Full wwPDB X-ray Structure Validation Report (i)

May 23, 2020 – 01:53 am BST

PDB ID	:	4ZC0
Title	:	Structure of a dodecameric bacterial helicase
Authors	:	Bazin, A.; Cherrier, M.V.; Gutsche, I.; Timmins, J.; Terradot, L.
Deposited on	:	2015-04-15
Resolution	:	6.70 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 (i) symbol.

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

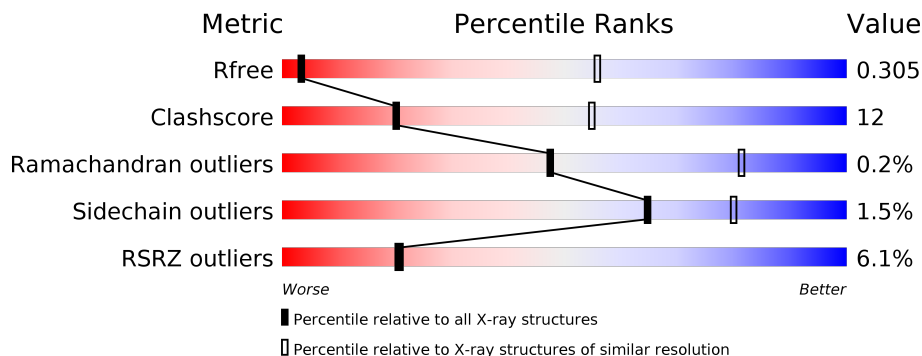|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 6.70 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	Percentile Ranks	Value
Rfree		0.305
Clashscore		12
Ramachandran outliers		0.2%
Sidechain outliers		1.5%
RSRZ outliers		6.1%

Worse ————————————————— *Better*

∎ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1002 (9.50-3.90)
Clashscore	141614	1066 (9.50-3.90)
Ramachandran outliers	138981	1000 (9.50-3.90)
Sidechain outliers	138945	1000 (9.50-3.86)
RSRZ outliers	127900	1004 (9.50-3.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria 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	521	3% — 60% / 25% / 15%
1	B	521	9% — 59% / 23% / • / 17%
1	C	521	2% — 20% / 8% / 72%
1	D	521	19% / 8% / 72%

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
2	TBR	B	501	-	-	X	-

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 9140 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 Replicative DNA helicase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	445	Total	C	N	O	S	0	0	0
			3491	2199	611	667	14			
1	B	434	Total	C	N	O	S	0	0	0
			3397	2141	595	647	14			
1	C	148	Total	C	N	O	S	0	0	0
			1122	714	193	212	3			
1	D	146	Total	C	N	O	S	0	0	0
			1112	708	191	210	3			

There are 132 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-32	MET	-	initiating methionine	UNP O25916
A	-31	HIS	-	expression tag	UNP O25916
A	-30	HIS	-	expression tag	UNP O25916
A	-29	HIS	-	expression tag	UNP O25916
A	-28	HIS	-	expression tag	UNP O25916
A	-27	HIS	-	expression tag	UNP O25916
A	-26	HIS	-	expression tag	UNP O25916
A	-25	GLY	-	expression tag	UNP O25916
A	-24	LYS	-	expression tag	UNP O25916
A	-23	PRO	-	expression tag	UNP O25916
A	-22	ILE	-	expression tag	UNP O25916
A	-21	PRO	-	expression tag	UNP O25916
A	-20	ASN	-	expression tag	UNP O25916
A	-19	PRO	-	expression tag	UNP O25916
A	-18	LEU	-	expression tag	UNP O25916
A	-17	LEU	-	expression tag	UNP O25916
A	-16	GLY	-	expression tag	UNP O25916
A	-15	LEU	-	expression tag	UNP O25916
A	-14	ASP	-	expression tag	UNP O25916
A	-13	SER	-	expression tag	UNP O25916
A	-12	THR	-	expression tag	UNP O25916

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	GLU	-	expression tag	UNP O25916
A	-10	ASN	-	expression tag	UNP O25916
A	-9	LEU	-	expression tag	UNP O25916
A	-8	TYR	-	expression tag	UNP O25916
A	-7	PHE	-	expression tag	UNP O25916
A	-6	GLN	-	expression tag	UNP O25916
A	-5	GLY	-	expression tag	UNP O25916
A	-4	ILE	-	expression tag	UNP O25916
A	-3	ASP	-	expression tag	UNP O25916
A	-2	PRO	-	expression tag	UNP O25916
A	-1	PHE	-	expression tag	UNP O25916
A	0	THR	-	expression tag	UNP O25916
B	-32	MET	-	initiating methionine	UNP O25916
B	-31	HIS	-	expression tag	UNP O25916
B	-30	HIS	-	expression tag	UNP O25916
B	-29	HIS	-	expression tag	UNP O25916
B	-28	HIS	-	expression tag	UNP O25916
B	-27	HIS	-	expression tag	UNP O25916
B	-26	HIS	-	expression tag	UNP O25916
B	-25	GLY	-	expression tag	UNP O25916
B	-24	LYS	-	expression tag	UNP O25916
B	-23	PRO	-	expression tag	UNP O25916
B	-22	ILE	-	expression tag	UNP O25916
B	-21	PRO	-	expression tag	UNP O25916
B	-20	ASN	-	expression tag	UNP O25916
B	-19	PRO	-	expression tag	UNP O25916
B	-18	LEU	-	expression tag	UNP O25916
B	-17	LEU	-	expression tag	UNP O25916
B	-16	GLY	-	expression tag	UNP O25916
B	-15	LEU	-	expression tag	UNP O25916
B	-14	ASP	-	expression tag	UNP O25916
B	-13	SER	-	expression tag	UNP O25916
B	-12	THR	-	expression tag	UNP O25916
B	-11	GLU	-	expression tag	UNP O25916
B	-10	ASN	-	expression tag	UNP O25916
B	-9	LEU	-	expression tag	UNP O25916
B	-8	TYR	-	expression tag	UNP O25916
B	-7	PHE	-	expression tag	UNP O25916
B	-6	GLN	-	expression tag	UNP O25916
B	-5	GLY	-	expression tag	UNP O25916
B	-4	ILE	-	expression tag	UNP O25916
B	-3	ASP	-	expression tag	UNP O25916

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	PRO	-	expression tag	UNP O25916
B	-1	PHE	-	expression tag	UNP O25916
B	0	THR	-	expression tag	UNP O25916
C	-32	MET	-	initiating methionine	UNP O25916
C	-31	HIS	-	expression tag	UNP O25916
C	-30	HIS	-	expression tag	UNP O25916
C	-29	HIS	-	expression tag	UNP O25916
C	-28	HIS	-	expression tag	UNP O25916
C	-27	HIS	-	expression tag	UNP O25916
C	-26	HIS	-	expression tag	UNP O25916
C	-25	GLY	-	expression tag	UNP O25916
C	-24	LYS	-	expression tag	UNP O25916
C	-23	PRO	-	expression tag	UNP O25916
C	-22	ILE	-	expression tag	UNP O25916
C	-21	PRO	-	expression tag	UNP O25916
C	-20	ASN	-	expression tag	UNP O25916
C	-19	PRO	-	expression tag	UNP O25916
C	-18	LEU	-	expression tag	UNP O25916
C	-17	LEU	-	expression tag	UNP O25916
C	-16	GLY	-	expression tag	UNP O25916
C	-15	LEU	-	expression tag	UNP O25916
C	-14	ASP	-	expression tag	UNP O25916
C	-13	SER	-	expression tag	UNP O25916
C	-12	THR	-	expression tag	UNP O25916
C	-11	GLU	-	expression tag	UNP O25916
C	-10	ASN	-	expression tag	UNP O25916
C	-9	LEU	-	expression tag	UNP O25916
C	-8	TYR	-	expression tag	UNP O25916
C	-7	PHE	-	expression tag	UNP O25916
C	-6	GLN	-	expression tag	UNP O25916
C	-5	GLY	-	expression tag	UNP O25916
C	-4	ILE	-	expression tag	UNP O25916
C	-3	ASP	-	expression tag	UNP O25916
C	-2	PRO	-	expression tag	UNP O25916
C	-1	PHE	-	expression tag	UNP O25916
C	0	THR	-	expression tag	UNP O25916
D	-32	MET	-	initiating methionine	UNP O25916
D	-31	HIS	-	expression tag	UNP O25916
D	-30	HIS	-	expression tag	UNP O25916
D	-29	HIS	-	expression tag	UNP O25916
D	-28	HIS	-	expression tag	UNP O25916
D	-27	HIS	-	expression tag	UNP O25916

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	-26	HIS	-	expression tag	UNP O25916
D	-25	GLY	-	expression tag	UNP O25916
D	-24	LYS	-	expression tag	UNP O25916
D	-23	PRO	-	expression tag	UNP O25916
D	-22	ILE	-	expression tag	UNP O25916
D	-21	PRO	-	expression tag	UNP O25916
D	-20	ASN	-	expression tag	UNP O25916
D	-19	PRO	-	expression tag	UNP O25916
D	-18	LEU	-	expression tag	UNP O25916
D	-17	LEU	-	expression tag	UNP O25916
D	-16	GLY	-	expression tag	UNP O25916
D	-15	LEU	-	expression tag	UNP O25916
D	-14	ASP	-	expression tag	UNP O25916
D	-13	SER	-	expression tag	UNP O25916
D	-12	THR	-	expression tag	UNP O25916
D	-11	GLU	-	expression tag	UNP O25916
D	-10	ASN	-	expression tag	UNP O25916
D	-9	LEU	-	expression tag	UNP O25916
D	-8	TYR	-	expression tag	UNP O25916
D	-7	PHE	-	expression tag	UNP O25916
D	-6	GLN	-	expression tag	UNP O25916
D	-5	GLY	-	expression tag	UNP O25916
D	-4	ILE	-	expression tag	UNP O25916
D	-3	ASP	-	expression tag	UNP O25916
D	-2	PRO	-	expression tag	UNP O25916
D	-1	PHE	-	expression tag	UNP O25916
D	0	THR	-	expression tag	UNP O25916

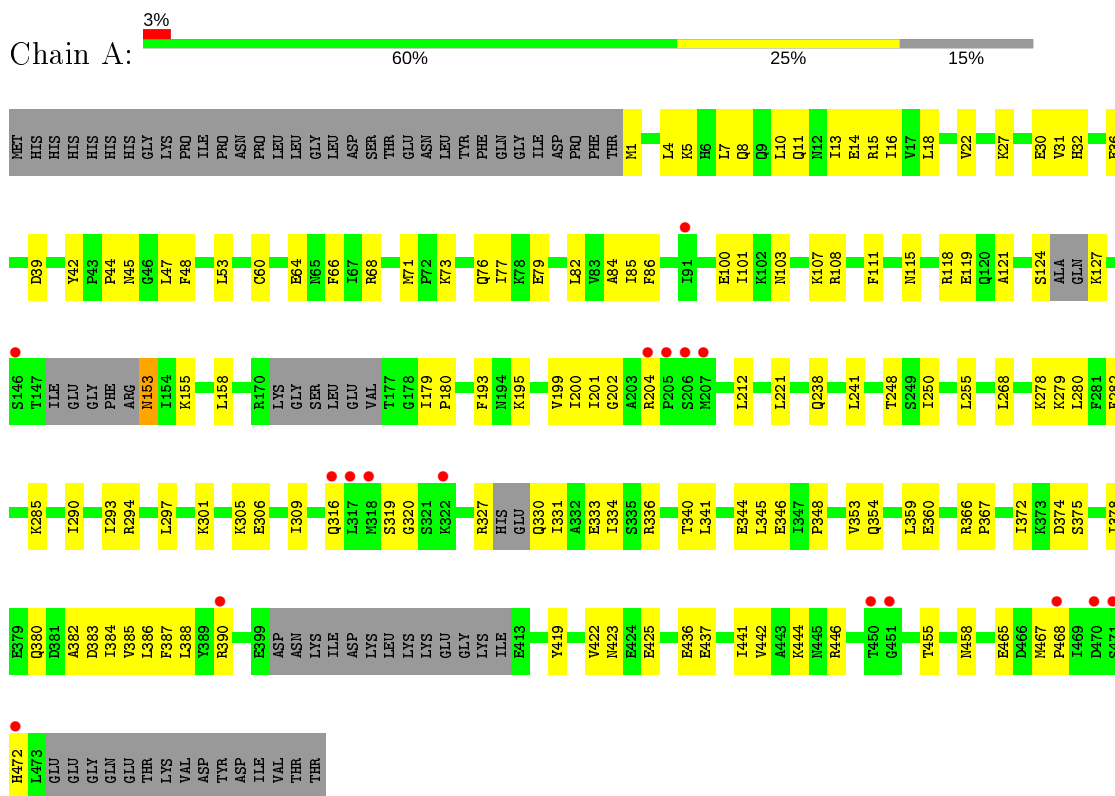- Molecule 2 is HEXATANTALUM DODECABROMIDE (three-letter code: TBR) (formula: $Br_{12}Ta_6$).
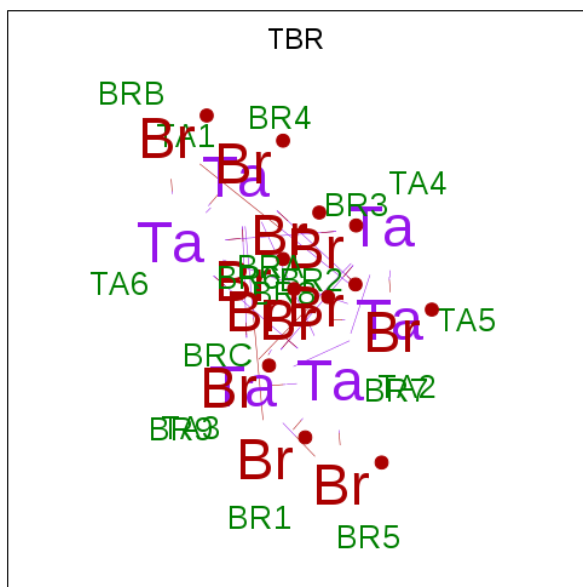
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Br	Ta		
2	B	1	18	12	6	0	0

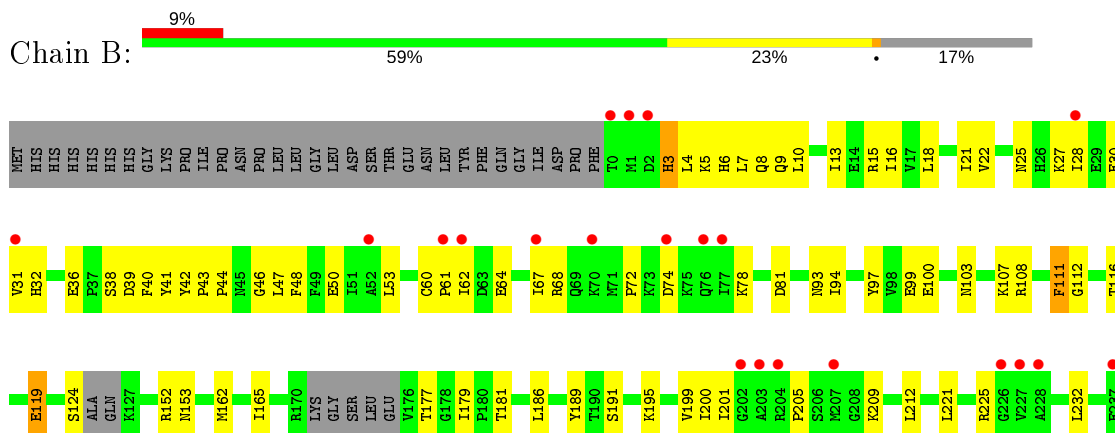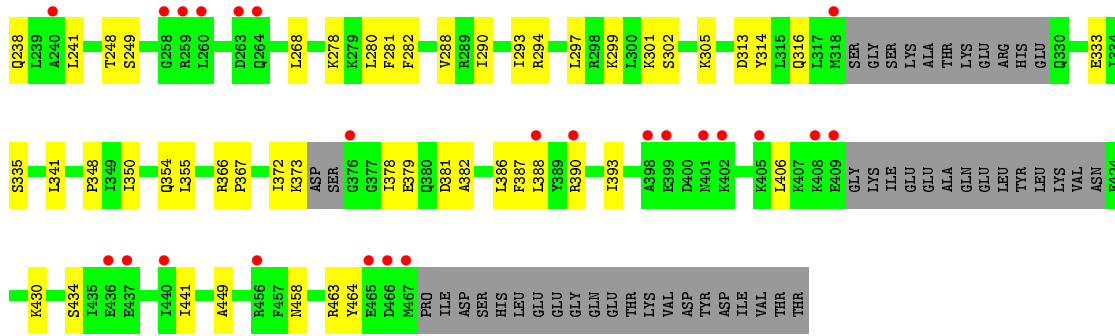# 3 Residue-property plots (i)

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.
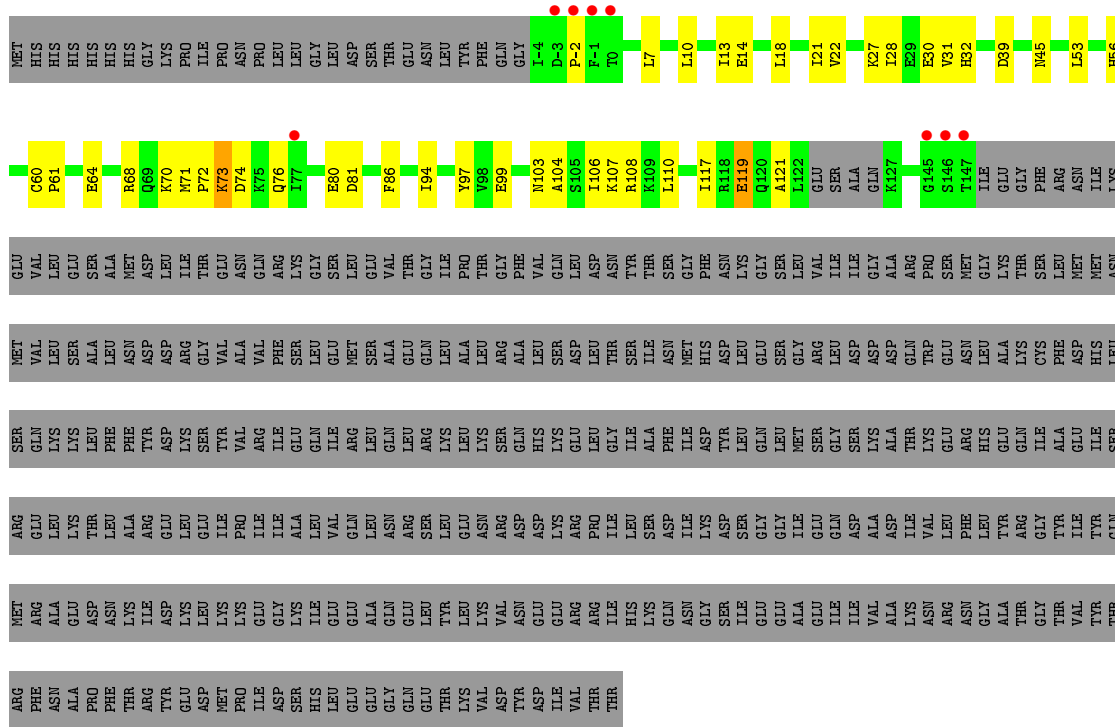
- Molecule 1: Replicative DNA helicase

Chain A:
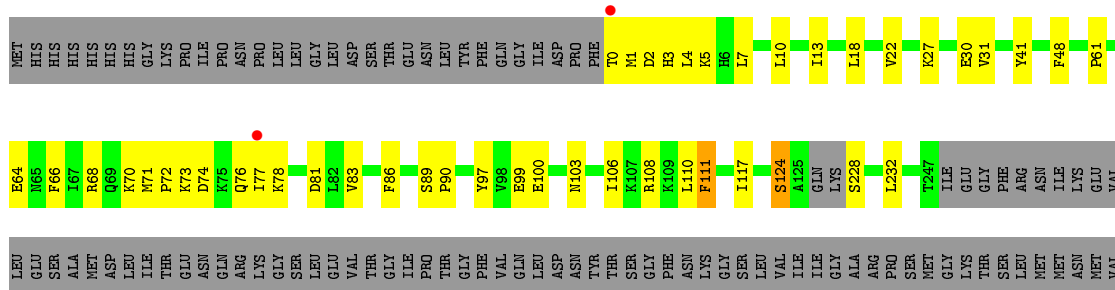
- Molecule 1: Replicative DNA helicase

Chain B:

- Molecule 1: Replicative DNA helicase

Chain C:

- Molecule 1: Replicative DNA helicase

Chain D:

LEU SER ALA LEU ASN ASP ASP ARG GLY VAL ALA VAL PHE SER LEU GLU MET SER ALA GLN GLU LEU ALA LEU ARG LEU SER ASP LEU THR SER ILE ASN MET HIS ASP LEU GLU SER GLY ARG LEU ASP ASP ASP GLN TRP GLU ASN LEU ALA LYS CYS PHE ASP HIS LEU SER GLN

LYS LYS LEU PHE TYR ASP SER LYS SER TYR VAL ARG ILE GLU GLN ILE ILE ARG GLN ILE LEU ARG LYS LYS SER GLN HIS LYS GLU GLY ILE GLY ILE ALA PHE ILE ASP TYR LEU GLN LEU MET GLU SER GLY SER LYS ALA THR GLU ARG HIS GLU GLN ILE ALA GLU ILE SER ARG GLU

LEU LYS THR LEU ALA ARG GLU LEU GLU ILE PRO ILE ALA LEU ILE VAL GLN LEU ASN ARG SER LEU GLU ASN ARG ASP ASP LYS ARG PRO ILE LEU SER ASP ILE LYS GLU SER GLY SER ILE GLU GLN ASP ALA ASP ILE VAL LEU PHE LEU TYR ARG GLY TYR ILE TYR GLN MET ARG

ALA GLU ASP ASN LYS ILE ASP LYS LEU LYS GLU LYS GLY LYS ILE GLU GLU ALA GLU LEU LEU LYS ASN GLU GLU ALA GLU ILE ILE ILE VAL ALA LYS ASN ARG ASN GLY ALA THR GLY THR VAL TYR THR ARG PHE

ASN ALA PRO PHE THR ARG TYR GLU TYR GLU ASP MET PRO ILE LEU ASP SER HIS LEU GLU GLU GLN GLU THR LYS VAL ASP TYR ASP ILE VAL THR THR

4   Data and refinement statistics (i)

Property	Value	Source
Space group	I 21 3	Depositor
Cell constants a, b, c, α, β, γ	283.47Å 283.47Å 283.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.24 – 6.70 47.24 – 6.70	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.24-6.70) 99.9 (47.24-6.70)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	0.18	Depositor
$< I/\sigma(I) >$ [1]	1.43 (at 6.67Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.258 , 0.299 0.266 , 0.305	Depositor DCC
R_{free} test set	355 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	579.5	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 363.5	EDS
L-test for twinning[2]	$< |L| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.037 for -l,-k,-h	Xtriage
F_o,F_c correlation	0.84	EDS
Total number of atoms	9140	wwPDB-VP
Average B, all atoms (Å^2)	315.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% 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 (i)

5.1 Standard geometry (i)

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

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	0.25	0/3536	0.46	0/4757
1	B	0.25	0/3439	0.45	0/4624
1	C	0.28	0/1140	0.50	1/1542 (0.1%)
1	D	0.28	0/1130	0.47	0/1528
All	All	0.26	0/9245	0.46	1/12451 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	-2	PRO	N-CA-CB	5.69	110.13	103.30

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	3491	0	3456	93	2
1	B	3397	0	3357	80	2
1	C	1122	0	1062	29	0
1	D	1112	0	1062	35	0
2	B	18	0	0	6	0
All	All	9140	0	8937	226	2

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 12.

All (226) 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:47:LEU:HG	2:B:501:TBR:BR9	2.15	1.01
1:B:301:LYS:NZ	1:B:305:LYS:O	2.07	0.86
1:A:301:LYS:NZ	1:A:305:LYS:O	2.08	0.84
1:C:99:GLU:O	1:C:103:ASN:ND2	2.13	0.81
1:B:39:ASP:O	1:B:108:ARG:NH2	2.14	0.80
1:A:200:ILE:HD12	1:A:382:ALA:HB2	1.66	0.77
1:D:10:LEU:HA	1:D:13:ILE:HD12	1.67	0.76
1:A:330:GLN:N	1:A:333:GLU:OE2	2.20	0.74
1:A:212:LEU:HD13	1:A:388:LEU:HD21	1.73	0.71
1:B:290:ILE:HA	1:B:293:ILE:HD12	1.74	0.70
1:A:73:LYS:HA	1:A:76:GLN:HE22	1.58	0.69
1:A:111:PHE:O	1:A:115:ASN:ND2	2.26	0.69
1:B:355:LEU:HD23	1:B:372:ILE:HB	1.75	0.69
1:D:71:MET:HG2	1:D:76:GLN:HG3	1.75	0.69
1:B:249:SER:HA	1:B:463:ARG:HH22	1.56	0.69
1:A:71:MET:HG2	1:A:76:GLN:HG3	1.74	0.68
1:B:47:LEU:HD21	2:B:501:TBR:BR7	2.48	0.68
1:C:94:ILE:HG13	1:C:97:TYR:HB2	1.74	0.68
1:D:64:GLU:OE1	1:D:68:ARG:NH2	2.27	0.67
1:A:331:ILE:HA	1:A:334:ILE:HB	1.76	0.66
1:A:330:GLN:HA	1:A:330:GLN:HE21	1.61	0.66
1:B:373:LYS:HG2	1:B:378:ILE:HG12	1.77	0.66
1:C:10:LEU:HA	1:C:13:ILE:HD12	1.78	0.65
1:A:195:LYS:HA	1:A:348:PRO:HD3	1.78	0.65
1:A:36:GLU:N	1:A:39:ASP:OD2	2.29	0.65
1:B:13:ILE:HA	1:B:16:ILE:HD12	1.79	0.65
1:C:39:ASP:O	1:C:108:ARG:NH2	2.30	0.65
1:B:212:LEU:HD13	1:B:388:LEU:HD21	1.79	0.64
1:A:124:SER:O	1:A:127:LYS:N	2.31	0.64
1:A:383:ASP:HA	1:A:446:ARG:HE	1.63	0.63
1:C:64:GLU:OE1	1:C:68:ARG:NH2	2.31	0.63
1:A:238:GLN:HA	1:A:241:LEU:HD12	1.79	0.63
1:C:21:ILE:HD11	1:C:31:VAL:HG21	1.79	0.62
1:A:221:LEU:HD22	1:A:278:LYS:HB3	1.82	0.62
1:C:70:LYS:NZ	1:C:70:LYS:HA	2.15	0.62
1:D:1:MET:HG3	1:D:5:LYS:HE3	1.82	0.61
1:A:39:ASP:O	1:A:108:ARG:NH2	2.28	0.61

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:36:GLU:N	1:B:39:ASP:OD2	2.32	0.61
1:D:99:GLU:O	1:D:103:ASN:ND2	2.31	0.61
1:D:228:SER:O	1:D:232:LEU:N	2.32	0.61
1:A:14:GLU:OE1	1:A:45:ASN:ND2	2.29	0.61
1:A:11:GLN:HG2	1:A:15:ARG:HE	1.65	0.60
1:A:13:ILE:HA	1:A:16:ILE:HD12	1.84	0.60
1:B:238:GLN:HA	1:B:241:LEU:HD12	1.83	0.60
1:B:62:ILE:HG23	1:B:67:ILE:HD11	1.84	0.60
1:A:387:PHE:HB2	1:A:441:ILE:HB	1.84	0.59
1:B:177:THR:OG1	1:B:191:SER:O	2.19	0.59
1:B:78:LYS:HB2	1:B:81:ASP:OD2	2.03	0.59
1:B:205:PRO:HA	1:B:209:LYS:HE3	1.85	0.59
1:A:290:ILE:HA	1:A:293:ILE:HD12	1.83	0.59
1:A:115:ASN:OD1	1:A:118:ARG:NH2	2.35	0.58
1:A:290:ILE:HD13	1:A:334:ILE:HG23	1.85	0.58
1:B:179:ILE:HG13	1:B:225:ARG:NH1	2.19	0.58
1:D:70:LYS:NZ	1:D:70:LYS:HA	2.18	0.58
1:B:41:TYR:HB2	1:B:108:ARG:NH1	2.17	0.58
1:B:38:SER:HB3	2:B:501:TBR:BR1	2.59	0.57
1:B:15:ARG:HH12	1:B:81:ASP:HA	1.70	0.57
1:B:32:HIS:HB2	1:B:53:LEU:HD21	1.86	0.57
1:C:107:LYS:HZ3	1:D:124:SER:HA	1.69	0.57
1:C:117:ILE:HG22	1:D:110:LEU:HD11	1.87	0.57
1:A:44:PRO:HB3	1:A:77:ILE:HG23	1.86	0.56
1:A:179:ILE:HB	1:A:193:PHE:HB2	1.87	0.56
1:B:335:SER:HB2	1:B:381:ASP:HB2	1.88	0.56
1:C:119:GLU:N	1:C:119:GLU:OE2	2.39	0.56
1:B:108:ARG:HA	1:B:111:PHE:CD2	2.40	0.56
1:B:50:GLU:OE2	2:B:501:TBR:BR5	2.79	0.56
1:D:27:LYS:O	1:D:30:GLU:HG2	2.06	0.55
1:A:32:HIS:HB2	1:A:53:LEU:HD21	1.88	0.55
1:B:112:GLY:O	1:B:116:THR:OG1	2.20	0.55
1:A:301:LYS:HG2	1:A:345:LEU:HD22	1.89	0.55
1:B:221:LEU:HD22	1:B:278:LYS:HB3	1.89	0.55
1:B:355:LEU:HA	1:B:372:ILE:HD13	1.89	0.54
1:D:73:LYS:HA	1:D:76:GLN:NE2	2.22	0.54
1:B:232:LEU:HD22	1:B:288:VAL:H	1.72	0.54
1:C:107:LYS:HZ3	1:D:124:SER:CA	2.18	0.54
1:D:2:ASP:OD1	1:D:3:HIS:N	2.40	0.54
1:B:373:LYS:HB2	1:B:373:LYS:NZ	2.23	0.54
1:A:73:LYS:HA	1:A:76:GLN:NE2	2.23	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:200:ILE:HD12	1:B:382:ALA:HB2	1.89	0.53
1:B:280:LEU:HD21	1:B:282:PHE:HE2	1.73	0.53
1:A:327:ARG:HH12	1:A:330:GLN:N	2.06	0.53
1:A:279:LYS:HD3	1:A:306:GLU:HG3	1.91	0.53
1:B:201:ILE:HG12	1:B:386:LEU:HB2	1.89	0.53
1:A:294:ARG:HA	1:A:341:LEU:HD22	1.91	0.53
1:B:64:GLU:OE1	1:B:68:ARG:NH2	2.38	0.53
1:D:73:LYS:HA	1:D:76:GLN:HE22	1.73	0.53
1:B:27:LYS:O	1:B:30:GLU:HG2	2.09	0.52
1:A:330:GLN:HB2	1:A:333:GLU:OE1	2.10	0.52
1:A:7:LEU:O	1:A:10:LEU:HG	2.10	0.52
1:D:7:LEU:O	1:D:10:LEU:HG	2.10	0.52
1:C:103:ASN:HA	1:C:106:ILE:HD12	1.91	0.52
1:B:99:GLU:O	1:B:103:ASN:ND2	2.40	0.51
1:D:41:TYR:HB2	1:D:108:ARG:NH1	2.25	0.51
1:A:280:LEU:HD21	1:A:282:PHE:HE2	1.75	0.51
1:A:13:ILE:HG22	1:A:101:ILE:HD11	1.93	0.51
1:A:4:LEU:HD22	1:D:4:LEU:HB3	1.92	0.51
1:A:82:LEU:HA	1:A:85:ILE:HD12	1.93	0.50
1:A:390:ARG:NH2	1:A:436:GLU:OE1	2.30	0.50
1:C:72:PRO:O	1:C:73:LYS:HG2	2.12	0.50
1:A:204:ARG:NH2	1:A:360:GLU:OE2	2.45	0.50
1:A:455:THR:OG1	1:A:465:GLU:O	2.30	0.50
1:B:18:LEU:O	1:B:22:VAL:HG23	2.11	0.50
1:D:61:PRO:HD2	1:D:66:PHE:CZ	2.47	0.50
1:A:7:LEU:HD23	1:A:10:LEU:HD21	1.93	0.49
1:A:201:ILE:O	1:A:353:VAL:N	2.42	0.49
1:A:437:GLU:OE1	1:A:472:HIS:HE1	1.95	0.49
1:B:100:GLU:O	1:B:103:ASN:HB2	2.12	0.49
1:B:38:SER:HA	2:B:501:TBR:BRC	2.67	0.49
1:A:10:LEU:HA	1:A:13:ILE:HD12	1.95	0.49
1:A:250:ILE:HB	1:A:255:LEU:HD11	1.94	0.49
1:C:27:LYS:O	1:C:30:GLU:HG2	2.13	0.49
1:B:248:THR:HG21	1:B:268:LEU:HA	1.95	0.49
1:D:71:MET:SD	1:D:72:PRO:HD2	2.53	0.48
1:D:78:LYS:HB2	1:D:81:ASP:OD2	2.14	0.48
1:B:27:LYS:O	1:B:31:VAL:HG23	2.13	0.48
1:A:319:SER:HA	1:A:375:SER:N	2.28	0.48
1:A:294:ARG:HG3	1:A:341:LEU:HD13	1.96	0.48
1:A:419:TYR:O	1:A:423:ASN:ND2	2.41	0.48
1:B:387:PHE:HB2	1:B:441:ILE:HB	1.94	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:ASN:HA	1:B:281:PHE:HA	1.95	0.48
1:B:195:LYS:HA	1:B:348:PRO:HD3	1.95	0.47
1:B:119:GLU:OE2	1:B:119:GLU:N	2.47	0.47
1:D:18:LEU:O	1:D:22:VAL:HG23	2.14	0.47
1:B:72:PRO:HB2	1:B:74:ASP:OD1	2.14	0.47
1:A:309:ILE:HD12	1:A:348:PRO:HG2	1.96	0.47
1:C:121:ALA:HB3	1:D:111:PHE:CE1	2.50	0.47
1:A:333:GLU:HA	1:A:336:ARG:NH1	2.30	0.47
1:C:7:LEU:O	1:C:10:LEU:HG	2.15	0.47
1:A:380:GLN:HG3	1:B:316:GLN:CG	2.45	0.47
1:B:94:ILE:HA	1:B:97:TYR:HD1	1.79	0.47
1:A:44:PRO:HA	1:A:47:LEU:HD12	1.97	0.46
1:C:71:MET:SD	1:C:72:PRO:HD2	2.54	0.46
1:A:153:ASN:N	1:B:282:PHE:H	2.13	0.46
1:A:11:GLN:O	1:A:15:ARG:HG3	2.15	0.46
1:B:25:ASN:O	1:B:28:ILE:HG22	2.16	0.46
1:A:366:ARG:HA	1:A:367:PRO:HD3	1.74	0.46
1:B:21:ILE:HD11	1:B:31:VAL:HG21	1.97	0.46
1:C:60:CYS:HA	1:C:61:PRO:HD3	1.82	0.46
1:A:18:LEU:HD22	1:A:48:PHE:CD1	2.51	0.46
1:B:47:LEU:CG	2:B:501:TBR:BR9	3.02	0.46
1:D:103:ASN:HA	1:D:106:ILE:HD12	1.96	0.46
1:B:294:ARG:HG3	1:B:341:LEU:HD13	1.97	0.46
1:D:27:LYS:O	1:D:31:VAL:HG23	2.16	0.45
1:A:79:GLU:OE2	1:A:82:LEU:HD23	2.16	0.45
1:B:199:VAL:O	1:B:350:ILE:HA	2.17	0.45
1:A:18:LEU:HD22	1:A:48:PHE:HD1	1.81	0.45
1:A:468:PRO:O	1:A:472:HIS:HB2	2.17	0.45
1:B:205:PRO:HG3	1:B:354:GLN:CD	2.37	0.45
1:A:4:LEU:HA	1:A:7:LEU:HB2	1.99	0.45
1:A:64:GLU:HG2	1:A:86:PHE:CZ	2.52	0.45
1:D:0:THR:O	1:D:1:MET:HG2	2.17	0.45
1:A:15:ARG:NH1	1:A:84:ALA:HB3	2.32	0.44
1:A:103:ASN:O	1:A:107:LYS:HG3	2.17	0.44
1:C:32:HIS:HB2	1:C:53:LEU:HD21	1.99	0.44
1:A:27:LYS:O	1:A:30:GLU:HG2	2.17	0.44
1:D:72:PRO:O	1:D:73:LYS:HG2	2.17	0.44
1:A:316:GLN:OE1	1:A:354:GLN:HB3	2.18	0.44
1:B:13:ILE:HG23	1:B:97:TYR:HD2	1.83	0.44
1:A:68:ARG:NH1	1:B:5:LYS:NZ	2.65	0.44
1:D:70:LYS:HZ2	1:D:70:LYS:HA	1.81	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:89:SER:HA	1:D:90:PRO:HD3	1.88	0.44
1:A:202:GLY:HA2	1:A:353:VAL:HB	2.00	0.43
1:A:320:GLY:N	1:A:375:SER:HB2	2.32	0.43
1:A:68:ARG:HH12	1:B:5:LYS:NZ	2.16	0.43
1:B:181:THR:HG21	1:B:186:LEU:HD23	2.00	0.43
1:B:379:GLU:OE2	1:B:381:ASP:N	2.50	0.43
1:C:104:ALA:O	1:C:108:ARG:HG3	2.17	0.43
1:A:155:LYS:HA	1:A:158:LEU:HD12	2.00	0.43
1:A:100:GLU:O	1:A:103:ASN:HB2	2.19	0.43
1:A:467:MET:HA	1:A:468:PRO:HD3	1.79	0.43
1:A:4:LEU:HA	1:A:7:LEU:HD12	1.98	0.43
1:A:18:LEU:O	1:A:22:VAL:HG23	2.19	0.43
1:D:97:TYR:HA	1:D:100:GLU:OE1	2.19	0.43
1:B:44:PRO:O	1:B:48:PHE:HB2	2.18	0.43
1:B:94:ILE:HA	1:B:97:TYR:CD1	2.54	0.43
1:B:6:HIS:O	1:B:9:GLN:HB2	2.19	0.43
1:D:83:VAL:HA	1:D:86:PHE:HD2	1.83	0.43
1:A:359:LEU:HD11	1:A:367:PRO:HA	2.00	0.43
1:B:5:LYS:O	1:B:8:GLN:HG2	2.19	0.43
1:B:3:HIS:ND1	1:B:4:LEU:HD13	2.33	0.43
1:A:331:ILE:HG13	1:A:374:ASP:CG	2.39	0.42
1:A:248:THR:HG21	1:A:268:LEU:HA	2.02	0.42
1:C:71:MET:SD	1:C:76:GLN:HA	2.58	0.42
1:D:18:LEU:HD22	1:D:48:PHE:HD1	1.83	0.42
1:D:72:PRO:HB2	1:D:74:ASP:OD1	2.18	0.42
1:B:366:ARG:HA	1:B:367:PRO:HD3	1.83	0.42
1:B:152:ARG:HA	1:B:153:ASN:HA	1.67	0.42
1:B:299:LYS:O	1:B:302:SER:OG	2.30	0.42
1:B:189:TYR:HD1	1:B:449:ALA:HB3	1.85	0.42
1:A:27:LYS:O	1:A:31:VAL:HG23	2.20	0.42
1:A:340:THR:O	1:A:344:GLU:HB2	2.18	0.42
1:A:422:VAL:HA	1:A:425:GLU:OE2	2.20	0.42
1:C:18:LEU:O	1:C:22:VAL:HG23	2.20	0.42
1:C:28:ILE:HG21	1:C:56:HIS:CG	2.54	0.42
1:A:4:LEU:O	1:A:8:GLN:HG3	2.19	0.42
1:B:60:CYS:HA	1:B:61:PRO:HD3	1.88	0.42
1:D:71:MET:SD	1:D:76:GLN:HA	2.59	0.42
1:B:7:LEU:HD23	1:B:10:LEU:HD13	2.00	0.42
1:C:99:GLU:HG2	1:C:103:ASN:HD21	1.83	0.42
1:C:72:PRO:C	1:C:74:ASP:H	2.24	0.42
1:C:110:LEU:HD11	1:D:117:ILE:HG13	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:LYS:HB3	1:A:346:GLU:O	2.20	0.41
1:B:212:LEU:HD12	1:B:464:TYR:CD1	2.55	0.41
1:B:297:LEU:HD23	1:B:297:LEU:HA	1.81	0.41
1:B:390:ARG:O	1:B:393:ILE:HG22	2.20	0.41
1:B:249:SER:HA	1:B:463:ARG:NH2	2.30	0.41
1:C:64:GLU:HG2	1:C:86:PHE:CZ	2.54	0.41
1:A:42:TYR:CD2	1:A:44:PRO:HD2	2.55	0.41
1:A:385:VAL:HG23	1:A:444:LYS:HD3	2.03	0.41
1:A:60:CYS:HB3	1:A:66:PHE:CE1	2.56	0.41
1:B:313:ASP:HA	1:B:314:TYR:HA	1.75	0.41
1:C:14:GLU:OE1	1:C:45:ASN:ND2	2.53	0.41
1:A:386:LEU:HD23	1:A:442:VAL:HA	2.02	0.41
1:A:293:ILE:O	1:A:297:LEU:HD13	2.20	0.41
1:D:48:PHE:HD2	1:D:77:ILE:HD13	1.85	0.41
1:A:285:LYS:HA	1:A:285:LYS:HD2	1.82	0.41
1:A:199:VAL:HG13	1:A:384:ILE:HB	2.02	0.41
1:B:162:MET:SD	1:B:165:ILE:HD11	2.61	0.41
1:B:406:LEU:HA	1:B:406:LEU:HD23	1.93	0.41
1:A:378:ILE:O	1:A:380:GLN:HG2	2.20	0.40
1:B:40:PHE:CD1	1:B:46:GLY:HA2	2.56	0.40
1:B:42:TYR:HA	1:B:43:PRO:HD3	1.93	0.40
1:A:1:MET:O	1:A:5:LYS:HG3	2.20	0.40
1:C:80:GLU:HG3	1:C:81:ASP:H	1.86	0.40
1:A:179:ILE:HA	1:A:180:PRO:HD3	1.91	0.40
1:B:42:TYR:CD2	1:B:44:PRO:HD2	2.56	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:ALA:O	1:B:107:LYS:NZ[9_555]	1.94	0.26
1:A:107:LYS:NZ	1:B:124:SER:O[9_555]	2.02	0.18

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	433/521 (83%)	423 (98%)	10 (2%)	0	100	100
1	B	422/521 (81%)	409 (97%)	13 (3%)	0	100	100
1	C	144/521 (28%)	138 (96%)	5 (4%)	1 (1%)	22	63
1	D	142/521 (27%)	136 (96%)	5 (4%)	1 (1%)	22	63
All	All	1141/2084 (55%)	1106 (97%)	33 (3%)	2 (0%)	47	81

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	124	SER
1	C	73	LYS

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	369/461 (80%)	365 (99%)	4 (1%)	73	84
1	B	356/461 (77%)	348 (98%)	8 (2%)	52	71
1	C	110/461 (24%)	109 (99%)	1 (1%)	78	87
1	D	110/461 (24%)	109 (99%)	1 (1%)	78	87
All	All	945/1844 (51%)	931 (98%)	14 (2%)	65	80

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	119	GLU
1	A	153	ASN
1	A	372	ILE
1	A	458	ASN
1	B	3	HIS
1	B	93	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	111	PHE
1	B	119	GLU
1	B	333	GLU
1	B	430	LYS
1	B	434	SER
1	B	458	ASN
1	C	119	GLU
1	D	111	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	76	GLN
1	A	472	HIS

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)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
2	TBR	B	501	-	0,36,36	0.00	-	-		

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.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	TBR	6	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 (i)

6.1 Protein, DNA and RNA chains (i)

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	445/521 (85%)	0.18	17 (3%)	40	36	58, 291, 466, 550	0
1	B	434/521 (83%)	0.55	45 (10%)	6	9	75, 341, 550, 550	0
1	C	148/521 (28%)	0.29	8 (5%)	25	26	118, 270, 425, 539	0
1	D	146/521 (28%)	-0.03	2 (1%)	75	66	114, 260, 386, 539	0
All	All	1173/2084 (56%)	0.30	72 (6%)	21	20	58, 301, 502, 550	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	388	LEU	6.7
1	B	467	MET	6.4
1	B	203	ALA	5.6
1	B	466	ASP	4.7
1	B	318	MET	4.7
1	C	146	SER	4.2
1	C	147	THR	4.2
1	B	62	ILE	4.2
1	B	465	GLU	3.7
1	B	259	ARG	3.7
1	D	0	THR	3.7
1	A	471	SER	3.7
1	B	76	GLN	3.6
1	B	77	ILE	3.5
1	B	398	ALA	3.4
1	C	0	THR	3.3
1	B	456	ARG	3.3
1	B	67	ILE	3.2
1	B	204	ARG	3.2
1	B	390	ARG	3.2
1	A	470	ASP	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	61	PRO	3.1
1	B	437	GLU	3.0
1	B	402	LYS	3.0
1	A	205	PRO	3.0
1	A	206	SER	2.9
1	B	1	MET	2.9
1	C	145	GLY	2.9
1	B	0	THR	2.9
1	A	316	GLN	2.8
1	A	318	MET	2.8
1	B	264	GLN	2.7
1	A	468	PRO	2.7
1	B	260	LEU	2.7
1	A	207	MET	2.7
1	A	317	LEU	2.7
1	B	207	MET	2.7
1	B	226	GLY	2.7
1	A	451	GLY	2.7
1	B	74	ASP	2.6
1	A	146	SER	2.6
1	B	399	GLU	2.6
1	B	263	ASP	2.6
1	B	376	GLY	2.6
1	B	202	GLY	2.5
1	B	240	ALA	2.5
1	B	405	LYS	2.4
1	A	204	ARG	2.4
1	C	-2	PRO	2.4
1	B	408	LYS	2.4
1	B	440	ILE	2.4
1	B	436	GLU	2.4
1	C	-3	ASP	2.3
1	C	77	ILE	2.3
1	A	91	ILE	2.3
1	A	390	ARG	2.3
1	B	31	VAL	2.2
1	B	409	GLU	2.2
1	A	472	HIS	2.1
1	B	52	ALA	2.1
1	B	70	LYS	2.1
1	B	237	GLU	2.1
1	A	322	LYS	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	2	ASP	2.1
1	A	450	THR	2.1
1	B	401	ASN	2.1
1	D	77	ILE	2.1
1	C	-1	PHE	2.1
1	B	258	GLY	2.0
1	B	227	VAL	2.0
1	B	228	ALA	2.0
1	B	28	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, 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	B-factors(Å^2)	Q<0.9
2	TBR	B	501	18/18	0.90	0.18	550,550,550,550	18

6.5 Other polymers (i)

There are no such residues in this entry.