C:638:ILE:O	1:C:665:THR:CG2	2.63	0.47
1:D:80:PRO:HB2	1:D:86:SER:HA	1.96	0.47
1:D:31:TYR:HA	1:D:60:TYR:OH	2.15	0.47
1:D:644:TRP:CE2	1:D:646:PRO:HG2	2.51	0.47
1:B:907:PHE:HA	1:B:918:PHE:CE2	2.50	0.46
1:A:1028:ASP:OD2	1:A:1030:ALA:N	2.48	0.46
1:B:1028:ASP:OD2	1:B:1030:ALA:N	2.48	0.46
1:D:634:ASP:HA	1:D:660:LYS:HD2	1.96	0.46
1:D:953:LEU:HD13	1:D:969:TYR:CG	2.51	0.46
1:C:408:ASP:HA	1:C:430:ILE:HD11	1.97	0.46
1:C:568:MET:SD	1:C:569:TRP:HB2	2.56	0.46
1:B:536:HIS:CG	1:B:544:LEU:HB2	2.50	0.46
1:B:645:LEU:N	1:B:646:PRO:CD	2.79	0.46
1:D:1028:ASP:OD2	1:D:1030:ALA:N	2.47	0.46
1:D:3:LYS:HG3	1:D:26:SER:HB3	1.97	0.46
1:D:676:SER:C	1:D:678:PRO:HD3	2.36	0.46
1:A:368:GLY:O	1:A:395:THR:HA	2.15	0.46
1:A:715:TYR:CD1	1:A:750:ALA:HB2	2.50	0.46
1:B:637:ARG:HG2	1:B:665:THR:HG21	1.97	0.46
1:B:953:LEU:HD13	1:B:969:TYR:CG	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:408:ASP:HA	1:A:430:ILE:HD11	1.98	0.46
1:B:3:LYS:HG3	1:B:26:SER:HB3	1.97	0.46
1:D:180:TYR:C	1:D:180:TYR:CD2	2.90	0.46
1:A:994:THR:N	1:A:995:PRO:CD	2.78	0.46
1:C:953:LEU:HD13	1:C:969:TYR:CG	2.49	0.46
1:D:4:LEU:HD23	1:D:4:LEU:C	2.37	0.46
1:A:637:ARG:HG2	1:A:665:THR:HG21	1.98	0.46
1:B:883:ASN:C	1:B:885:LEU:HD23	2.37	0.46
1:C:947:GLU:OE1	1:C:947:GLU:HA	2.16	0.46
1:D:149:THR:O	1:D:150:TYR:HB2	2.15	0.46
1:B:267:TYR:OH	1:B:289:PRO:HA	2.16	0.45
1:B:41:ARG:HH11	1:C:1016:THR:HG23	1.81	0.45
1:B:63:ILE:HG23	1:B:91:PHE:HD1	1.81	0.45
1:C:362:ARG:NH1	1:C:1042:GLN:HG3	2.31	0.45
1:C:476:PHE:CG	1:C:477:PRO:HD2	2.51	0.45
1:C:651:SER:O	1:C:655:VAL:HG23	2.17	0.45
1:C:907:PHE:HA	1:C:918:PHE:CE2	2.52	0.45
1:D:775:TYR:C	1:D:775:TYR:CD1	2.90	0.45
1:A:4:LEU:HD23	1:A:4:LEU:C	2.37	0.45
1:A:80:PRO:HB2	1:A:86:SER:HA	1.97	0.45
1:C:868:PRO:HA	1:C:871:LYS:HE3	1.98	0.45
1:D:1024:ILE:HG23	1:D:1035:LEU:HD22	1.99	0.45
1:A:408:ASP:O	1:A:412:HIS:CD2	2.69	0.45
1:C:3:LYS:HG3	1:C:26:SER:HB3	1.99	0.45
1:D:225:GLU:OE1	1:D:225:GLU:N	2.49	0.45
1:D:866:VAL:HG22	1:D:867:THR:N	2.31	0.45
1:A:568:MET:SD	1:A:568:MET:C	2.95	0.45
1:A:633:ILE:HG22	1:A:636:PHE:CE1	2.52	0.45
1:A:63:ILE:HG23	1:A:91:PHE:HD1	1.82	0.45
1:C:425:PHE:O	1:C:429:VAL:HG23	2.17	0.45
1:C:523:LYS:HD2	1:C:523:LYS:N	2.32	0.45
1:C:51:GLY:O	1:C:52:GLN:C	2.56	0.45
1:C:867:THR:O	1:C:867:THR:HG23	2.16	0.45
1:A:536:HIS:CG	1:A:544:LEU:HB2	2.52	0.44
1:B:116:LYS:O	1:B:120:LYS:HG3	2.17	0.44
1:B:634:ASP:HA	1:B:660:LYS:HD2	1.98	0.44
1:B:31:TYR:HA	1:B:60:TYR:OH	2.17	0.44
1:C:63:ILE:HG23	1:C:91:PHE:HD1	1.82	0.44
1:C:564:PHE:CD2	1:C:754:ILE:HD13	2.53	0.44
1:D:425:PHE:O	1:D:429:VAL:HG23	2.18	0.44
1:D:867:THR:HG23	1:D:867:THR:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:907:PHE:HA	1:D:918:PHE:CE2	2.52	0.44
1:A:459:ASP:O	1:A:461:GLY:N	2.51	0.44
1:B:676:SER:C	1:B:678:PRO:HD3	2.38	0.44
1:B:770:SER:HB3	1:B:773:SER:HB2	1.99	0.44
1:B:964:HIS:HA	1:B:967:ILE:HG22	1.98	0.44
1:A:964:HIS:HA	1:A:967:ILE:HG22	1.98	0.44
1:B:867:THR:HG23	1:B:867:THR:O	2.17	0.44
1:C:645:LEU:N	1:C:646:PRO:CD	2.80	0.44
1:A:425:PHE:O	1:A:429:VAL:HG23	2.17	0.44
1:C:39:VAL:H	1:C:375:ASN:ND2	2.16	0.44
1:B:568:MET:SD	1:B:569:TRP:HB2	2.58	0.44
1:C:856:VAL:CG1	1:C:873:VAL:HG13	2.47	0.44
1:D:1049:ASN:C	1:D:1049:ASN:HD22	2.21	0.44
1:D:637:ARG:HG2	1:D:665:THR:HG21	1.99	0.44
1:A:666:ILE:HG21	1:A:685:TYR:HD1	1.83	0.44
1:D:63:ILE:HG23	1:D:91:PHE:HD1	1.82	0.44
1:C:1024:ILE:HG23	1:C:1035:LEU:HD22	2.00	0.44
1:D:564:PHE:CD2	1:D:754:ILE:HD13	2.52	0.44
1:A:568:MET:SD	1:A:569:TRP:HB2	2.57	0.44
1:D:638:ILE:O	1:D:665:THR:CG2	2.66	0.44
1:A:267:TYR:OH	1:A:289:PRO:HA	2.18	0.43
1:A:409:ARG:HD3	1:D:22:GLU:HG3	2.00	0.43
1:A:634:ASP:HA	1:A:660:LYS:HD2	1.99	0.43
1:A:645:LEU:N	1:A:646:PRO:CD	2.81	0.43
1:D:149:THR:O	1:D:150:TYR:CB	2.66	0.43
1:A:360:THR:HG21	1:A:417:ARG:NH1	2.33	0.43
1:B:476:PHE:CG	1:B:477:PRO:HD2	2.52	0.43
1:C:761:SER:O	1:C:803:ARG:NH1	2.48	0.43
1:D:408:ASP:HA	1:D:430:ILE:HD11	1.99	0.43
1:B:959:TYR:N	1:B:959:TYR:CD2	2.86	0.43
1:B:1015:LYS:HA	1:B:1015:LYS:HD2	1.76	0.43
1:D:807:ALA:HB3	1:D:808:PRO:HD3	2.00	0.43
1:B:564:PHE:CD2	1:B:754:ILE:HD13	2.53	0.43
1:B:651:SER:O	1:B:655:VAL:HG23	2.19	0.43
1:C:432:ASN:ND2	1:C:434:ASN:H	2.16	0.43
1:C:634:ASP:HA	1:C:660:LYS:HD2	2.00	0.43
1:A:22:GLU:O	1:D:405:ARG:HD2	2.19	0.43
1:B:759:THR:HG21	1:B:799:TRP:CD1	2.54	0.43
1:B:225:GLU:OE1	1:B:225:GLU:N	2.52	0.43
1:B:823:HIS:CD2	1:B:825:MET:HB2	2.54	0.43
1:C:204:ASN:N	1:C:205:PRO:HD3	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:232:ARG:HB2	1:D:445:ILE:HG21	2.01	0.43
1:A:770:SER:HB3	1:A:773:SER:HB2	1.99	0.43
1:B:432:ASN:ND2	1:B:434:ASN:H	2.17	0.43
1:C:866:VAL:HG22	1:C:867:THR:N	2.33	0.43
1:D:338:ILE:O	1:D:394:CYS:HA	2.19	0.43
1:D:109:HIS:HE1	1:D:265:VAL:O	2.02	0.43
1:D:368:GLY:O	1:D:395:THR:HA	2.19	0.43
1:A:225:GLU:N	1:A:225:GLU:OE1	2.52	0.42
1:B:360:THR:HG21	1:B:417:ARG:NH1	2.34	0.42
1:B:51:GLY:O	1:B:52:GLN:C	2.57	0.42
1:C:338:ILE:O	1:C:394:CYS:HA	2.18	0.42
1:B:856:VAL:CG1	1:B:873:VAL:HG13	2.49	0.42
1:B:994:THR:N	1:B:995:PRO:CD	2.82	0.42
1:A:338:ILE:O	1:A:394:CYS:HA	2.19	0.42
1:A:676:SER:C	1:A:678:PRO:HD3	2.39	0.42
1:D:203:GLU:HB2	1:D:278:LYS:HE2	2.01	0.42
1:D:79:HIS:NE2	1:D:310:GLN:OE1	2.43	0.42
1:D:201:TYR:CE2	1:D:203:GLU:HG2	2.54	0.42
1:A:637:ARG:HA	1:A:663:GLU:HB2	2.02	0.42
1:B:360:THR:HG23	1:B:1042:GLN:HE22	1.84	0.42
1:C:1028:ASP:OD2	1:C:1030:ALA:N	2.51	0.42
1:D:144:LEU:HD23	1:D:173:ASP:OD2	2.19	0.42
1:D:964:HIS:HA	1:D:967:ILE:HG22	2.00	0.42
1:B:425:PHE:O	1:B:429:VAL:HG23	2.19	0.42
1:B:542:THR:HG21	1:B:572:ALA:HB3	2.01	0.42
1:D:138:VAL:CG1	1:D:142:GLY:HA3	2.49	0.42
1:D:51:GLY:O	1:D:52:GLN:C	2.57	0.42
1:B:1024:ILE:HG23	1:B:1035:LEU:HD22	2.02	0.42
1:D:108:HIS:O	1:D:112:ILE:HG22	2.19	0.42
1:A:578:TYR:CZ	1:A:585:PRO:HD2	2.54	0.42
1:B:691:GLU:O	1:B:694:ALA:HB3	2.20	0.42
1:D:267:TYR:OH	1:D:289:PRO:HA	2.20	0.42
1:A:856:VAL:CG1	1:A:873:VAL:HG13	2.49	0.42
1:B:117:ILE:H	1:B:117:ILE:HD12	1.84	0.42
1:D:856:VAL:CG1	1:D:873:VAL:HG13	2.49	0.42
1:A:823:HIS:CD2	1:A:825:MET:HB2	2.55	0.42
1:B:338:ILE:O	1:B:394:CYS:HA	2.19	0.42
1:B:666:ILE:HG21	1:B:685:TYR:HD1	1.85	0.42
1:C:691:GLU:O	1:C:694:ALA:HB3	2.20	0.42
1:D:51:GLY:HA3	1:D:59:ALA:CB	2.50	0.42
1:A:651:SER:O	1:A:655:VAL:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:883:ASN:C	1:A:885:LEU:HD23	2.40	0.41
1:B:4:LEU:HD23	1:B:4:LEU:C	2.41	0.41
1:D:787:ILE:HA	1:D:787:ILE:HD12	1.90	0.41
1:A:31:TYR:HA	1:A:60:TYR:OH	2.20	0.41
1:B:885:LEU:HD12	1:B:890:VAL:HG22	2.03	0.41
1:A:363:SER:HB2	1:A:371:LEU:CD1	2.50	0.41
1:A:866:VAL:HG22	1:A:867:THR:N	2.35	0.41
1:C:770:SER:HB3	1:C:773:SER:HB2	2.01	0.41
1:C:823:HIS:CD2	1:C:825:MET:H	2.26	0.41
1:D:171:ARG:HB2	1:D:171:ARG:NH1	2.35	0.41
1:D:651:SER:O	1:D:655:VAL:HG23	2.21	0.41
1:A:51:GLY:O	1:A:52:GLN:C	2.57	0.41
1:C:31:TYR:HA	1:C:60:TYR:OH	2.20	0.41
1:D:677:ARG:HG2	1:D:677:ARG:HH21	1.85	0.41
1:D:12:ILE:HB	1:D:82:TYR:CE2	2.55	0.41
1:C:1049:ASN:C	1:C:1049:ASN:HD22	2.24	0.41
1:D:637:ARG:HA	1:D:663:GLU:HB2	2.03	0.41
1:D:645:LEU:N	1:D:646:PRO:CD	2.83	0.41
1:A:1024:ILE:HG23	1:A:1035:LEU:HD22	2.03	0.41
1:B:232:ARG:HB2	1:B:445:ILE:HG21	2.01	0.41
1:B:270:ALA:HB3	1:B:310:GLN:HE21	1.85	0.41
1:B:408:ASP:O	1:B:412:HIS:CD2	2.73	0.41
1:C:352:LEU:HA	1:C:353:PRO:HD2	1.89	0.41
1:C:232:ARG:HB2	1:C:445:ILE:HG21	2.01	0.41
1:C:4:LEU:HD23	1:C:4:LEU:C	2.40	0.41
1:D:757:VAL:CG2	1:D:771:MET:HB2	2.50	0.41
1:A:232:ARG:HB2	1:A:445:ILE:HG21	2.03	0.41
1:B:362:ARG:NH1	1:B:1042:GLN:HG3	2.35	0.41
1:B:432:ASN:HD22	1:B:434:ASN:H	1.69	0.41
1:C:363:SER:HB2	1:C:371:LEU:CD1	2.51	0.41
1:C:637:ARG:HA	1:C:663:GLU:HB2	2.02	0.41
1:C:12:ILE:HB	1:C:82:TYR:CE2	2.56	0.41
1:D:883:ASN:C	1:D:885:LEU:HD23	2.40	0.41
1:C:868:PRO:O	1:C:871:LYS:HG2	2.21	0.41
1:B:523:LYS:HD2	1:B:523:LYS:N	2.36	0.41
1:D:770:SER:HB3	1:D:773:SER:HB2	2.01	0.41
1:A:691:GLU:O	1:A:694:ALA:HB3	2.21	0.41
1:A:933:ILE:HD11	1:A:937:PRO:HG3	2.03	0.41
1:C:559:GLY:O	1:C:560:LEU:HD23	2.21	0.41
1:D:925:ILE:O	1:D:928:LYS:HE3	2.20	0.41
1:A:523:LYS:HD2	1:A:523:LYS:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:605:PHE:CD1	1:B:605:PHE:C	2.93	0.41
1:D:885:LEU:HD12	1:D:890:VAL:HG22	2.03	0.40
1:B:22:GLU:HG3	1:C:409:ARG:HD3	2.02	0.40
1:C:225:GLU:N	1:C:225:GLU:OE1	2.54	0.40
1:C:883:ASN:C	1:C:885:LEU:HD23	2.42	0.40
1:C:933:ILE:HD11	1:C:937:PRO:HG3	2.03	0.40
1:D:844:HIS:ND1	1:D:845:ARG:HG3	2.36	0.40
1:B:844:HIS:ND1	1:B:845:ARG:HG3	2.36	0.40
1:C:109:HIS:HE1	1:C:265:VAL:O	2.05	0.40
1:C:807:ALA:HB3	1:C:808:PRO:HD3	2.03	0.40
1:C:823:HIS:CD2	1:C:825:MET:HB2	2.56	0.40
1:D:2:LYS:N	1:D:76:ASP:OD2	2.35	0.40
1:A:807:ALA:HB3	1:A:808:PRO:HD3	2.04	0.40
1:B:787:ILE:HA	1:B:787:ILE:HD12	1.89	0.40
1:B:925:ILE:O	1:B:928:LYS:HE3	2.22	0.40
1:B:933:ILE:HD11	1:B:937:PRO:HG3	2.02	0.40
1:C:527:LEU:HD12	1:C:787:ILE:HB	2.03	0.40
1:A:360:THR:HG23	1:A:1042:GLN:HE22	1.86	0.40
1:B:883:ASN:CB	1:B:885:LEU:CD2	2.99	0.40
1:C:925:ILE:O	1:C:928:LYS:HE3	2.21	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	977/1143 (86%)	919 (94%)	56 (6%)	2 (0%)	47	79
1	B	975/1143 (85%)	922 (95%)	52 (5%)	1 (0%)	51	83
1	C	974/1143 (85%)	917 (94%)	56 (6%)	1 (0%)	51	83
1	D	1042/1143 (91%)	983 (94%)	56 (5%)	3 (0%)	41	73
All	All	3968/4572 (87%)	3741 (94%)	220 (6%)	7 (0%)	47	79

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	460	ARG
1	B	269	ASN
1	C	269	ASN
1	D	269	ASN
1	A	269	ASN
1	D	84	LEU
1	D	610	ALA

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	832/955 (87%)	777 (93%)	55 (7%)	16	47
1	B	830/955 (87%)	778 (94%)	52 (6%)	18	48
1	C	831/955 (87%)	779 (94%)	52 (6%)	18	48
1	D	872/955 (91%)	812 (93%)	60 (7%)	15	45
All	All	3365/3820 (88%)	3146 (94%)	219 (6%)	17	47

All (219) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	GLU
1	A	76	ASP
1	A	125	GLU
1	A	131	ILE
1	A	216	ARG
1	A	233	ARG
1	A	330	GLU
1	A	333	LEU
1	A	341	ARG
1	A	363	SER
1	A	372	ASP
1	A	388	SER
1	A	409	ARG

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Mol	Chain	Res	Type
1	A	421	THR
1	A	442	THR
1	A	457	LEU
1	A	481	ASN
1	A	494	LEU
1	A	523	LYS
1	A	542	THR
1	A	544	LEU
1	A	569	TRP
1	A	591	LYS
1	A	606	ARG
1	A	609	ASN
1	A	619	ASN
1	A	647	GLN
1	A	665	THR
1	A	681	ASN
1	A	688	LEU
1	A	705	MET
1	A	712	GLN
1	A	727	LEU
1	A	748	THR
1	A	783	ARG
1	A	814	THR
1	A	835	SER
1	A	854	ARG
1	A	868	PRO
1	A	878	LEU
1	A	885	LEU
1	A	886	THR
1	A	888	GLU
1	A	893	ARG
1	A	896	GLU
1	A	921	LYS
1	A	940	HIS
1	A	990	THR
1	A	1003	LEU
1	A	1011	ILE
1	A	1016	THR
1	A	1035	LEU
1	A	1039	LEU
1	A	1049	ASN
1	A	1052	SER

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Mol	Chain	Res	Type
1	B	11	GLU
1	B	76	ASP
1	B	125	GLU
1	B	233	ARG
1	B	260	LYS
1	B	330	GLU
1	B	333	LEU
1	B	341	ARG
1	B	363	SER
1	B	372	ASP
1	B	388	SER
1	B	409	ARG
1	B	421	THR
1	B	480	GLU
1	B	481	ASN
1	B	494	LEU
1	B	523	LYS
1	B	542	THR
1	B	544	LEU
1	B	569	TRP
1	B	591	LYS
1	B	606	ARG
1	B	609	ASN
1	B	619	ASN
1	B	647	GLN
1	B	665	THR
1	B	681	ASN
1	B	688	LEU
1	B	705	MET
1	B	727	LEU
1	B	748	THR
1	B	749	GLN
1	B	783	ARG
1	B	814	THR
1	B	835	SER
1	B	854	ARG
1	B	878	LEU
1	B	885	LEU
1	B	886	THR
1	B	893	ARG
1	B	896	GLU
1	B	921	LYS

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Mol	Chain	Res	Type
1	B	940	HIS
1	B	959	TYR
1	B	990	THR
1	B	1003	LEU
1	B	1011	ILE
1	B	1016	THR
1	B	1029	LEU
1	B	1035	LEU
1	B	1039	LEU
1	B	1049	ASN
1	C	76	ASP
1	C	125	GLU
1	C	233	ARG
1	C	321	ARG
1	C	330	GLU
1	C	333	LEU
1	C	341	ARG
1	C	363	SER
1	C	372	ASP
1	C	388	SER
1	C	409	ARG
1	C	421	THR
1	C	442	THR
1	C	481	ASN
1	C	494	LEU
1	C	523	LYS
1	C	542	THR
1	C	544	LEU
1	C	569	TRP
1	C	591	LYS
1	C	606	ARG
1	C	609	ASN
1	C	619	ASN
1	C	647	GLN
1	C	665	THR
1	C	681	ASN
1	C	688	LEU
1	C	705	MET
1	C	727	LEU
1	C	748	THR
1	C	783	ARG
1	C	814	THR

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Mol	Chain	Res	Type
1	C	835	SER
1	C	855	LYS
1	C	868	PRO
1	C	871	LYS
1	C	878	LEU
1	C	885	LEU
1	C	886	THR
1	C	888	GLU
1	C	893	ARG
1	C	896	GLU
1	C	898	ASN
1	C	940	HIS
1	C	990	THR
1	C	1003	LEU
1	C	1011	ILE
1	C	1016	THR
1	C	1029	LEU
1	C	1035	LEU
1	C	1039	LEU
1	C	1049	ASN
1	D	76	ASP
1	D	112	ILE
1	D	116	LYS
1	D	125	GLU
1	D	135	ASN
1	D	149	THR
1	D	180	TYR
1	D	182	ARG
1	D	233	ARG
1	D	235	GLN
1	D	330	GLU
1	D	333	LEU
1	D	341	ARG
1	D	363	SER
1	D	372	ASP
1	D	388	SER
1	D	409	ARG
1	D	417	ARG
1	D	421	THR
1	D	442	THR
1	D	457	LEU
1	D	481	ASN

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Mol	Chain	Res	Type
1	D	492	GLN
1	D	494	LEU
1	D	523	LYS
1	D	542	THR
1	D	544	LEU
1	D	569	TRP
1	D	591	LYS
1	D	606	ARG
1	D	609	ASN
1	D	619	ASN
1	D	647	GLN
1	D	665	THR
1	D	677	ARG
1	D	681	ASN
1	D	682	ILE
1	D	688	LEU
1	D	705	MET
1	D	719	SER
1	D	727	LEU
1	D	748	THR
1	D	783	ARG
1	D	878	LEU
1	D	885	LEU
1	D	886	THR
1	D	893	ARG
1	D	896	GLU
1	D	921	LYS
1	D	940	HIS
1	D	990	THR
1	D	1003	LEU
1	D	1011	ILE
1	D	1012	GLU
1	D	1013	LYS
1	D	1016	THR
1	D	1035	LEU
1	D	1039	LEU
1	D	1043	ARG
1	D	1049	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (86) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	109	HIS
1	A	217	HIS
1	A	308	GLN
1	A	375	ASN
1	A	412	HIS
1	A	432	ASN
1	A	439	GLN
1	A	474	ASN
1	A	505	ASN
1	A	547	GLN
1	A	615	ASN
1	A	647	GLN
1	A	653	GLN
1	A	681	ASN
1	A	739	ASN
1	A	794	GLN
1	A	823	HIS
1	A	829	GLN
1	A	1010	GLN
1	A	1042	GLN
1	A	1049	ASN
1	B	109	HIS
1	B	308	GLN
1	B	375	ASN
1	B	412	HIS
1	B	432	ASN
1	B	439	GLN
1	B	474	ASN
1	B	505	ASN
1	B	547	GLN
1	B	615	ASN
1	B	647	GLN
1	B	653	GLN
1	B	681	ASN
1	B	739	ASN
1	B	780	HIS
1	B	794	GLN
1	B	823	HIS
1	B	829	GLN
1	B	851	GLN
1	B	1010	GLN
1	B	1042	GLN
1	B	1049	ASN

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Mol	Chain	Res	Type
1	C	109	HIS
1	C	252	ASN
1	C	308	GLN
1	C	375	ASN
1	C	412	HIS
1	C	432	ASN
1	C	439	GLN
1	C	474	ASN
1	C	481	ASN
1	C	505	ASN
1	C	547	GLN
1	C	615	ASN
1	C	647	GLN
1	C	653	GLN
1	C	681	ASN
1	C	739	ASN
1	C	794	GLN
1	C	823	HIS
1	C	1010	GLN
1	C	1049	ASN
1	D	0	HIS
1	D	109	HIS
1	D	135	ASN
1	D	252	ASN
1	D	308	GLN
1	D	375	ASN
1	D	412	HIS
1	D	432	ASN
1	D	439	GLN
1	D	474	ASN
1	D	505	ASN
1	D	547	GLN
1	D	615	ASN
1	D	647	GLN
1	D	653	GLN
1	D	681	ASN
1	D	712	GLN
1	D	739	ASN
1	D	794	GLN
1	D	823	HIS
1	D	1010	GLN
1	D	1042	GLN

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Mol	Chain	Res	Type
1	D	1049	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 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	BTN	A	1202	-	14,17,17	1.18	2 (14%)	19,23,23	1.86	6 (31%)

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	BTN	A	1202	-	-	1/5/28/28	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1202	BTN	C2-S1	-2.60	1.78	1.82
3	A	1202	BTN	C3-N1	-2.20	1.31	1.35

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1202	BTN	C6-C5-C4	3.93	112.07	108.66
3	A	1202	BTN	C6-C5-N1	-3.16	109.01	113.03
3	A	1202	BTN	C5-C6-S1	-3.03	103.71	106.31
3	A	1202	BTN	O3-C3-N1	-2.66	122.12	125.94
3	A	1202	BTN	C6-S1-C2	2.56	95.15	89.89
3	A	1202	BTN	O3-C3-N2	2.13	128.99	125.94

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1202	BTN	C2-C7-C8-C9

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	981/1143 (85%)	-0.27	4 (0%) 92 84	40, 71, 108, 160	0
1	B	979/1143 (85%)	0.05	45 (4%) 32 16	36, 86, 149, 219	0
1	C	978/1143 (85%)	0.20	59 (6%) 21 10	37, 90, 168, 255	0
1	D	1046/1143 (91%)	-0.25	6 (0%) 89 78	40, 71, 108, 177	0
All	All	3984/4572 (87%)	-0.07	114 (2%) 51 28	36, 76, 144, 255	0

All (114) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	284	PHE	9.0
1	C	283	TYR	8.6
1	C	265	VAL	6.0
1	B	277	VAL	5.6
1	C	105	PRO	5.6
1	C	281	LYS	5.5
1	C	258	ALA	5.2
1	C	264	ASN	4.9
1	C	284	PHE	4.9
1	C	255	CYS	4.8
1	C	262	CYS	4.7
1	B	287	VAL	4.4
1	B	213	LEU	4.4
1	C	267	TYR	4.4
1	D	193	SER	4.3
1	B	273	VAL	4.1
1	B	278	LYS	4.0
1	B	262	CYS	4.0
1	B	451	LEU	4.0
1	C	243	ALA	4.0
1	C	285	ILE	4.0

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Mol	Chain	Res	Type	RSRZ
1	C	276	LEU	4.0
1	C	104	GLY	3.9
1	B	281	LYS	3.9
1	C	277	VAL	3.8
1	B	206	LYS	3.7
1	B	429	VAL	3.7
1	C	257	ALA	3.5
1	B	442	THR	3.5
1	B	929	ASP	3.5
1	C	216	ARG	3.5
1	B	245	GLY	3.4
1	C	895	ASN	3.3
1	D	190	ALA	3.3
1	C	127	LYS	3.3
1	B	282	PHE	3.2
1	C	234	ASN	3.2
1	B	275	PHE	3.2
1	C	251	ARG	3.2
1	C	325	LEU	3.2
1	B	450	SER	3.1
1	C	272	THR	3.1
1	D	137	ALA	3.1
1	C	116	LYS	3.1
1	B	239	GLU	3.1
1	C	214	GLY	3.1
1	C	892	ALA	3.1
1	B	452	PHE	3.0
1	C	218	GLY	3.0
1	B	365	GLY	3.0
1	A	283	TYR	3.0
1	B	243	ALA	3.0
1	C	204	ASN	3.0
1	C	326	PRO	3.0
1	C	260	LYS	3.0
1	B	103	VAL	2.9
1	B	425	PHE	2.9
1	C	253	GLU	2.9
1	D	189	GLY	2.9
1	D	194	GLY	2.9
1	B	446	ASP	2.9
1	B	366	GLY	2.9
1	B	839	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	329	SER	2.8
1	C	261	LEU	2.8
1	C	222	HIS	2.8
1	C	886	THR	2.8
1	B	280	ASP	2.8
1	B	269	ASN	2.7
1	C	205	PRO	2.7
1	C	317	LYS	2.7
1	C	110	LEU	2.7
1	C	246	LEU	2.6
1	B	430	ILE	2.6
1	C	207	HIS	2.5
1	C	280	ASP	2.5
1	A	129	PRO	2.5
1	C	372	ASP	2.5
1	C	120	LYS	2.4
1	C	889	ASP	2.4
1	A	131	ILE	2.4
1	C	896	GLU	2.4
1	B	265	VAL	2.4
1	B	443	THR	2.4
1	B	896	GLU	2.4
1	C	1029	LEU	2.4
1	B	448	THR	2.4
1	C	249	ASP	2.4
1	B	268	VAL	2.3
1	B	895	ASN	2.3
1	C	212	ILE	2.3
1	C	331	ILE	2.3
1	B	204	ASN	2.3
1	C	394	CYS	2.3
1	B	276	LEU	2.3
1	C	77	ALA	2.3
1	D	196	ILE	2.3
1	C	316	GLY	2.2
1	C	320	HIS	2.2
1	B	231	GLN	2.1
1	B	892	ALA	2.1
1	C	275	PHE	2.1
1	C	282	PHE	2.1
1	B	264	ASN	2.1
1	B	205	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	363	SER	2.1
1	B	890	VAL	2.1
1	B	1029	LEU	2.1
1	C	323	ILE	2.1
1	B	246	LEU	2.1
1	A	281	LYS	2.0
1	B	99	GLY	2.0
1	C	929	ASP	2.0
1	C	859	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. 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	MN	C	2000	1/1	0.85	0.28	99,99,99,99	0
2	MN	A	1201	1/1	0.91	0.22	98,98,98,98	0
3	BTN	A	1202	16/16	0.92	0.24	88,114,121,123	0
2	MN	D	2000	1/1	0.96	0.23	88,88,88,88	0
2	MN	B	2000	1/1	0.97	0.25	90,90,90,90	0

6.5 Other polymers (i)

There are no such residues in this entry.