



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 08:58 PM GMT

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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026982
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20026982

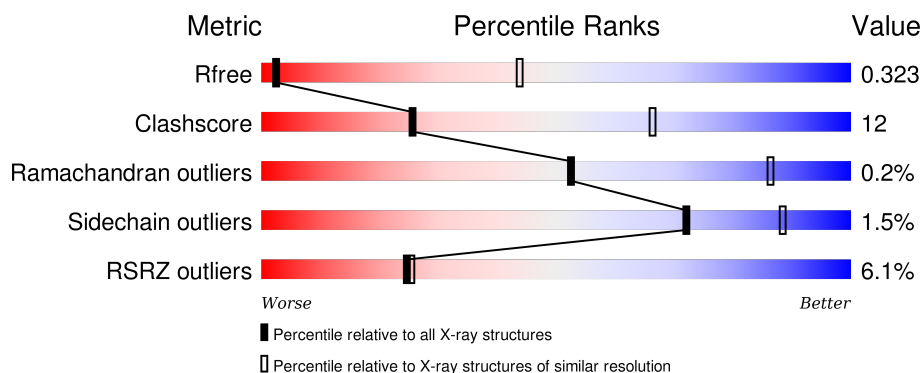
1 Overall quality at a glance ⓘ

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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1014 (9.50-3.66)
Clashscore	102246	1062 (9.50-3.70)
Ramachandran outliers	100387	1035 (9.50-3.66)
Sidechain outliers	100360	1005 (9.50-3.66)
RSRZ outliers	91569	1013 (9.50-3.66)

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

Mol	Chain	Length	Quality of chain
1	A	521	<div> <div>3%</div> <div>60%</div> <div>25%</div> <div>15%</div> </div>
1	B	521	<div> <div>8%</div> <div>59%</div> <div>23%</div> <div>17%</div> </div>
1	C	521	<div> <div>2%</div> <div>20%</div> <div>8%</div> <div>72%</div> </div>
1	D	521	<div> <div>19%</div> <div>8%</div> <div>72%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	TBR	B	501	-	-	X	-

2 Entry composition

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

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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

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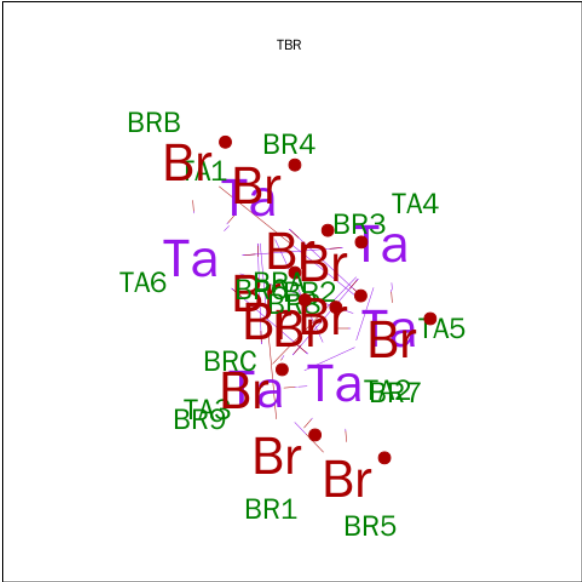
Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	PRO	-	expression tag	UNP O25916
B	-1	PHE	-	expression tag	UNP O25916
B	0	THR	-	expression tag	UNP O25916
C	-32	MET	-	initiating methionine	UNP O25916
C	-31	HIS	-	expression tag	UNP O25916
C	-30	HIS	-	expression tag	UNP O25916
C	-29	HIS	-	expression 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

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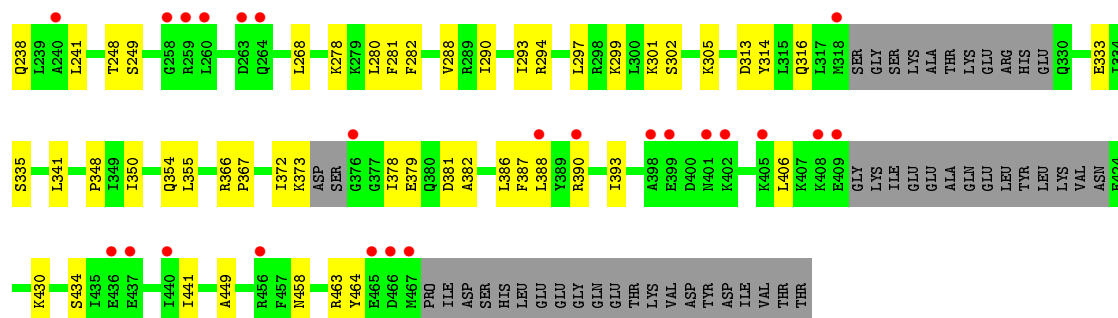
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Chain	Residue	Modelled	Actual	Comment	Reference
D	-26	HIS	-	expression tag	UNP O25916
D	-25	GLY	-	expression tag	UNP O25916
D	-24	LYS	-	expression tag	UNP O25916
D	-23	PRO	-	expression tag	UNP O25916
D	-22	ILE	-	expression tag	UNP O25916
D	-21	PRO	-	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

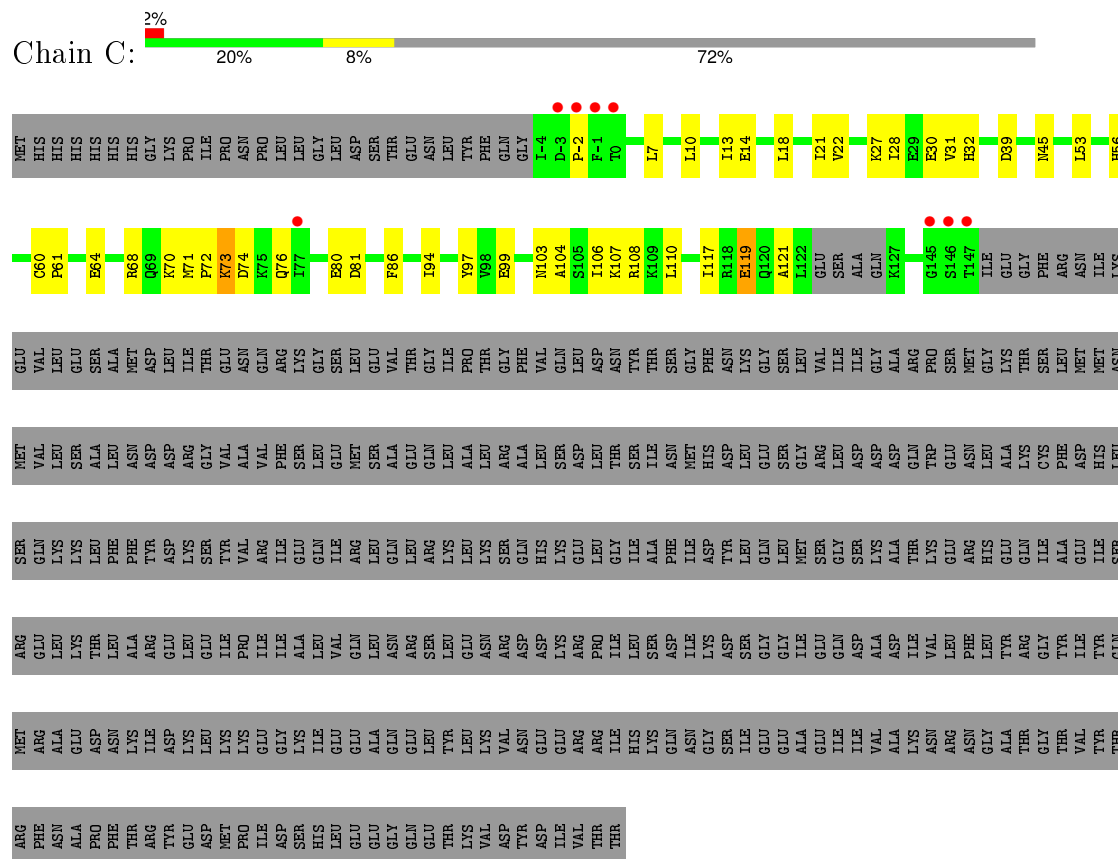
- Molecule 2 is HEXATANTALUM DODECABROMIDE (three-letter code: TBR) (formula: Br₁₂Ta₆).



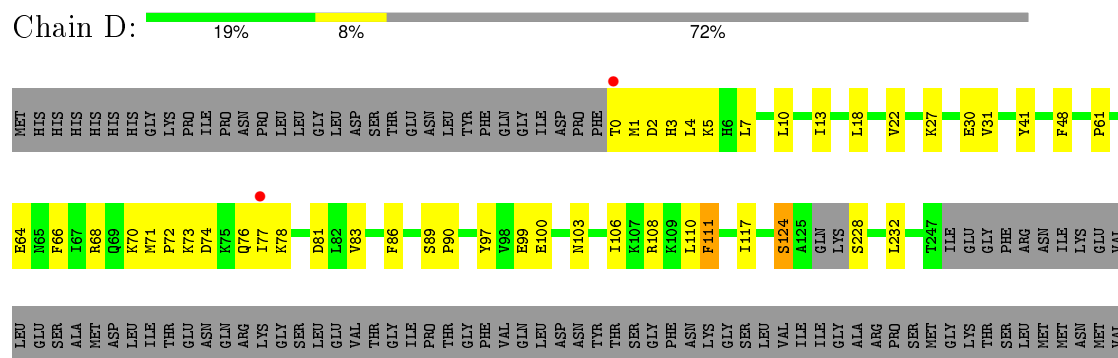
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	Br	Ta	0	0
			18	12	6		



• Molecule 1: Replicative DNA helicase



• Molecule 1: Replicative DNA helicase



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

4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	1.43 (at 6.67Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.258 , 0.299 0.297 , 0.323	Depositor DCC
R_{free} test set	356 reflections (5.40%)	DCC
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 , 364.1	EDS
Estimated twinning fraction	0.037 for -l,-k,-h	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 6954 reflections	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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(°)	Ideal(°)
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:B:13:ILE:HA	1:B:16:ILE:HD12	1.79	0.65
1:A:36:GLU:N	1:A:39:ASP:OD2	2.29	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:C:64:GLU:OE1	1:C:68:ARG:NH2	2.31	0.63
1:A:383:ASP:HA	1:A:446:ARG:HE	1.63	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:C:70:LYS:NZ	1:C:70:LYS:HA	2.15	0.62
1:A:221:LEU:HD22	1:A:278:LYS:HB3	1.82	0.62
1:D:1:MET:HG3	1:D:5:LYS:HE3	1.82	0.61
1:B:36:GLU:N	1:B:39:ASP:OD2	2.32	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:ASP:O	1:A:108:ARG:NH2	2.28	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:62:ILE:HG23	1:B:67:ILE:HD11	1.84	0.60
1:B:238:GLN:HA	1:B:241:LEU:HD12	1.83	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:C:119:GLU:N	1:C:119:GLU:OE2	2.39	0.56
1:B:335:SER:HB2	1:B:381:ASP:HB2	1.88	0.56
1:A:179:ILE:HB	1:A:193:PHE:HB2	1.87	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:C:107:LYS:HZ3	1:D:124:SER:CA	2.18	0.54
1:B:232:LEU:HD22	1:B:288:VAL:H	1.72	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

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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:D:7:LEU:O	1:D:10:LEU:HG	2.10	0.52
1:A:7:LEU:O	1:A: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:D:61:PRO:HD2	1:D:66:PHE:CZ	2.47	0.50
1:A:204:ARG:NH2	1:A:360:GLU:OE2	2.45	0.50
1:B:18:LEU:O	1:B:22:VAL:HG23	2.11	0.50
1:A:455:THR:OG1	1:A:465:GLU:O	2.30	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:C:27:LYS:O	1:C:30:GLU:HG2	2.13	0.49
1:A:250:ILE:HB	1:A:255:LEU:HD11	1.94	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:B:387:PHE:HB2	1:B:441:ILE:HB	1.94	0.48
1:A:419:TYR:O	1:A:423:ASN:ND2	2.41	0.48

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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:B:94:ILE:HA	1:B:97:TYR:HD1	1.79	0.47
1:A:380:GLN:HG3	1:B:316:GLN:CG	2.45	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:11:GLN:O	1:A:15:ARG:HG3	2.15	0.46
1:A:153:ASN:N	1:B:282:PHE:H	2.13	0.46
1:B:25:ASN:O	1:B:28:ILE:HG22	2.16	0.46
1:B:21:ILE:HD11	1:B:31:VAL:HG21	1.97	0.46
1:A:366:ARG:HA	1:A:367:PRO:HD3	1.74	0.46
1:C:60:CYS:HA	1:C:61:PRO:HD3	1.82	0.46
1:B:47:LEU:CG	2:B:501:TBR:BR9	3.02	0.46
1:A:18:LEU:HD22	1:A:48:PHE:CD1	2.51	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:B:205:PRO:HG3	1:B:354:GLN:CD	2.37	0.45
1:A:468:PRO:O	1:A:472:HIS:HB2	2.17	0.45
1:D:0:THR:O	1:D:1:MET:HG2	2.17	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: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:D:72:PRO:O	1:D:73:LYS:HG2	2.17	0.44
1:A:27:LYS:O	1:A:30:GLU: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:D:70:LYS:HZ2	1:D:70:LYS:HA	1.81	0.44
1:A:68:ARG:NH1	1:B:5:LYS:NZ	2.65	0.44

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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:C:104:ALA:O	1:C:108:ARG:HG3	2.17	0.43
1:B:379:GLU:OE2	1:B:381:ASP:N	2.50	0.43
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:A:155:LYS:HA	1:A:158:LEU:HD12	2.00	0.43
1:A:4:LEU:HA	1:A:7:LEU:HD12	1.98	0.43
1:A:467:MET:HA	1:A:468:PRO:HD3	1.79	0.43
1:A:100:GLU:O	1:A:103:ASN:HB2	2.19	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:D:72:PRO:HB2	1:D:74:ASP:OD1	2.18	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:A:248:THR:HG21	1:A:268:LEU:HA	2.02	0.42
1:B:366:ARG:HA	1:B:367:PRO:HD3	1.83	0.42
1:B:299:LYS:O	1:B:302:SER:OG	2.30	0.42
1:B:152:ARG:HA	1:B:153:ASN:HA	1.67	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:C:28:ILE:HG21	1:C:56:HIS:CG	2.54	0.42
1:A:422:VAL:HA	1:A:425:GLU:OE2	2.20	0.42
1:A:340:THR:O	1:A:344:GLU:HB2	2.18	0.42
1:C:18:LEU:O	1:C:22:VAL:HG23	2.20	0.42
1:D:71:MET:SD	1:D:76:GLN:HA	2.59	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:C:99:GLU:HG2	1:C:103:ASN:HD21	1.83	0.42
1:B:7:LEU:HD23	1:B:10:LEU:HD13	2.00	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

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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:B:406:LEU:HA	1:B:406:LEU:HD23	1.93	0.41
1:B:162:MET:SD	1:B:165:ILE:HD11	2.61	0.41
1:A:199:VAL:HG13	1:A:384:ILE:HB	2.02	0.41
1:A:378:ILE:O	1:A:380:GLN:HG2	2.20	0.40
1:B:42:TYR:HA	1:B:43:PRO:HD3	1.93	0.40
1:B:40:PHE:CD1	1:B:46:GLY:HA2	2.56	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%)	26	71
1	D	142/521 (27%)	136 (96%)	5 (4%)	1 (1%)	26	71
All	All	1141/2084 (55%)	1106 (97%)	33 (3%)	2 (0%)	52	86

All (2) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

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%)	80	91
1	B	356/461 (77%)	348 (98%)	8 (2%)	60	83
1	C	110/461 (24%)	109 (99%)	1 (1%)	84	93
1	D	110/461 (24%)	109 (99%)	1 (1%)	84	93
All	All	945/1844 (51%)	931 (98%)	14 (2%)	72	88

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

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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	-	0,180,180	0.00	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TBR	B	501	-	-	0/0/696/696	0/0/19/19

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	445/521 (85%)	0.17	17 (3%) 44 42	58, 291, 466, 550	0
1	B	434/521 (83%)	0.54	44 (10%) 9 14	75, 341, 550, 550	0
1	C	148/521 (28%)	0.29	8 (5%) 29 30	118, 270, 425, 539	0
1	D	146/521 (28%)	-0.03	2 (1%) 78 72	114, 260, 386, 539	0
All	All	1173/2084 (56%)	0.30	71 (6%) 25 25	58, 301, 502, 550	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	388	LEU	6.7
1	B	467	MET	6.3
1	B	203	ALA	5.7
1	B	318	MET	4.8
1	B	466	ASP	4.6
1	C	146	SER	4.3
1	C	147	THR	4.3
1	B	62	ILE	4.1
1	B	259	ARG	3.8
1	D	0	THR	3.7
1	A	471	SER	3.7
1	B	465	GLU	3.7
1	B	76	GLN	3.6
1	B	398	ALA	3.5
1	B	77	ILE	3.5
1	C	0	THR	3.4
1	B	204	ARG	3.2
1	B	456	ARG	3.2
1	B	67	ILE	3.2
1	B	390	ARG	3.2
1	A	470	ASP	3.1

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

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Mol	Chain	Res	Type	RSRZ
1	B	401	ASN	2.1
1	B	237	GLU	2.1
1	A	450	THR	2.1
1	B	258	GLY	2.1
1	B	228	ALA	2.0
1	B	227	VAL	2.0
1	A	322	LYS	2.0
1	B	70	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	TBR	B	501	18/18	0.90	0.18	-0.45	550,550,550,550	18

6.5 Other polymers [i](#)

There are no such residues in this entry.