



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:34 PM GMT

PDB ID : 4FFI  
Title : Crystal Structure of Levan Fructotransferase D54N mutant from *Arthrobacter ureafaciens* in complex with levanbiose  
Authors : Park, J.; Rhee, S.  
Deposited on : 2012-06-01  
Resolution : 2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
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) : trunk26865

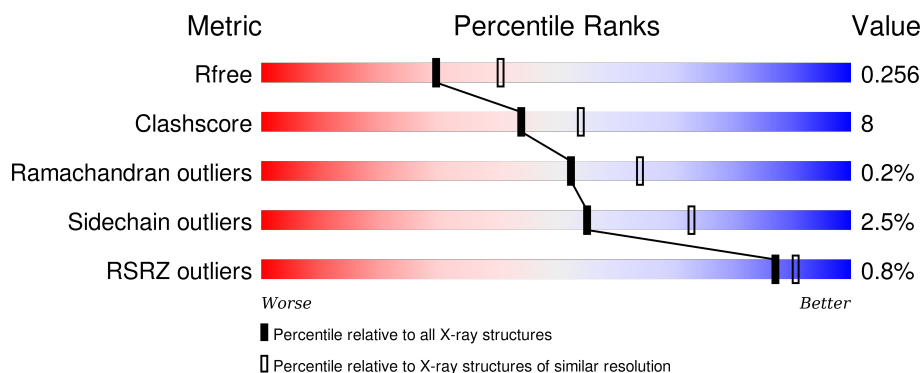
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	492	<div> <div></div> <div>81%15%..</div> </div>
1	B	492	<div> <div></div> <div>78%17%..</div> </div>
1	C	492	<div> <div></div> <div>85%12%..</div> </div>
1	D	492	<div> <div></div> <div>81%15%..</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	LBS	A	602	-	-	-	X
2	LBS	C	601	-	-	-	X
2	LBS	D	601	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16025 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 Levan fructotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	480	Total	C	N	O	S	0	0	0
			3739	2375	646	710	8			
1	B	480	Total	C	N	O	S	0	0	0
			3739	2375	646	710	8			
1	C	479	Total	C	N	O	S	0	0	0
			3734	2372	645	709	8			
1	D	478	Total	C	N	O	S	0	0	0
			3725	2367	643	707	8			

There are 52 discrepancies between the modelled and reference sequences:

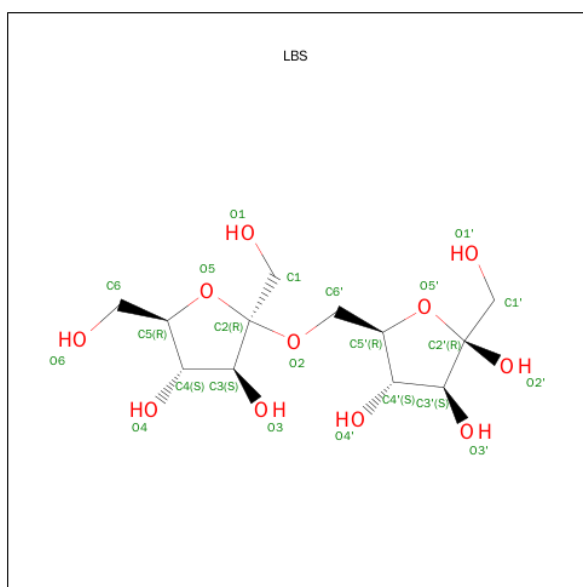
Chain	Residue	Modelled	Actual	Comment	Reference
A	40	MET	-	EXPRESSION TAG	UNP Q9KJD0
A	54	ASN	ASP	ENGINEERED MUTATION	UNP Q9KJD0
A	115	ASP	GLY	CONFLICT	UNP Q9KJD0
A	522	LEU	-	EXPRESSION TAG	UNP Q9KJD0
A	523	GLU	-	EXPRESSION TAG	UNP Q9KJD0
A	524	HIS	-	EXPRESSION TAG	UNP Q9KJD0
A	525	HIS	-	EXPRESSION TAG	UNP Q9KJD0
A	526	HIS	-	EXPRESSION TAG	UNP Q9KJD0
A	527	HIS	-	EXPRESSION TAG	UNP Q9KJD0
A	528	HIS	-	EXPRESSION TAG	UNP Q9KJD0
A	529	HIS	-	EXPRESSION TAG	UNP Q9KJD0
A	530	HIS	-	EXPRESSION TAG	UNP Q9KJD0
A	531	HIS	-	EXPRESSION TAG	UNP Q9KJD0
B	40	MET	-	EXPRESSION TAG	UNP Q9KJD0
B	54	ASN	ASP	ENGINEERED MUTATION	UNP Q9KJD0
B	115	ASP	GLY	CONFLICT	UNP Q9KJD0
B	522	LEU	-	EXPRESSION TAG	UNP Q9KJD0
B	523	GLU	-	EXPRESSION TAG	UNP Q9KJD0
B	524	HIS	-	EXPRESSION TAG	UNP Q9KJD0
B	525	HIS	-	EXPRESSION TAG	UNP Q9KJD0
B	526	HIS	-	EXPRESSION TAG	UNP Q9KJD0

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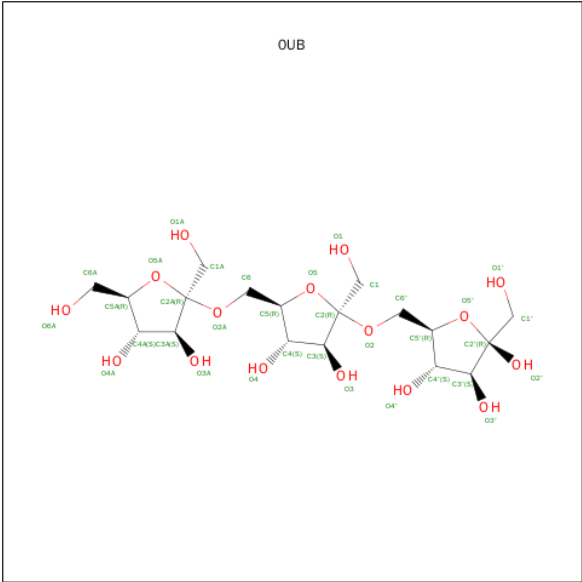
Chain	Residue	Modelled	Actual	Comment	Reference
B	527	HIS	-	EXPRESSION TAG	UNP Q9KJD0
B	528	HIS	-	EXPRESSION TAG	UNP Q9KJD0
B	529	HIS	-	EXPRESSION TAG	UNP Q9KJD0
B	530	HIS	-	EXPRESSION TAG	UNP Q9KJD0
B	531	HIS	-	EXPRESSION TAG	UNP Q9KJD0
C	40	MET	-	EXPRESSION TAG	UNP Q9KJD0
C	54	ASN	ASP	ENGINEERED MUTATION	UNP Q9KJD0
C	115	ASP	GLY	CONFLICT	UNP Q9KJD0
C	522	LEU	-	EXPRESSION TAG	UNP Q9KJD0
C	523	GLU	-	EXPRESSION TAG	UNP Q9KJD0
C	524	HIS	-	EXPRESSION TAG	UNP Q9KJD0
C	525	HIS	-	EXPRESSION TAG	UNP Q9KJD0
C	526	HIS	-	EXPRESSION TAG	UNP Q9KJD0
C	527	HIS	-	EXPRESSION TAG	UNP Q9KJD0
C	528	HIS	-	EXPRESSION TAG	UNP Q9KJD0
C	529	HIS	-	EXPRESSION TAG	UNP Q9KJD0
C	530	HIS	-	EXPRESSION TAG	UNP Q9KJD0
C	531	HIS	-	EXPRESSION TAG	UNP Q9KJD0
D	40	MET	-	EXPRESSION TAG	UNP Q9KJD0
D	54	ASN	ASP	ENGINEERED MUTATION	UNP Q9KJD0
D	115	ASP	GLY	CONFLICT	UNP Q9KJD0
D	522	LEU	-	EXPRESSION TAG	UNP Q9KJD0
D	523	GLU	-	EXPRESSION TAG	UNP Q9KJD0
D	524	HIS	-	EXPRESSION TAG	UNP Q9KJD0
D	525	HIS	-	EXPRESSION TAG	UNP Q9KJD0
D	526	HIS	-	EXPRESSION TAG	UNP Q9KJD0
D	527	HIS	-	EXPRESSION TAG	UNP Q9KJD0
D	528	HIS	-	EXPRESSION TAG	UNP Q9KJD0
D	529	HIS	-	EXPRESSION TAG	UNP Q9KJD0
D	530	HIS	-	EXPRESSION TAG	UNP Q9KJD0
D	531	HIS	-	EXPRESSION TAG	UNP Q9KJD0

- Molecule 2 is 6-O-BETA-D-FRUCTOFURANOSYL-BETA-D-FRUCTOFURANOSE (three-letter code: LBS) (formula: C<sub>12</sub>H<sub>22</sub>O<sub>11</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			23	12	11		
2	A	1	Total	C	O	0	0
			23	12	11		
2	B	1	Total	C	O	0	0
			23	12	11		
2	C	1	Total	C	O	0	0
			23	12	11		
2	C	1	Total	C	O	0	0
			23	12	11		
2	C	1	Total	C	O	0	0
			23	12	11		
2	D	1	Total	C	O	0	0
			23	12	11		
2	D	1	Total	C	O	0	0
			23	12	11		
2	D	1	Total	C	O	0	0
			23	12	11		

- Molecule 3 is BETA-D-FRUCTOFURANOSYL-(2->6)-BETA-D-FRUCTOFURANOSYL-(2->6)-BETA-D-FRUCTOFURANOSE (three-letter code: 0UB) (formula: C<sub>18</sub>H<sub>32</sub>O<sub>16</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			34	18	16		

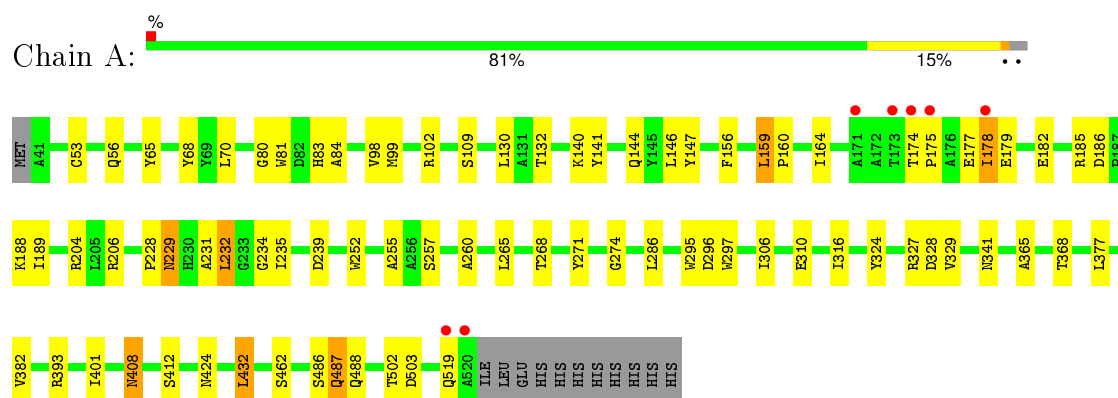
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	193	Total	O	0	0
			193	193		
4	B	192	Total	O	0	0
			192	192		
4	C	227	Total	O	0	0
			227	227		
4	D	235	Total	O	0	0
			235	235		

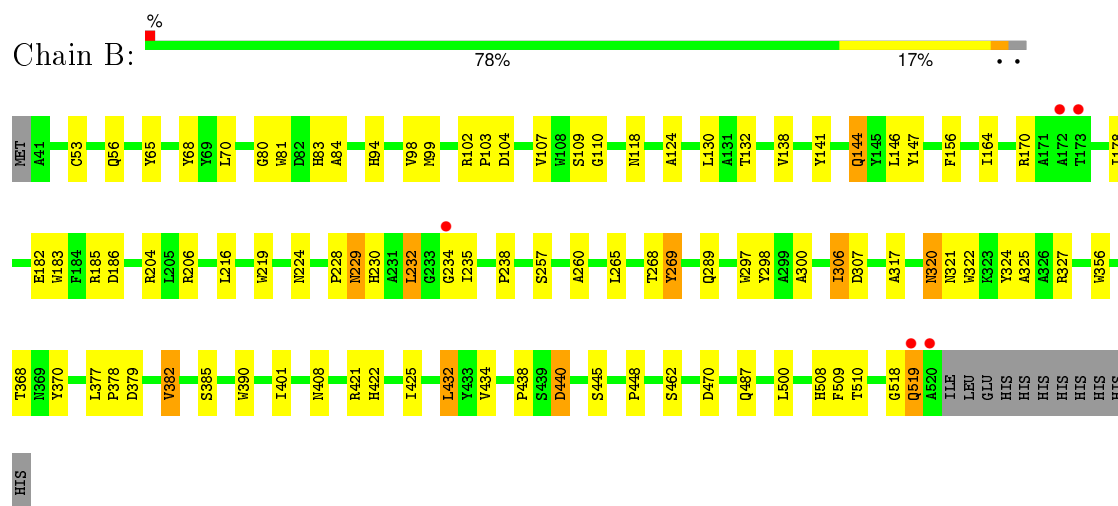
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

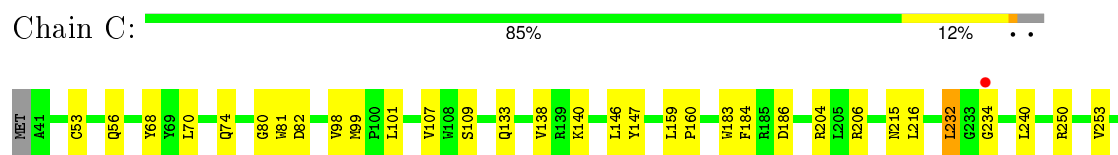
- Molecule 1: Levan fructotransferase

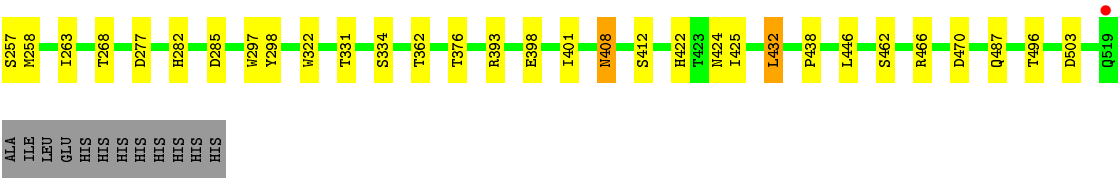


- Molecule 1: Levan fructotransferase

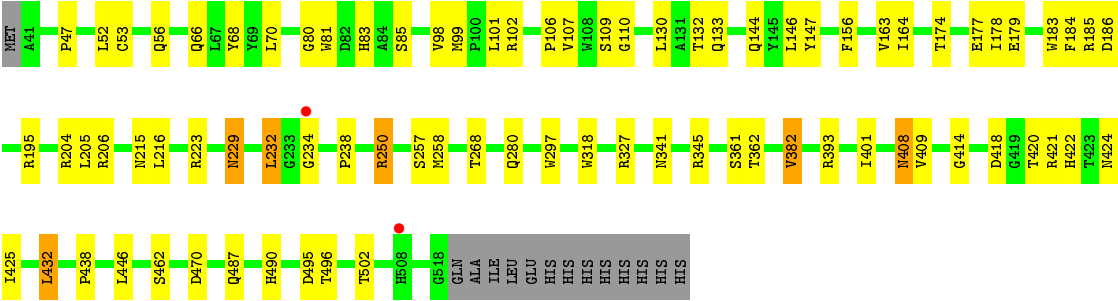
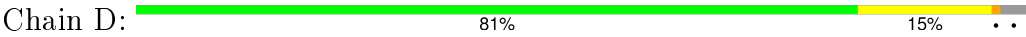


- Molecule 1: Levan fructotransferase





● Molecule 1: Levan fructotransferase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	82.51Å 168.12Å 263.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.30 44.40 – 2.30	Depositor EDS
% Data completeness (in resolution range)	89.4 (50.00-2.30) 92.9 (44.40-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.00 (at 2.29Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.215 , 0.251 0.220 , 0.256	Depositor DCC
$R_{free}$ test set	15149 reflections (9.98%)	DCC
Wilson B-factor (Å <sup>2</sup> )	23.6	Xtriage
Anisotropy	0.310	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 34.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 153850 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	16025	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.40% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LBS, 0UB

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	0.33	0/3863	0.63	1/5312 (0.0%)
1	B	0.32	0/3863	0.64	1/5312 (0.0%)
1	C	0.33	0/3858	0.64	1/5305 (0.0%)
1	D	0.34	0/3849	0.64	1/5293 (0.0%)
All	All	0.33	0/15433	0.64	4/21222 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	432	LEU	N-CA-C	-6.06	94.65	111.00
1	D	432	LEU	N-CA-C	-5.91	95.06	111.00
1	B	432	LEU	N-CA-C	-5.86	95.17	111.00
1	A	432	LEU	N-CA-C	-5.82	95.29	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	269	TYR	Sidechain

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3739	0	3491	60	0
1	B	3739	0	3491	62	0
1	C	3734	0	3486	46	0
1	D	3725	0	3478	63	0
2	A	46	0	44	1	0
2	B	23	0	22	2	0
2	C	69	0	66	1	0
2	D	69	0	65	3	0
3	B	34	0	30	0	0
4	A	193	0	0	3	0
4	B	192	0	0	8	0
4	C	227	0	0	7	0
4	D	235	0	0	3	0
All	All	16025	0	14173	234	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 8.

All (234) 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:102:ARG:HD3	4:B:784:HOH:O	1.80	0.80
1:A:81:TRP:HB2	1:A:99:MET:HB2	1.66	0.78
1:D:250:ARG:HH11	1:D:250:ARG:HG2	1.52	0.75
1:D:53:CYS:HB3	1:D:70:LEU:HB2	1.68	0.74
1:B:206:ARG:HH11	1:B:234:GLY:HA3	1.52	0.74
1:C:53:CYS:HB3	1:C:70:LEU:HB2	1.72	0.71
1:C:393:ARG:HD3	1:C:496:THR:HG22	1.74	0.70
1:A:175:PRO:HA	1:A:178:ILE:HD12	1.75	0.69
2:D:602:LBS:H8	2:D:602:LBS:H3	1.76	0.68
1:A:206:ARG:HH11	1:A:234:GLY:HA3	1.59	0.67
2:A:601:LBS:H8	2:A:601:LBS:H3	1.76	0.67
1:D:327:ARG:HH22	1:D:490:HIS:HE1	1.43	0.67
1:A:206:ARG:NH1	1:A:234:GLY:HA3	2.10	0.66
1:D:81:TRP:HB2	1:D:99:MET:HB2	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:206:ARG:HH11	1:D:234:GLY:CA	2.10	0.65
1:B:206:ARG:NH1	1:B:234:GLY:HA3	2.12	0.64
1:B:401:ILE:O	1:B:462:SER:HA	1.96	0.64
1:A:53:CYS:HB3	1:A:70:LEU:HB2	1.80	0.63
1:A:140:LYS:HG3	1:A:141:TYR:CD1	2.33	0.63
1:B:53:CYS:HB3	1:B:70:LEU:HB2	1.82	0.62
1:D:206:ARG:NH1	1:D:234:GLY:H	1.98	0.61
1:B:229:ASN:O	1:B:232:LEU:HB2	2.01	0.61
1:D:422:HIS:CD2	1:D:424:ASN:HD21	2.18	0.61
1:D:418:ASP:OD1	1:D:420:THR:HG22	2.00	0.61
1:D:66:GLN:NE2	1:D:85:SER:HB3	2.15	0.61
1:D:206:ARG:NH1	1:D:234:GLY:N	2.48	0.61
1:C:80:GLY:HA2	1:C:107:VAL:HB	1.82	0.60
1:A:146:LEU:HD23	1:A:147:TYR:N	2.16	0.60
1:D:250:ARG:HG2	1:D:250:ARG:NH1	2.17	0.60
1:D:327:ARG:HH22	1:D:490:HIS:CE1	2.19	0.60
1:D:345:ARG:HD3	1:D:361:SER:HB3	1.84	0.60
1:D:66:GLN:HE22	1:D:85:SER:HB3	1.66	0.60
1:C:277:ASP:OD1	1:C:282:HIS:HE1	1.85	0.59
1:D:133:GLN:NE2	1:D:147:TYR:OH	2.35	0.59
1:D:102:ARG:HD3	4:D:830:HOH:O	2.01	0.59
1:C:446:LEU:HD23	4:C:718:HOH:O	2.01	0.59
1:C:206:ARG:NH1	1:C:234:GLY:N	2.50	0.58
1:A:159:LEU:HD23	1:A:160:PRO:HD2	1.84	0.58
1:A:324:TYR:O	1:A:327:ARG:HG2	2.03	0.58
1:B:98:VAL:HG22	1:B:156:PHE:HD1	1.67	0.58
1:C:206:ARG:HH11	1:C:234:GLY:CA	2.17	0.58
1:A:98:VAL:HG22	1:A:156:PHE:HD1	1.69	0.57
1:C:81:TRP:HB2	1:C:99:MET:HB2	1.86	0.57
1:B:300:ALA:HB2	1:B:317:ALA:HB2	1.84	0.57
1:A:368:THR:HG23	4:A:773:HOH:O	2.05	0.57
1:D:146:LEU:HD23	1:D:146:LEU:C	2.25	0.57
1:C:206:ARG:NH1	1:C:234:GLY:H	2.02	0.57
1:C:206:ARG:HD3	1:C:234:GLY:HA2	1.87	0.57
1:A:401:ILE:O	1:A:462:SER:HA	2.03	0.57
1:D:422:HIS:HD2	1:D:424:ASN:HD21	1.51	0.56
1:B:146:LEU:HD23	1:B:147:TYR:N	2.21	0.56
1:C:74:GLN:HG2	4:C:877:HOH:O	2.06	0.56
1:B:183:TRP:O	1:B:204:ARG:HD3	2.05	0.56
1:B:94:HIS:HB3	4:B:802:HOH:O	2.04	0.56
1:B:440:ASP:OD2	1:B:445:SER:HB2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:486:SER:O	1:A:487:GLN:HG3	2.06	0.55
1:B:141:TYR:CE1	1:B:170:ARG:HD3	2.40	0.55
1:B:422:HIS:O	1:B:438:PRO:HB2	2.07	0.55
1:A:204:ARG:O	1:A:234:GLY:O	2.24	0.54
1:A:56:GLN:HB2	1:A:68:TYR:HB2	1.90	0.54
1:B:80:GLY:HA2	1:B:107:VAL:HB	1.89	0.54
1:A:206:ARG:HD3	1:A:234:GLY:HA2	1.89	0.54
1:A:140:LYS:HG3	1:A:141:TYR:HD1	1.72	0.54
1:C:470:ASP:HB3	4:C:712:HOH:O	2.07	0.54
1:C:215:ASN:O	1:C:216:LEU:HB2	2.07	0.54
1:D:183:TRP:O	1:D:204:ARG:HD2	2.08	0.53
1:D:362:THR:HG22	4:D:746:HOH:O	2.07	0.53
1:B:324:TYR:O	1:B:327:ARG:HG2	2.08	0.53
1:D:257:SER:HA	1:D:268:THR:O	2.09	0.53
1:A:178:ILE:HD13	1:A:179:GLU:N	2.23	0.53
1:C:376:THR:HG23	4:C:825:HOH:O	2.09	0.53
1:B:508:HIS:HB3	4:B:702:HOH:O	2.09	0.53
1:C:160:PRO:HG2	4:C:871:HOH:O	2.09	0.53
1:A:174:THR:O	1:A:178:ILE:HG23	2.09	0.53
1:C:257:SER:HA	1:C:268:THR:O	2.09	0.53
1:B:204:ARG:O	1:B:234:GLY:O	2.27	0.52
1:C:393:ARG:CD	1:C:496:THR:HG22	2.39	0.52
1:A:178:ILE:HD13	1:A:179:GLU:H	1.75	0.52
1:C:109:SER:HB2	1:C:186:ASP:OD1	2.09	0.52
1:B:228:PRO:HG2	4:B:820:HOH:O	2.10	0.52
1:D:109:SER:HB2	1:D:186:ASP:OD1	2.09	0.52
1:A:174:THR:HG23	1:A:177:GLU:OE2	2.10	0.51
1:B:98:VAL:CG2	1:B:156:PHE:HD1	2.24	0.51
1:D:144:GLN:HG2	1:D:164:ILE:HB	1.93	0.51
1:A:408:ASN:HB3	1:A:503:ASP:HB3	1.91	0.51
1:B:306:ILE:C	1:B:306:ILE:HD13	2.30	0.51
1:B:83:HIS:CD2	1:B:84:ALA:N	2.79	0.51
1:C:412:SER:OG	1:C:424:ASN:ND2	2.43	0.51
1:B:224:ASN:OD1	2:B:601:LBS:H12	2.11	0.51
1:A:229:ASN:O	1:A:232:LEU:HB2	2.10	0.50
1:C:232:LEU:HD12	1:C:263:ILE:HD11	1.92	0.50
1:D:401:ILE:O	1:D:462:SER:HA	2.12	0.50
1:D:393:ARG:CD	1:D:496:THR:HG22	2.41	0.50
1:A:178:ILE:O	1:A:182:GLU:HG3	2.12	0.50
1:D:132:THR:HG21	1:D:185:ARG:HB3	1.92	0.50
1:B:110:GLY:HA3	1:B:130:LEU:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:518:GLY:C	1:B:519:GLN:OE1	2.49	0.50
1:B:425:ILE:HD12	1:B:425:ILE:N	2.27	0.50
1:D:56:GLN:HB2	1:D:68:TYR:HB2	1.93	0.50
1:B:206:ARG:HD3	1:B:234:GLY:HA2	1.94	0.49
1:B:385:SER:HA	1:B:500:LEU:O	2.11	0.49
1:B:56:GLN:HB2	1:B:68:TYR:HB2	1.95	0.49
1:D:422:HIS:HD2	1:D:424:ASN:ND2	2.09	0.49
1:A:146:LEU:C	1:A:146:LEU:HD23	2.33	0.49
1:C:184:PHE:HA	1:C:204:ARG:HD3	1.94	0.49
1:D:98:VAL:HG22	1:D:156:PHE:HD1	1.78	0.49
1:B:257:SER:HB3	1:B:298:TYR:CE2	2.48	0.49
1:D:425:ILE:N	1:D:425:ILE:HD12	2.28	0.49
1:A:140:LYS:HE3	1:A:141:TYR:HE1	1.78	0.48
1:C:183:TRP:O	1:C:204:ARG:HD2	2.12	0.48
1:B:118:ASN:HB2	1:B:124:ALA:HA	1.95	0.48
1:D:206:ARG:HH11	1:D:234:GLY:HA3	1.78	0.48
1:B:257:SER:HA	1:B:268:THR:O	2.14	0.48
1:B:138:VAL:HB	1:B:141:TYR:CD2	2.48	0.48
1:D:229:ASN:O	1:D:232:LEU:HB2	2.14	0.48
1:B:216:LEU:HA	1:B:219:TRP:CZ2	2.49	0.48
1:D:232:LEU:O	1:D:258:MET:HB3	2.14	0.48
1:D:414:GLY:O	1:D:495:ASP:HB3	2.13	0.48
1:A:188:LYS:HG2	1:A:239:ASP:HA	1.95	0.47
1:C:184:PHE:HD1	1:C:204:ARG:HD3	1.79	0.47
1:A:206:ARG:HH11	1:A:234:GLY:CA	2.24	0.47
1:D:179:GLU:HG2	1:D:205:LEU:HD22	1.95	0.47
1:D:206:ARG:HH11	1:D:234:GLY:N	2.12	0.47
1:D:146:LEU:HD23	1:D:147:TYR:N	2.29	0.47
1:D:393:ARG:HD2	1:D:496:THR:HG22	1.96	0.47
1:A:140:LYS:HG3	1:A:141:TYR:CE1	2.49	0.47
1:C:206:ARG:HD3	1:C:234:GLY:CA	2.45	0.47
1:D:186:ASP:HB2	1:D:238:PRO:HD2	1.96	0.47
1:D:215:ASN:O	1:D:216:LEU:HB2	2.15	0.47
1:B:146:LEU:HD23	1:B:146:LEU:C	2.36	0.47
1:D:206:ARG:HD3	1:D:234:GLY:HA2	1.97	0.47
1:A:109:SER:HB2	1:A:186:ASP:OD1	2.15	0.47
1:B:144:GLN:HG2	1:B:164:ILE:HB	1.97	0.47
1:A:365:ALA:HB3	4:A:738:HOH:O	2.15	0.47
1:D:422:HIS:O	1:D:438:PRO:HB2	2.15	0.46
1:A:377:LEU:N	1:A:377:LEU:HD12	2.29	0.46
1:C:401:ILE:O	1:C:462:SER:HA	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:VAL:HG11	4:A:823:HOH:O	2.15	0.46
1:B:132:THR:HG21	1:B:185:ARG:HB3	1.98	0.46
1:B:109:SER:HB2	1:B:186:ASP:OD1	2.15	0.46
2:D:602:LBS:H8	2:D:602:LBS:C6	2.43	0.46
1:B:224:ASN:HD21	2:B:601:LBS:H12	1.80	0.46
1:B:432:LEU:HA	1:B:432:LEU:HD22	1.83	0.46
1:D:184:PHE:HD1	1:D:204:ARG:HD3	1.80	0.46
1:A:519:GLN:NE2	1:A:519:GLN:HA	2.30	0.46
1:D:66:GLN:NE2	1:D:83:HIS:NE2	2.60	0.45
1:C:159:LEU:HD12	1:C:160:PRO:HD2	1.98	0.45
1:A:132:THR:HG21	1:A:185:ARG:HB3	1.98	0.45
1:C:206:ARG:HH11	1:C:234:GLY:N	2.15	0.45
1:A:229:ASN:HD21	1:A:231:ALA:HB3	1.82	0.45
1:C:398:GLU:HG2	1:C:466:ARG:HG3	1.97	0.45
1:D:223:ARG:HB2	1:D:280:GLN:HB3	1.99	0.45
1:C:257:SER:HB3	1:C:298:TYR:CE2	2.52	0.45
1:B:206:ARG:HA	1:B:234:GLY:HA2	1.99	0.45
1:A:296:ASP:OD2	1:A:488:GLN:HG2	2.16	0.45
1:C:146:LEU:HD23	1:C:146:LEU:C	2.37	0.45
1:A:260:ALA:HB1	1:A:265:LEU:HB2	1.99	0.45
1:C:232:LEU:O	1:C:258:MET:HB3	2.17	0.45
1:A:393:ARG:HH11	1:A:393:ARG:HG3	1.83	0.45
1:A:130:LEU:HD13	1:A:189:ILE:HD11	1.98	0.45
1:C:99:MET:HG2	1:C:147:TYR:CD1	2.52	0.44
1:A:144:GLN:HG2	1:A:164:ILE:HB	1.99	0.44
1:B:81:TRP:HB2	1:B:99:MET:HB2	1.99	0.44
1:B:186:ASP:HB2	1:B:238:PRO:HD2	2.00	0.44
1:A:70:LEU:HA	1:A:80:GLY:O	2.18	0.44
1:B:289:GLN:NE2	1:B:356:TRP:HZ3	2.15	0.44
1:C:138:VAL:HG12	1:C:140:LYS:HG2	2.00	0.44
1:A:83:HIS:CD2	1:A:84:ALA:N	2.86	0.44
1:C:432:LEU:HA	1:C:432:LEU:HD22	1.88	0.44
1:C:206:ARG:HH11	1:C:234:GLY:HA3	1.83	0.43
1:D:174:THR:O	1:D:178:ILE:HG13	2.18	0.43
1:A:432:LEU:HD22	1:A:432:LEU:HA	1.73	0.43
1:D:80:GLY:HA2	1:D:107:VAL:HB	2.00	0.43
1:B:98:VAL:HG22	1:B:156:PHE:CD1	2.51	0.43
1:B:368:THR:HG23	4:B:875:HOH:O	2.17	0.43
1:D:204:ARG:HH21	2:D:602:LBS:H15	1.83	0.43
1:D:420:THR:HG23	1:D:421:ARG:HG3	1.99	0.43
1:A:98:VAL:HG22	1:A:156:PHE:CD1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:300:ALA:CB	1:B:317:ALA:HB2	2.49	0.43
1:D:144:GLN:CD	1:D:144:GLN:N	2.70	0.43
1:B:379:ASP:HB3	1:B:510:THR:HG22	2.01	0.43
1:B:382:VAL:HG13	1:B:509:PHE:CD2	2.54	0.43
1:D:47:PRO:HD3	1:D:52:LEU:HB2	2.01	0.43
1:B:421:ARG:O	1:B:422:HIS:HB3	2.19	0.43
1:A:486:SER:C	1:A:487:GLN:HG3	2.39	0.43
1:A:255:ALA:HB2	1:A:271:TYR:HB3	2.00	0.43
1:A:228:PRO:HD3	1:A:286:LEU:HD13	2.01	0.43
1:A:65:TYR:OH	1:A:306:ILE:HG22	2.18	0.43
1:A:252:TRP:HB2	1:A:274:GLY:O	2.18	0.43
1:C:408:ASN:HB3	1:C:503:ASP:HB3	2.01	0.42
1:B:65:TYR:OH	1:B:306:ILE:HG22	2.19	0.42
1:D:382:VAL:HG22	1:D:502:THR:HG23	2.01	0.42
1:C:68:TYR:HA	1:C:82:ASP:O	2.19	0.42
1:B:320:ASN:HD22	1:B:321:ASN:H	1.67	0.42
1:A:295:TRP:H	1:A:487:GLN:HG3	1.85	0.42
1:D:195:ARG:HG3	1:D:195:ARG:HH11	1.84	0.42
1:C:331:THR:HA	1:C:334:SER:OG	2.20	0.42
1:A:316:ILE:HD11	1:A:341:ASN:HB3	2.00	0.42
1:B:434:VAL:HG11	1:B:487:GLN:NE2	2.35	0.42
1:D:110:GLY:HA3	1:D:130:LEU:O	2.20	0.42
1:C:362:THR:HG22	4:C:766:HOH:O	2.20	0.42
1:C:425:ILE:HD12	1:C:425:ILE:N	2.35	0.42
1:C:56:GLN:HB2	1:C:68:TYR:HB2	2.02	0.41
1:A:206:ARG:NH1	1:A:234:GLY:CA	2.81	0.41
1:B:370:TYR:HD2	1:B:519:GLN:HA	1.85	0.41
1:C:322:TRP:CZ2	2:C:601:LBS:H10	2.55	0.41
1:D:408:ASN:HD22	1:D:409:VAL:N	2.18	0.41
1:B:260:ALA:CB	1:B:265:LEU:HB2	2.51	0.41
1:D:206:ARG:NH1	1:D:234:GLY:CA	2.81	0.41
1:D:174:THR:OG1	1:D:177:GLU:HG3	2.20	0.41
1:B:470:ASP:HB3	4:B:746:HOH:O	2.21	0.41
1:C:285:ASP:HB3	4:C:851:HOH:O	2.20	0.41
1:B:269:TYR:HB2	4:B:724:HOH:O	2.19	0.41
1:D:163:VAL:HG23	1:D:164:ILE:HG13	2.02	0.41
1:B:178:ILE:O	1:B:182:GLU:HG3	2.21	0.41
1:B:322:TRP:CE3	1:B:325:ALA:HB3	2.56	0.41
1:B:390:TRP:HA	4:B:759:HOH:O	2.20	0.41
1:C:422:HIS:O	1:C:438:PRO:HB2	2.21	0.41
1:B:118:ASN:HB2	1:B:124:ALA:CA	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:382:VAL:HG23	1:A:502:THR:HG23	2.03	0.41
1:C:240:LEU:HA	1:C:253:VAL:O	2.21	0.41
1:A:206:ARG:HA	1:A:234:GLY:HA2	2.03	0.40
1:A:310:GLU:HA	1:A:310:GLU:OE2	2.22	0.40
1:D:432:LEU:HA	1:D:432:LEU:HD22	1.91	0.40
1:C:133:GLN:NE2	1:C:147:TYR:OH	2.53	0.40
1:A:519:GLN:HE21	1:A:519:GLN:HA	1.86	0.40
1:B:377:LEU:HA	1:B:378:PRO:HD3	1.95	0.40
1:D:318:TRP:HA	1:D:341:ASN:HD22	1.86	0.40
1:D:183:TRP:CE3	1:D:205:LEU:HD13	2.56	0.40
1:A:519:GLN:HE21	1:A:519:GLN:CA	2.35	0.40
1:D:470:ASP:HB3	4:D:752:HOH:O	2.21	0.40
1:A:412:SER:OG	1:A:424:ASN:ND2	2.54	0.40
1:D:101:LEU:HD12	1:D:106:PRO:HA	2.02	0.40
1:A:257:SER:HA	1:A:268:THR:O	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	478/492 (97%)	448 (94%)	29 (6%)	1 (0%)	52	64
1	B	478/492 (97%)	446 (93%)	30 (6%)	2 (0%)	39	48
1	C	477/492 (97%)	452 (95%)	25 (5%)	0	100	100
1	D	476/492 (97%)	443 (93%)	33 (7%)	0	100	100
All	All	1909/1968 (97%)	1789 (94%)	117 (6%)	3 (0%)	52	64

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	235	ILE
1	B	235	ILE
1	B	103	PRO

### 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	381/393 (97%)	372 (98%)	9 (2%)	57	74
1	B	381/393 (97%)	367 (96%)	14 (4%)	41	55
1	C	381/393 (97%)	374 (98%)	7 (2%)	66	82
1	D	380/393 (97%)	372 (98%)	8 (2%)	61	78
All	All	1523/1572 (97%)	1485 (98%)	38 (2%)	55	73

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	102	ARG
1	A	159	LEU
1	A	178	ILE
1	A	229	ASN
1	A	232	LEU
1	A	297	TRP
1	A	328	ASP
1	A	408	ASN
1	A	487	GLN
1	B	104	ASP
1	B	144	GLN
1	B	229	ASN
1	B	230	HIS
1	B	232	LEU
1	B	297	TRP
1	B	306	ILE
1	B	307	ASP
1	B	320	ASN
1	B	382	VAL

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Mol	Chain	Res	Type
1	B	408	ASN
1	B	440	ASP
1	B	448	PRO
1	B	519	GLN
1	C	98	VAL
1	C	101	LEU
1	C	232	LEU
1	C	250	ARG
1	C	297	TRP
1	C	408	ASN
1	C	487	GLN
1	D	229	ASN
1	D	232	LEU
1	D	250	ARG
1	D	297	TRP
1	D	382	VAL
1	D	408	ASN
1	D	446	LEU
1	D	487	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	GLN
1	A	75	ASN
1	A	133	GLN
1	A	229	ASN
1	A	289	GLN
1	A	408	ASN
1	A	424	ASN
1	A	479	ASN
1	A	519	GLN
1	B	133	GLN
1	B	144	GLN
1	B	229	ASN
1	B	289	GLN
1	B	320	ASN
1	B	341	ASN
1	B	408	ASN
1	B	488	GLN
1	C	133	GLN
1	C	144	GLN

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Mol	Chain	Res	Type
1	C	282	HIS
1	C	341	ASN
1	C	391	ASN
1	C	408	ASN
1	C	422	HIS
1	C	424	ASN
1	C	487	GLN
1	C	519	GLN
1	D	66	GLN
1	D	74	GLN
1	D	133	GLN
1	D	180	ASN
1	D	229	ASN
1	D	341	ASN
1	D	408	ASN
1	D	422	HIS
1	D	424	ASN
1	D	487	GLN
1	D	490	HIS

### 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 ⓘ

10 ligands are 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	LBS	A	601	-	23,24,24	1.33	2 (8%)	28,37,37	1.36	3 (10%)
2	LBS	A	602	-	23,24,24	1.22	1 (4%)	28,37,37	1.15	5 (17%)
2	LBS	B	601	-	23,24,24	1.39	2 (8%)	28,37,37	1.29	5 (17%)
3	0UB	B	602	-	35,36,36	1.36	5 (14%)	46,56,56	1.34	4 (8%)
2	LBS	C	601	-	23,24,24	1.19	1 (4%)	28,37,37	1.50	5 (17%)
2	LBS	C	602	-	23,24,24	1.34	4 (17%)	28,37,37	1.46	4 (14%)
2	LBS	C	603	-	23,24,24	1.40	5 (21%)	28,37,37	1.32	4 (14%)
2	LBS	D	601	-	23,24,24	1.23	1 (4%)	28,37,37	1.63	6 (21%)
2	LBS	D	602	-	23,24,24	1.45	4 (17%)	28,37,37	1.47	4 (14%)
2	LBS	D	603	-	23,24,24	1.33	2 (8%)	28,37,37	1.57	6 (21%)

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	LBS	A	601	-	-	0/14/52/52	0/2/2/2
2	LBS	A	602	-	-	0/14/52/52	0/2/2/2
2	LBS	B	601	-	-	0/14/52/52	0/2/2/2
3	0UB	B	602	-	-	0/23/80/80	0/3/3/3
2	LBS	C	601	-	-	0/14/52/52	0/2/2/2
2	LBS	C	602	-	-	0/14/52/52	0/2/2/2
2	LBS	C	603	-	-	0/14/52/52	0/2/2/2
2	LBS	D	601	-	-	0/14/52/52	0/2/2/2
2	LBS	D	602	-	-	0/14/52/52	0/2/2/2
2	LBS	D	603	-	-	0/14/52/52	0/2/2/2

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	602	0UB	O4'-C4'	-3.23	1.35	1.43
3	B	602	0UB	O4-C4	-3.07	1.35	1.43
2	D	602	LBS	O3'-C3'	-2.97	1.36	1.42
3	B	602	0UB	O5'-C2'	-2.90	1.38	1.43
2	C	602	LBS	O3'-C3'	-2.59	1.37	1.42
2	D	601	LBS	O3-C3	-2.42	1.37	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	603	LBS	O3'-C3'	-2.40	1.37	1.42
2	C	603	LBS	O3'-C3'	-2.35	1.37	1.42
3	B	602	0UB	C4'-C3'	-2.34	1.41	1.52
2	C	601	LBS	O3-C3	-2.33	1.37	1.42
2	B	601	LBS	O3'-C3'	-2.31	1.37	1.42
2	A	601	LBS	O3'-C3'	-2.30	1.37	1.42
2	C	603	LBS	O2'-C2'	-2.29	1.37	1.41
2	A	601	LBS	O3-C3	-2.28	1.38	1.42
2	C	602	LBS	O2'-C2'	-2.27	1.37	1.41
2	C	602	LBS	O3-C3	-2.21	1.38	1.42
2	C	603	LBS	O3-C3	-2.17	1.38	1.42
2	A	602	LBS	O3-C3	-2.16	1.38	1.42
2	D	602	LBS	O3-C3	-2.16	1.38	1.42
3	B	602	0UB	O3A-C3A	-2.15	1.38	1.42
2	B	601	LBS	O3-C3	-2.15	1.38	1.42
2	C	603	LBS	O4'-C4'	-2.08	1.38	1.43
2	C	603	LBS	C4-C3	-2.07	1.43	1.52
2	D	602	LBS	O2-C2	-2.04	1.38	1.41
2	D	602	LBS	O2'-C2'	-2.03	1.37	1.41
2	C	602	LBS	O4'-C4'	-2.01	1.38	1.43
2	D	603	LBS	O2'-C2'	-2.01	1.37	1.41

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	603	LBS	O4'-C4'-C3'	-2.15	105.17	112.01
2	D	601	LBS	O4'-C4'-C3'	-2.11	105.32	112.01
2	A	602	LBS	C6'-O2-C2	2.06	119.95	116.08
2	A	602	LBS	O1'-C1'-C2'	2.07	115.41	111.39
2	B	601	LBS	O5-C5-C6	2.08	114.86	108.57
2	A	601	LBS	O6-C6-C5	2.08	118.20	111.33
2	D	601	LBS	O1-C1-C2	2.10	118.62	111.91
2	C	601	LBS	O6-C6-C5	2.11	118.30	111.33
2	B	601	LBS	O1-C1-C2	2.24	119.06	111.91
2	D	603	LBS	O1-C1-C2	2.25	119.12	111.91
2	A	602	LBS	O6-C6-C5	2.27	118.82	111.33
2	C	601	LBS	O5-C5-C6	2.29	115.50	108.57
2	B	601	LBS	O2-C6'-C5'	2.29	113.07	107.77
2	D	603	LBS	O6-C6-C5	2.32	118.98	111.33
2	C	603	LBS	C6'-O2-C2	2.36	120.50	116.08
2	D	603	LBS	O1'-C1'-C2'	2.39	116.04	111.39
2	A	602	LBS	O1-C1-C2	2.48	119.83	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	LBS	O1'-C1'-C2'	2.52	116.29	111.39
2	D	601	LBS	O5-C5-C6	2.53	116.22	108.57
2	D	602	LBS	O6-C6-C5	2.55	119.75	111.33
2	C	603	LBS	O6-C6-C5	2.57	119.84	111.33
2	C	603	LBS	O1'-C1'-C2'	2.58	116.40	111.39
2	D	602	LBS	C6'-O2-C2	2.65	121.05	116.08
2	C	602	LBS	O6-C6-C5	2.68	120.18	111.33
3	B	602	0UB	O6A-C6A-C5A	2.80	120.60	111.33
2	A	602	LBS	O2-C6'-C5'	2.82	114.29	107.77
2	C	602	LBS	C6'-O2-C2	2.85	121.43	116.08
2	B	601	LBS	O6-C6-C5	2.87	120.82	111.33
3	B	602	0UB	C6'-O2-C2	3.08	121.86	116.08
2	B	601	LBS	O1'-C1'-C2'	3.10	117.41	111.39
2	C	601	LBS	C6'-O2-C2	3.19	122.06	116.08
2	D	602	LBS	O2-C6'-C5'	3.49	115.84	107.77
2	D	603	LBS	C6'-O2-C2	3.51	122.67	116.08
2	C	601	LBS	O2-C6'-C5'	3.55	115.98	107.77
3	B	602	0UB	O2-C6'-C5'	3.61	116.12	107.77
2	C	602	LBS	O2-C6'-C5'	3.62	116.13	107.77
2	C	601	LBS	O1'-C1'-C2'	3.65	118.48	111.39
2	C	603	LBS	O2-C6'-C5'	3.65	116.22	107.77
2	D	601	LBS	O1'-C1'-C2'	3.66	118.51	111.39
2	D	601	LBS	C6'-O2-C2	3.81	123.22	116.08
2	C	602	LBS	O1'-C1'-C2'	3.82	118.82	111.39
2	A	601	LBS	O2-C6'-C5'	3.98	116.97	107.77
3	B	602	0UB	O2A-C6-C5	4.06	117.16	107.77
2	D	602	LBS	O1'-C1'-C2'	4.11	119.38	111.39
2	D	601	LBS	O2-C6'-C5'	4.28	117.66	107.77
2	D	603	LBS	O2-C6'-C5'	4.89	119.08	107.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	LBS	1	0
2	B	601	LBS	2	0
2	C	601	LBS	1	0
2	D	602	LBS	3	0

## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	480/492 (97%)	-0.23	7 (1%) 76 81	11, 23, 37, 55	0
1	B	480/492 (97%)	-0.26	5 (1%) 84 88	12, 22, 36, 58	0
1	C	479/492 (97%)	-0.37	2 (0%) 93 95	9, 20, 29, 48	0
1	D	478/492 (97%)	-0.36	2 (0%) 93 95	8, 21, 33, 42	0
All	All	1917/1968 (97%)	-0.30	16 (0%) 87 90	8, 21, 34, 58	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	519	GLN	3.5
1	B	173	THR	3.1
1	A	173	THR	3.0
1	A	519	GLN	2.9
1	A	171	ALA	2.9
1	B	172	ALA	2.9
1	C	234	GLY	2.9
1	A	520	ALA	2.8
1	A	178	ILE	2.6
1	D	234	GLY	2.6
1	B	234	GLY	2.5
1	D	508	HIS	2.4
1	B	520	ALA	2.4
1	A	175	PRO	2.3
1	C	519	GLN	2.3
1	A	174	THR	2.3

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
2	LBS	D	601	23/23	0.78	0.22	5.24	54,60,63,64	0
2	LBS	C	601	23/23	0.86	0.16	4.12	45,48,49,50	0
2	LBS	A	602	23/23	0.89	0.16	2.55	23,32,40,43	0
2	LBS	B	601	23/23	0.93	0.15	0.72	33,35,36,40	0
2	LBS	C	603	23/23	0.92	0.13	0.49	25,34,43,45	0
2	LBS	D	602	23/23	0.94	0.14	0.28	21,25,32,35	0
2	LBS	A	601	23/23	0.95	0.13	0.20	24,32,35,37	0
3	0UB	B	602	34/34	0.93	0.13	0.15	18,34,40,43	0
2	LBS	D	603	23/23	0.94	0.12	-0.02	19,24,32,35	0
2	LBS	C	602	23/23	0.94	0.12	-0.24	21,26,31,34	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.