



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 12, 2016 – 12:38 PM EDT

PDB ID : 5B0I  
Title : Structure of MoeN5-Sso7d fusion protein in complex with beta-octyl glucoside  
Authors : Ko, T.-P.; Zhang, L.; Chen, C.-C.; Guo, R.-T.; Oldfield, E.O.  
Deposited on : 2015-10-30  
Resolution : 2.26 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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027107  
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-20027107

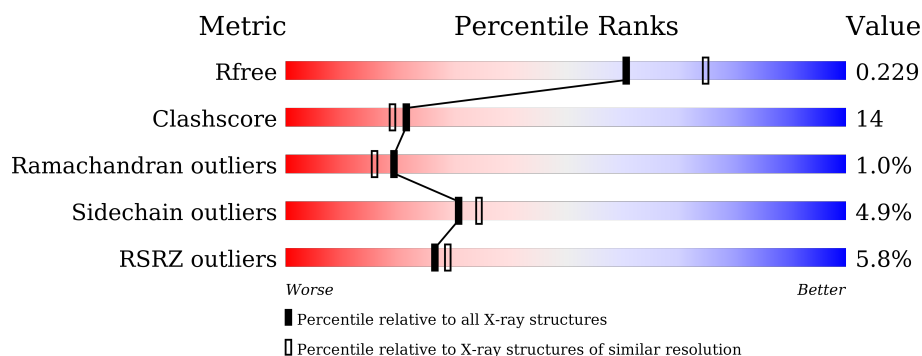
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.26 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	1640 (2.28-2.24)
Clashscore	102246	1095 (2.26-2.26)
Ramachandran outliers	100387	1063 (2.26-2.26)
Sidechain outliers	100360	1063 (2.26-2.26)
RSRZ outliers	91569	1647 (2.28-2.24)

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	343	<div> <div>4%</div> <div> <div></div> <div>63%</div> <div>12%</div> <div>•</div> <div>22%</div> </div> </div>
1	B	343	<div> <div>7%</div> <div> <div></div> <div>71%</div> <div>23%</div> <div>• •</div> </div> </div>
1	C	343	<div> <div>%</div> <div> <div></div> <div>55%</div> <div>18%</div> <div>• •</div> <div>24%</div> </div> </div>
1	D	343	<div> <div>8%</div> <div> <div></div> <div>70%</div> <div>25%</div> <div>• •</div> </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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	BOG	A	501	-	-	-	X
2	BOG	C	401	-	-	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9876 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 MoeN5,DNA-binding protein 7d.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	266	Total	C	N	O	S	0	0	0
			2026	1250	376	389	11			
1	B	332	Total	C	N	O	S	0	0	0
			2533	1571	463	485	14			
1	C	262	Total	C	N	O	S	0	0	0
			1998	1234	372	381	11			
1	D	333	Total	C	N	O	S	0	0	0
			2543	1579	466	484	14			

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	expression tag	UNP A0A010
A	-12	ALA	-	expression tag	UNP A0A010
A	-11	HIS	-	expression tag	UNP A0A010
A	-10	HIS	-	expression tag	UNP A0A010
A	-9	HIS	-	expression tag	UNP A0A010
A	-8	HIS	-	expression tag	UNP A0A010
A	-7	HIS	-	expression tag	UNP A0A010
A	-6	HIS	-	expression tag	UNP A0A010
A	-5	VAL	-	expression tag	UNP A0A010
A	-4	ASP	-	expression tag	UNP A0A010
A	-3	ASP	-	expression tag	UNP A0A010
A	-2	ASP	-	expression tag	UNP A0A010
A	-1	ASP	-	expression tag	UNP A0A010
A	0	LYS	-	expression tag	UNP A0A010
A	261	ALA	-	linker	UNP A0A010
A	262	GLY	-	linker	UNP A0A010
A	263	ALA	-	linker	UNP A0A010
A	264	GLY	-	linker	UNP A0A010
A	265	ALA	-	linker	UNP A0A010
B	-13	MET	-	expression tag	UNP A0A010
B	-12	ALA	-	expression tag	UNP A0A010

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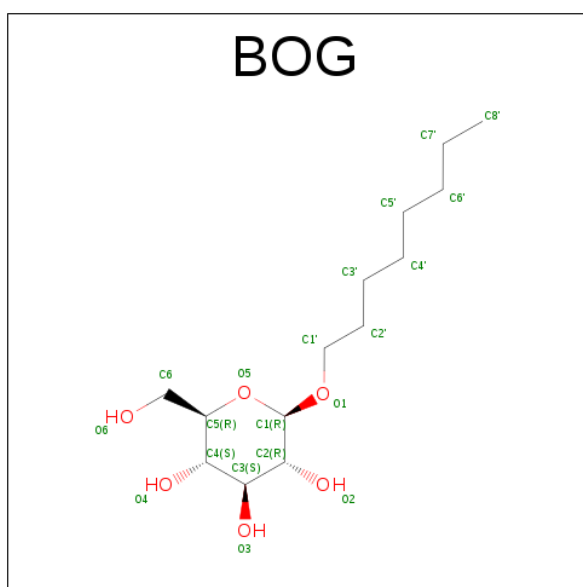
Chain	Residue	Modelled	Actual	Comment	Reference
B	-11	HIS	-	expression tag	UNP A0A010
B	-10	HIS	-	expression tag	UNP A0A010
B	-9	HIS	-	expression tag	UNP A0A010
B	-8	HIS	-	expression tag	UNP A0A010
B	-7	HIS	-	expression tag	UNP A0A010
B	-6	HIS	-	expression tag	UNP A0A010
B	-5	VAL	-	expression tag	UNP A0A010
B	-4	ASP	-	expression tag	UNP A0A010
B	-3	ASP	-	expression tag	UNP A0A010
B	-2	ASP	-	expression tag	UNP A0A010
B	-1	ASP	-	expression tag	UNP A0A010
B	0	LYS	-	expression tag	UNP A0A010
B	261	ALA	-	linker	UNP A0A010
B	262	GLY	-	linker	UNP A0A010
B	263	ALA	-	linker	UNP A0A010
B	264	GLY	-	linker	UNP A0A010
B	265	ALA	-	linker	UNP A0A010
C	-13	MET	-	expression tag	UNP A0A010
C	-12	ALA	-	expression tag	UNP A0A010
C	-11	HIS	-	expression tag	UNP A0A010
C	-10	HIS	-	expression tag	UNP A0A010
C	-9	HIS	-	expression tag	UNP A0A010
C	-8	HIS	-	expression tag	UNP A0A010
C	-7	HIS	-	expression tag	UNP A0A010
C	-6	HIS	-	expression tag	UNP A0A010
C	-5	VAL	-	expression tag	UNP A0A010
C	-4	ASP	-	expression tag	UNP A0A010
C	-3	ASP	-	expression tag	UNP A0A010
C	-2	ASP	-	expression tag	UNP A0A010
C	-1	ASP	-	expression tag	UNP A0A010
C	0	LYS	-	expression tag	UNP A0A010
C	261	ALA	-	linker	UNP A0A010
C	262	GLY	-	linker	UNP A0A010
C	263	ALA	-	linker	UNP A0A010
C	264	GLY	-	linker	UNP A0A010
C	265	ALA	-	linker	UNP A0A010
D	-13	MET	-	expression tag	UNP A0A010
D	-12	ALA	-	expression tag	UNP A0A010
D	-11	HIS	-	expression tag	UNP A0A010
D	-10	HIS	-	expression tag	UNP A0A010
D	-9	HIS	-	expression tag	UNP A0A010
D	-8	HIS	-	expression tag	UNP A0A010

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-7	HIS	-	expression tag	UNP A0A010
D	-6	HIS	-	expression tag	UNP A0A010
D	-5	VAL	-	expression tag	UNP A0A010
D	-4	ASP	-	expression tag	UNP A0A010
D	-3	ASP	-	expression tag	UNP A0A010
D	-2	ASP	-	expression tag	UNP A0A010
D	-1	ASP	-	expression tag	UNP A0A010
D	0	LYS	-	expression tag	UNP A0A010
D	261	ALA	-	linker	UNP A0A010
D	262	GLY	-	linker	UNP A0A010
D	263	ALA	-	linker	UNP A0A010
D	264	GLY	-	linker	UNP A0A010
D	265	ALA	-	linker	UNP A0A010

- Molecule 2 is B-OCTYLGLUCOSIDE (three-letter code: BOG) (formula:  $C_{14}H_{28}O_6$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			20	14	6		
2	A	1	Total	C	O	0	0
			20	14	6		
2	B	1	Total	C	O	0	0
			20	14	6		
2	C	1	Total	C	O	0	0
			20	14	6		
2	D	1	Total	C	O	0	0
			20	14	6		

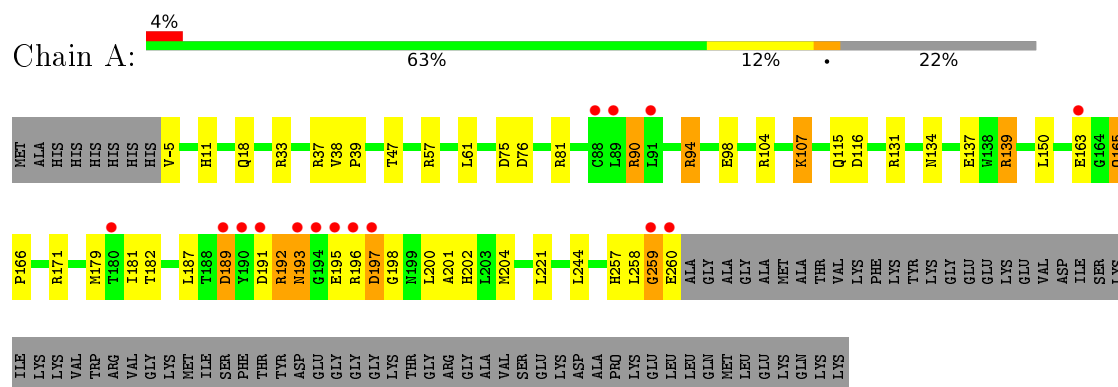
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	164	Total 164	O 164	0	0
3	B	187	Total 187	O 187	0	0
3	C	157	Total 157	O 157	0	0
3	D	168	Total 168	O 168	0	0

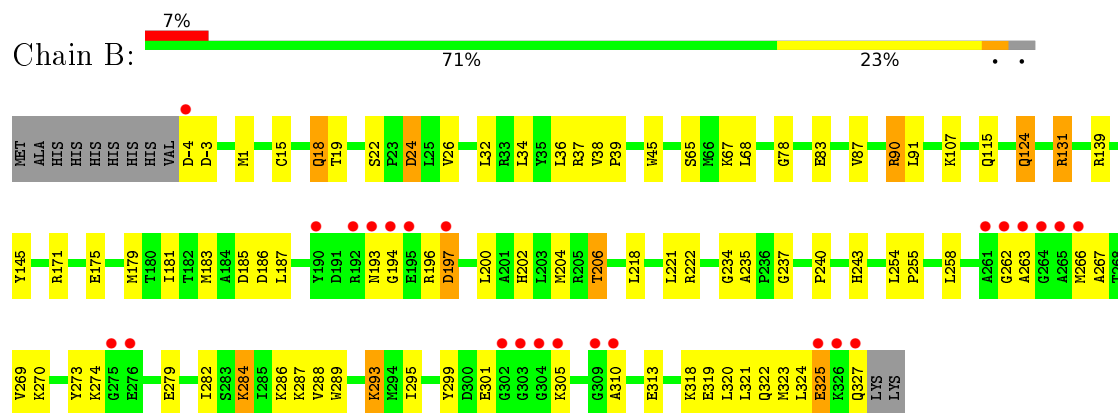
### 3 Residue-property plots [i](#)

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

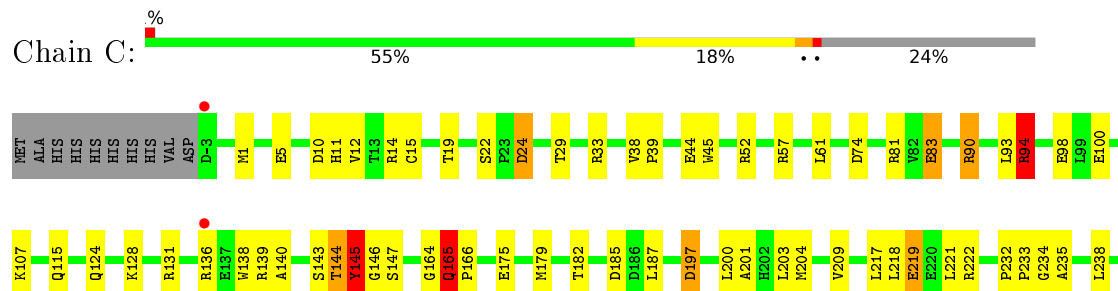
#### • Molecule 1: MoeN5,DNA-binding protein 7d



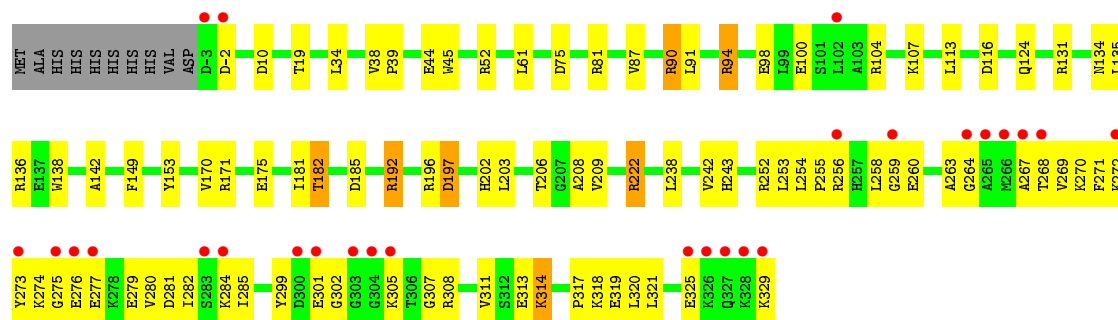
#### • Molecule 1: MoeN5,DNA-binding protein 7d



#### • Molecule 1: MoeN5,DNA-binding protein 7d







## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	137.53Å 218.39Å 104.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.26 24.99 – 2.26	Depositor EDS
% Data completeness (in resolution range)	97.0 (25.00-2.26) 96.9 (24.99-2.26)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.81 (at 2.26Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.183 , 0.229 0.183 , 0.229	Depositor DCC
$R_{free}$ test set	3624 reflections (5.07%)	DCC
Wilson B-factor (Å <sup>2</sup> )	40.9	Xtriage
Anisotropy	0.394	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 44.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 71469 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	9876	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.56% 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: BOG

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	0.81	0/2058	0.91	3/2797 (0.1%)
1	B	0.77	1/2572 (0.0%)	0.87	0/3478
1	C	0.86	3/2030 (0.1%)	0.93	3/2759 (0.1%)
1	D	0.74	0/2582	0.85	4/3489 (0.1%)
All	All	0.79	4/9242 (0.0%)	0.89	10/12523 (0.1%)

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	D	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	83	GLU	CB-CG	-5.58	1.41	1.52
1	C	219	GLU	CG-CD	5.45	1.60	1.51
1	B	15	CYS	CB-SG	-5.21	1.73	1.81
1	C	15	CYS	CB-SG	-5.14	1.73	1.81

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	94	ARG	NE-CZ-NH2	-8.14	116.23	120.30
1	D	52	ARG	NE-CZ-NH1	-8.09	116.26	120.30
1	C	94	ARG	NE-CZ-NH1	7.93	124.26	120.30
1	A	94	ARG	NE-CZ-NH1	7.55	124.08	120.30
1	A	37	ARG	NE-CZ-NH2	7.13	123.86	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	94	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	D	-2	ASP	N-CA-C	-5.36	96.53	111.00
1	D	222	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	C	145	TYR	N-CA-C	-5.09	97.26	111.00
1	A	171	ARG	NE-CZ-NH2	-5.01	117.79	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	153	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	2026	0	2005	51	0
1	B	2533	0	2532	67	0
1	C	1998	0	1983	61	0
1	D	2543	0	2554	80	0
2	A	40	0	56	5	0
2	B	20	0	28	1	0
2	C	20	0	28	5	0
2	D	20	0	28	4	0
3	A	164	0	0	4	0
3	B	187	0	0	5	0
3	C	157	0	0	9	0
3	D	168	0	0	4	0
All	All	9876	0	9214	259	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 14.

All (259) 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:1:MET:CE	1:B:1:MET:SD	2.05	1.43
2:D:401:BOG:H2	3:D:583:HOH:O	1.62	0.98
1:D:131:ARG:HG2	1:D:131:ARG:HH11	1.30	0.96
2:D:401:BOG:H4	3:D:524:HOH:O	1.66	0.94
1:D:325:GLU:HB2	1:D:329:LYS:HD2	1.52	0.90
1:D:192:ARG:HH11	1:D:192:ARG:HG2	1.39	0.87
1:C:219:GLU:OE1	1:C:222:ARG:NE	2.08	0.86
1:B:318:LYS:HG3	1:B:319:GLU:OE2	1.77	0.84
1:D:282:ILE:HA	1:D:285:ILE:HD13	1.59	0.83
1:C:145:TYR:CE1	2:C:401:BOG:H61	2.14	0.83
1:A:150:LEU:HD13	2:A:501:BOG:H8'1	1.62	0.81
1:A:193:ASN:HB3	1:A:195:GLU:HG3	1.62	0.81
1:D:192:ARG:CG	1:D:192:ARG:HH11	1.94	0.79
1:C:136:ARG:NH1	1:C:136:ARG:HB3	1.98	0.78
1:B:1:MET:HG2	1:B:37:ARG:HD3	1.65	0.78
1:B:179:MET:HE3	1:B:221:LEU:HD21	1.67	0.77
1:D:131:ARG:NH1	1:D:131:ARG:HG2	2.00	0.76
1:D:222:ARG:HH11	1:D:243:HIS:HD2	1.34	0.76
1:B:22:SER:O	1:B:26:VAL:HG23	1.85	0.76
1:B:222:ARG:HH11	1:B:243:HIS:HD2	1.34	0.74
1:A:200:LEU:HG	1:A:204:MET:CE	2.17	0.74
1:A:38:VAL:HG12	1:A:39:PRO:HD3	1.69	0.73
1:A:94:ARG:HD2	1:A:98:GLU:OE2	1.87	0.73
1:B:124:GLN:HE21	1:B:124:GLN:HA	1.54	0.72
1:D:301:GLU:HG3	1:D:305:LYS:HB3	1.72	0.71
1:A:195:GLU:C	1:A:196:ARG:HH11	1.95	0.70
1:C:131:ARG:HH11	1:C:131:ARG:HG2	1.57	0.70
1:C:124:GLN:NE2	2:C:401:BOG:H5'2	2.07	0.70
1:C:139:ARG:HG3	1:C:179:MET:HE3	1.74	0.69
1:D:203:LEU:HA	1:D:206:THR:HG22	1.74	0.69
1:D:142:ALA:HB1	1:D:182:THR:HG21	1.73	0.69
1:B:22:SER:OG	1:B:24:ASP:HB2	1.93	0.69
1:C:179:MET:HE2	1:C:217:LEU:HD11	1.75	0.69
1:C:22:SER:N	1:C:83:GLU:OE1	2.26	0.69
1:D:94:ARG:HD2	1:D:98:GLU:OE2	1.93	0.69
1:C:187:LEU:HD21	1:C:204:MET:HE3	1.75	0.68
1:A:131:ARG:HG3	1:A:197:ASP:HB3	1.75	0.68
1:D:252:ARG:O	1:D:255:PRO:HD2	1.93	0.67
1:A:192:ARG:HA	1:A:192:ARG:NE	2.09	0.67
1:B:131:ARG:HG3	1:B:197:ASP:HB3	1.77	0.66
1:A:61:LEU:HD13	1:A:94:ARG:HG3	1.77	0.66
1:B:179:MET:CE	1:B:221:LEU:HD21	2.24	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:273:TYR:CE2	1:B:274:LYS:HD2	2.30	0.66
1:D:203:LEU:HA	1:D:206:THR:CG2	2.26	0.65
1:B:301:GLU:OE2	1:B:305:LYS:HE3	1.98	0.64
1:D:135:LEU:HB2	1:D:209:VAL:HG22	1.80	0.63
1:A:131:ARG:HG3	1:A:197:ASP:CB	2.29	0.63
1:D:124:GLN:HG2	2:D:401:BOG:H7'1	1.81	0.63
1:C:200:LEU:HG	1:C:204:MET:HE2	1.80	0.63
1:D:267:ALA:HB1	1:D:282:ILE:HG13	1.81	0.62
1:A:104:ARG:HD2	3:A:688:HOH:O	1.99	0.62
1:C:140:ALA:O	1:C:144:THR:HG23	2.00	0.62
1:A:195:GLU:O	1:A:196:ARG:NH1	2.29	0.61
1:D:280:VAL:HG21	1:D:299:TYR:CZ	2.36	0.61
1:D:134:ASN:HD21	1:D:136:ARG:NH2	1.98	0.60
1:B:323:MET:O	1:B:327:GLN:HB2	2.01	0.60
1:A:189:ASP:O	1:A:193:ASN:HB2	2.02	0.60
1:C:218:LEU:HD11	1:C:249:VAL:HG11	1.83	0.60
1:B:179:MET:HG2	1:B:221:LEU:HD11	1.84	0.60
1:C:94:ARG:HD2	1:C:98:GLU:OE2	2.00	0.60
1:A:38:VAL:CG1	1:A:39:PRO:HD3	2.33	0.59
1:D:149:PHE:CD1	2:D:401:BOG:H2'2	2.38	0.58
1:D:138:TRP:HH2	1:D:182:THR:HG22	1.69	0.58
1:D:238:LEU:O	1:D:242:VAL:HG23	2.04	0.58
1:D:34:LEU:HD21	1:D:181:ILE:HG21	1.84	0.58
1:D:61:LEU:HD13	1:D:94:ARG:HG3	1.86	0.58
1:D:313:GLU:HG2	1:D:314:LYS:N	2.19	0.58
1:D:269:VAL:HG22	1:D:317:PRO:HG3	1.86	0.57
1:D:192:ARG:NH1	1:D:192:ARG:HB3	2.19	0.57
1:D:203:LEU:CA	1:D:206:THR:HG22	2.34	0.57
1:D:259:GLY:C	1:D:260:GLU:HG2	2.26	0.56
1:B:243:HIS:HE1	3:B:626:HOH:O	1.88	0.56
1:C:187:LEU:HD21	1:C:204:MET:CE	2.36	0.56
1:B:287:LYS:HG3	1:B:288:VAL:N	2.20	0.56
1:C:139:ARG:HG3	1:C:179:MET:CE	2.34	0.55
1:D:272:LYS:HA	1:D:276:GLU:O	2.07	0.55
1:B:301:GLU:HB3	1:B:305:LYS:HD3	1.89	0.55
1:A:90:ARG:HD3	1:A:90:ARG:C	2.27	0.55
1:B:200:LEU:HG	1:B:204:MET:HE2	1.89	0.55
1:B:266:MET:HE3	1:B:266:MET:HA	1.88	0.55
1:C:81:ARG:HD3	1:D:81:ARG:NH2	2.21	0.55
1:B:267:ALA:O	1:B:282:ILE:HG12	2.07	0.54
1:C:61:LEU:HD13	1:C:94:ARG:HB3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:584:HOH:O	1:D:107:LYS:HD3	2.06	0.54
1:C:81:ARG:NH2	3:C:501:HOH:O	2.40	0.54
1:C:136:ARG:CZ	1:C:136:ARG:HB3	2.37	0.54
1:C:10:ASP:CG	1:C:14:ARG:HH22	2.11	0.54
1:A:107:LYS:HD3	1:A:107:LYS:O	2.08	0.54
1:A:200:LEU:HG	1:A:204:MET:HE2	1.90	0.54
1:B:19:THR:O	1:B:19:THR:HG22	2.07	0.53
1:C:11:HIS:CD2	1:C:57:ARG:HD2	2.43	0.53
1:A:182:THR:HG23	2:A:502:BOG:O6	2.09	0.53
1:C:74:ASP:OD1	1:C:128:LYS:NZ	2.41	0.53
1:A:192:ARG:HG3	3:C:617:HOH:O	2.09	0.53
1:D:268:THR:HG22	1:D:281:ASP:HA	1.90	0.53
1:C:218:LEU:HD11	1:C:249:VAL:CG1	2.39	0.53
1:B:284:LYS:HE3	1:B:284:LYS:HA	1.91	0.52
1:C:147:SER:O	1:C:175:GLU:HG2	2.08	0.52
1:D:325:GLU:O	1:D:329:LYS:HB3	2.09	0.52
1:A:259:GLY:O	1:D:131:ARG:NH2	2.41	0.52
1:D:192:ARG:HH11	1:D:192:ARG:CB	2.21	0.52
1:B:266:MET:HE2	1:B:267:ALA:N	2.25	0.52
1:C:219:GLU:CD	1:C:222:ARG:HH21	2.13	0.52
1:A:187:LEU:HD21	1:A:204:MET:CE	2.40	0.52
1:A:61:LEU:CD1	1:A:94:ARG:HG3	2.40	0.52
1:B:321:LEU:O	1:B:324:LEU:HB2	2.10	0.51
1:A:139:ARG:HD3	1:A:179:MET:HE1	1.91	0.51
1:C:179:MET:HG2	1:C:221:LEU:HD11	1.93	0.51
1:B:270:LYS:HE2	1:B:279:GLU:OE2	2.10	0.51
1:D:259:GLY:O	1:D:260:GLU:HG2	2.11	0.51
1:B:266:MET:CE	1:B:267:ALA:H	2.23	0.51
1:C:38:VAL:N	1:C:39:PRO:CD	2.74	0.51
1:D:269:VAL:HG22	1:D:317:PRO:CG	2.40	0.50
1:B:286:LYS:HE2	1:B:299:TYR:O	2.10	0.50
1:C:164:GLY:N	3:C:503:HOH:O	2.44	0.50
1:B:266:MET:CE	1:B:267:ALA:N	2.74	0.50
1:C:19:THR:O	1:C:19:THR:HG22	2.11	0.50
1:D:192:ARG:HH11	1:D:192:ARG:HB3	1.76	0.50
1:C:145:TYR:HE1	2:C:401:BOG:H61	1.72	0.50
1:A:200:LEU:HG	1:A:204:MET:HE1	1.93	0.50
1:B:115:GLN:HG2	3:B:643:HOH:O	2.10	0.50
1:B:301:GLU:CD	1:B:305:LYS:HE3	2.31	0.50
1:D:90:ARG:HD3	1:D:90:ARG:C	2.32	0.50
1:C:11:HIS:CG	1:C:57:ARG:HD2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:131:ARG:NH1	1:C:131:ARG:HG2	2.25	0.49
1:A:131:ARG:CG	1:A:197:ASP:HB3	2.43	0.49
1:D:202:HIS:O	1:D:206:THR:HG22	2.12	0.49
1:B:90:ARG:C	1:B:90:ARG:HD3	2.33	0.49
1:A:179:MET:HE2	1:A:221:LEU:HD21	1.94	0.49
1:B:318:LYS:O	1:B:322:GLN:HG3	2.12	0.48
1:D:280:VAL:HG21	1:D:299:TYR:CE1	2.48	0.48
1:B:266:MET:HE3	1:B:267:ALA:H	1.78	0.48
1:B:139:ARG:NH1	3:B:503:HOH:O	2.34	0.48
1:D:269:VAL:HG21	1:D:320:LEU:HD22	1.96	0.48
1:C:219:GLU:HG3	3:C:515:HOH:O	2.14	0.48
2:C:401:BOG:O2	2:C:401:BOG:H1'2	2.14	0.48
1:A:260:GLU:HG3	1:D:131:ARG:HH21	1.78	0.48
1:B:171:ARG:O	1:B:175:GLU:HG3	2.14	0.47
1:B:293:LYS:HG2	1:B:313:GLU:OE2	2.14	0.47
1:D:301:GLU:CG	1:D:305:LYS:HB3	2.42	0.47
1:D:192:ARG:CG	1:D:192:ARG:NH1	2.64	0.47
1:B:202:HIS:O	1:B:206:THR:HB	2.15	0.47
1:D:45:TRP:CE3	1:D:170:VAL:HG22	2.49	0.47
1:D:267:ALA:HB1	1:D:282:ILE:CG1	2.44	0.47
1:C:232:PRO:HA	1:C:233:PRO:C	2.34	0.47
1:D:192:ARG:NH1	1:D:192:ARG:HG2	2.17	0.47
1:D:196:ARG:O	1:D:197:ASP:C	2.53	0.47
1:D:267:ALA:HA	1:D:319:GLU:OE1	2.15	0.47
1:D:87:VAL:O	1:D:91:LEU:HG	2.14	0.47
1:C:83:GLU:HG3	3:C:565:HOH:O	2.13	0.47
1:A:134:ASN:OD1	1:A:137:GLU:HG3	2.15	0.47
1:C:187:LEU:CD2	1:C:204:MET:HE3	2.43	0.47
1:A:150:LEU:HD13	2:A:501:BOG:C8'	2.42	0.46
1:B:183:MET:HE1	1:B:218:LEU:HG	1.97	0.46
1:B:287:LYS:HG3	1:B:288:VAL:H	1.79	0.46
1:B:107:LYS:NZ	3:B:508:HOH:O	2.49	0.46
1:A:192:ARG:HD2	3:C:532:HOH:O	2.15	0.46
1:D:254:LEU:CD1	1:D:258:LEU:HD13	2.45	0.46
1:B:254:LEU:HB2	1:B:255:PRO:HD3	1.98	0.46
1:D:271:PHE:HB3	1:D:311:VAL:CG1	2.44	0.46
1:A:181:ILE:HD11	2:A:501:BOG:H8'3	1.98	0.46
1:B:67:LYS:NZ	2:B:401:BOG:O2	2.50	0.45
1:B:287:LYS:HG2	1:B:289:TRP:CE3	2.51	0.45
1:C:1:MET:HE2	3:C:589:HOH:O	2.16	0.45
1:D:318:LYS:HA	1:D:321:LEU:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:75:ASP:HB2	1:D:81:ARG:NH1	2.32	0.45
1:A:131:ARG:HB3	1:A:198:GLY:N	2.31	0.45
1:D:270:LYS:HG3	1:D:279:GLU:HG3	1.98	0.45
1:A:75:ASP:CG	1:A:81:ARG:NH1	2.71	0.45
1:C:143:SER:O	1:C:147:SER:HB2	2.17	0.44
1:D:10:ASP:HB2	3:D:594:HOH:O	2.17	0.44
1:D:45:TRP:CD2	1:D:170:VAL:HG22	2.52	0.44
1:A:192:ARG:HA	1:A:192:ARG:CZ	2.47	0.44
1:A:187:LEU:HD21	1:A:204:MET:HE3	1.99	0.44
1:D:277:GLU:OE1	1:D:277:GLU:HA	2.18	0.44
1:A:244:LEU:HD12	3:A:651:HOH:O	2.18	0.44
1:A:196:ARG:HD2	1:A:202:HIS:ND1	2.33	0.44
1:D:281:ASP:O	1:D:284:LYS:HB2	2.17	0.44
1:B:1:MET:CG	1:B:37:ARG:HD3	2.43	0.44
1:D:252:ARG:NH1	1:D:253:LEU:HD21	2.33	0.44
1:B:187:LEU:HD21	1:B:204:MET:CE	2.48	0.43
1:D:171:ARG:O	1:D:175:GLU:HG3	2.17	0.43
1:D:192:ARG:NH1	1:D:192:ARG:CB	2.80	0.43
1:D:307:GLY:C	1:D:308:ARG:HG3	2.37	0.43
1:C:165:GLN:HA	1:C:166:PRO:HD2	1.87	0.43
1:C:232:PRO:HA	1:C:234:GLY:N	2.32	0.43
1:C:252:ARG:NH1	1:C:253:LEU:HD21	2.32	0.43
1:B:187:LEU:HD21	1:B:204:MET:HE1	1.99	0.43
2:C:401:BOG:H2'2	2:C:401:BOG:H5'1	1.59	0.43
1:C:90:ARG:HD3	1:C:90:ARG:C	2.39	0.43
1:A:179:MET:CE	1:A:221:LEU:HD21	2.49	0.43
1:B:237:GLY:O	1:B:240:PRO:HD2	2.18	0.43
1:D:138:TRP:CH2	1:D:182:THR:HG22	2.50	0.43
1:A:131:ARG:HH11	1:A:131:ARG:HG2	1.83	0.43
1:A:165:GLN:HA	1:A:166:PRO:HD2	1.90	0.43
1:B:269:VAL:HG21	1:B:320:LEU:HD22	2.01	0.43
1:C:93:LEU:HD22	1:D:113:LEU:HB3	2.01	0.43
1:D:38:VAL:N	1:D:39:PRO:CD	2.82	0.43
1:B:194:GLY:C	1:B:196:ARG:NH1	2.72	0.42
1:C:44:GLU:HG2	1:C:238:LEU:HG	2.01	0.42
1:B:32:LEU:O	1:B:36:LEU:HD12	2.18	0.42
1:C:222:ARG:NH1	1:C:243:HIS:HD2	2.17	0.42
1:B:131:ARG:HA	1:B:131:ARG:HD2	1.72	0.42
1:C:136:ARG:HH11	1:C:136:ARG:HB3	1.77	0.42
1:C:131:ARG:HD2	1:C:197:ASP:OD1	2.19	0.42
1:B:322:GLN:HA	1:B:325:GLU:OE2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:206:THR:HG23	1:D:208:ALA:H	1.85	0.42
1:A:165:GLN:H	1:A:165:GLN:HG2	1.77	0.42
1:C:187:LEU:HD23	1:C:201:ALA:HB2	2.01	0.42
1:C:166:PRO:HD3	1:C:233:PRO:HD2	2.00	0.42
1:D:276:GLU:OE1	1:D:276:GLU:HA	2.19	0.42
1:A:116:ASP:N	1:A:116:ASP:OD1	2.51	0.42
1:A:75:ASP:CG	1:A:81:ARG:HH11	2.23	0.42
1:B:258:LEU:HB3	1:B:262:GLY:HA3	2.01	0.42
1:C:179:MET:CE	1:C:217:LEU:HD11	2.47	0.42
1:D:273:TYR:O	1:D:274:LYS:C	2.57	0.42
1:A:187:LEU:HD21	1:A:204:MET:HE1	2.01	0.42
1:C:203:LEU:HB3	1:C:209:VAL:HG23	2.01	0.42
1:A:187:LEU:CD2	1:A:204:MET:HE3	2.50	0.42
1:D:61:LEU:CD1	1:D:94:ARG:HG3	2.49	0.42
1:C:5:GLU:OE2	1:C:33:ARG:HG2	2.18	0.42
1:C:100:GLU:OE1	1:D:100:GLU:OE1	2.37	0.42
1:D:269:VAL:O	1:D:279:GLU:HA	2.20	0.41
2:A:502:BOG:H2'2	2:A:502:BOG:H5'1	1.80	0.41
1:A:76:ASP:OD1	1:A:76:ASP:N	2.53	0.41
1:B:124:GLN:NE2	1:B:145:TYR:HB3	2.35	0.41
1:B:34:LEU:HD21	1:B:181:ILE:HD12	2.02	0.41
1:B:78:GLY:N	3:B:501:HOH:O	2.21	0.41
1:A:81:ARG:HD2	3:A:713:HOH:O	2.19	0.41
1:C:24:ASP:HB2	3:C:554:HOH:O	2.20	0.41
1:C:251:VAL:HG13	1:C:252:ARG:N	2.36	0.41
1:D:256:ARG:HE	1:D:256:ARG:HB2	1.59	0.41
1:C:1:MET:C	1:C:1:MET:SD	2.98	0.41
1:C:12:VAL:HG12	1:C:29:THR:HG21	2.02	0.41
1:A:201:ALA:HB1	1:A:257:HIS:CE1	2.56	0.41
1:B:194:GLY:C	1:B:196:ARG:HH12	2.24	0.41
1:B:83:GLU:O	1:B:87:VAL:HG23	2.21	0.41
1:B:65:SER:HB2	1:B:91:LEU:HB2	2.01	0.41
1:C:136:ARG:HH11	1:C:136:ARG:CB	2.33	0.41
1:B:295:ILE:O	1:B:310:ALA:HA	2.21	0.41
1:B:319:GLU:CD	1:B:319:GLU:H	2.23	0.41
1:B:68:LEU:HD23	1:B:68:LEU:HA	1.89	0.41
1:D:116:ASP:HA	3:D:584:HOH:O	2.21	0.41
1:D:44:GLU:HG2	1:D:238:LEU:HG	2.03	0.41
1:B:18:GLN:HE21	1:B:18:GLN:HB2	1.65	0.41
1:B:269:VAL:O	1:B:279:GLU:HA	2.21	0.41
1:A:150:LEU:HD12	1:A:150:LEU:HA	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:254:LEU:N	1:C:255:PRO:CD	2.84	0.41
1:A:11:HIS:CE1	1:A:57:ARG:CZ	3.03	0.41
1:B:38:VAL:N	1:B:39:PRO:CD	2.84	0.40
1:B:45:TRP:CE2	1:B:235:ALA:HB2	2.56	0.40
1:C:138:TRP:CZ2	1:C:182:THR:HG22	2.56	0.40
1:D:203:LEU:C	1:D:206:THR:HG22	2.41	0.40
1:D:273:TYR:C	1:D:275:GLY:N	2.74	0.40
1:B:273:TYR:O	1:B:274:LYS:HB2	2.21	0.40
1:D:254:LEU:N	1:D:255:PRO:CD	2.84	0.40
1:A:33:ARG:HD3	3:A:627:HOH:O	2.21	0.40
1:C:45:TRP:CE2	1:C:235:ALA:HB2	2.56	0.40
1:D:252:ARG:CZ	1:D:253:LEU:HD21	2.52	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	264/343 (77%)	248 (94%)	13 (5%)	3 (1%)	17	13
1	B	330/343 (96%)	307 (93%)	21 (6%)	2 (1%)	30	30
1	C	260/343 (76%)	251 (96%)	6 (2%)	3 (1%)	16	11
1	D	331/343 (96%)	307 (93%)	20 (6%)	4 (1%)	16	11
All	All	1185/1372 (86%)	1113 (94%)	60 (5%)	12 (1%)	19	16

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	263	ALA
1	C	165	GLN
1	D	263	ALA

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Mol	Chain	Res	Type
1	D	264	GLY
1	A	165	GLN
1	A	259	GLY
1	C	146	GLY
1	A	193	ASN
1	D	197	ASP
1	C	145	TYR
1	D	302	GLY
1	B	234	GLY

### 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	209/270 (77%)	196 (94%)	13 (6%)	23	22
1	B	260/270 (96%)	245 (94%)	15 (6%)	25	25
1	C	206/270 (76%)	195 (95%)	11 (5%)	28	30
1	D	261/270 (97%)	254 (97%)	7 (3%)	52	63
All	All	936/1080 (87%)	890 (95%)	46 (5%)	31	34

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-5	VAL
1	A	18	GLN
1	A	47	THR
1	A	90	ARG
1	A	107	LYS
1	A	115	GLN
1	A	139	ARG
1	A	163	GLU
1	A	189	ASP
1	A	191	ASP
1	A	192	ARG
1	A	197	ASP

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Mol	Chain	Res	Type
1	A	258	LEU
1	B	-4	ASP
1	B	-3	ASP
1	B	18	GLN
1	B	24	ASP
1	B	90	ARG
1	B	124	GLN
1	B	131	ARG
1	B	185	ASP
1	B	186	ASP
1	B	193	ASN
1	B	197	ASP
1	B	206	THR
1	B	284	LYS
1	B	293	LYS
1	B	325	GLU
1	C	24	ASP
1	C	52	ARG
1	C	90	ARG
1	C	94	ARG
1	C	107	LYS
1	C	115	GLN
1	C	144	THR
1	C	165	GLN
1	C	185	ASP
1	C	197	ASP
1	C	254	LEU
1	D	19	THR
1	D	90	ARG
1	D	104	ARG
1	D	182	THR
1	D	185	ASP
1	D	192	ARG
1	D	314	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	119	HIS
1	B	18	GLN
1	B	124	GLN
1	B	243	HIS

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Mol	Chain	Res	Type
1	C	115	GLN
1	C	124	GLN
1	C	243	HIS
1	D	243	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](#)

5 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	BOG	A	501	-	20,20,20	1.05	1 (5%)	25,25,25	0.70	0
2	BOG	A	502	-	20,20,20	0.85	1 (5%)	25,25,25	0.96	1 (4%)
2	BOG	B	401	-	20,20,20	0.94	1 (5%)	25,25,25	1.03	1 (4%)
2	BOG	C	401	-	20,20,20	0.92	1 (5%)	25,25,25	0.68	0
2	BOG	D	401	-	20,20,20	0.96	1 (5%)	25,25,25	0.78	1 (4%)

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	BOG	A	501	-	-	0/11/31/31	0/1/1/1
2	BOG	A	502	-	-	0/11/31/31	0/1/1/1
2	BOG	B	401	-	-	0/11/31/31	0/1/1/1
2	BOG	C	401	-	-	0/11/31/31	0/1/1/1
2	BOG	D	401	-	-	0/11/31/31	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	502	BOG	O1-C1'	3.20	1.51	1.42
2	C	401	BOG	O1-C1'	3.48	1.52	1.42
2	B	401	BOG	O1-C1'	3.69	1.53	1.42
2	D	401	BOG	O1-C1'	3.70	1.53	1.42
2	A	501	BOG	O1-C1'	3.75	1.53	1.42

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	BOG	C1'-O1-C1	-2.81	109.08	114.00
2	A	502	BOG	C1'-O1-C1	-2.48	109.67	114.00
2	D	401	BOG	C1-C2-C3	2.19	114.32	109.98

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	BOG	3	0
2	A	502	BOG	2	0
2	B	401	BOG	1	0
2	C	401	BOG	5	0
2	D	401	BOG	4	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	266/343 (77%)	-0.14	15 (5%)	28 31	32, 43, 73, 103	0
1	B	332/343 (96%)	-0.02	24 (7%)	18 20	32, 47, 92, 100	0
1	C	262/343 (76%)	-0.32	3 (1%)	82 84	29, 44, 61, 85	0
1	D	333/343 (97%)	0.08	27 (8%)	15 16	30, 47, 116, 134	0
All	All	1193/1372 (86%)	-0.09	69 (5%)	26 29	29, 45, 94, 134	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	266	MET	8.0
1	D	264	GLY	6.5
1	D	265	ALA	5.9
1	D	305	LYS	5.6
1	B	261	ALA	5.3
1	B	194	GLY	5.3
1	D	267	ALA	5.1
1	B	264	GLY	5.0
1	A	193	ASN	5.0
1	D	259	GLY	4.9
1	D	329	LYS	4.8
1	D	268	THR	4.6
1	D	325	GLU	4.5
1	D	303	GLY	4.4
1	D	328	LYS	4.3
1	D	275	GLY	4.3
1	B	325	GLU	3.9
1	B	304	GLY	3.9
1	D	276	GLU	3.8
1	B	262	GLY	3.7
1	D	284	LYS	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	327	GLN	3.6
1	A	197	ASP	3.6
1	D	326	LYS	3.6
1	D	300	ASP	3.6
1	B	326	LYS	3.5
1	A	195	GLU	3.5
1	D	304	GLY	3.4
1	B	263	ALA	3.3
1	B	195	GLU	3.1
1	A	190	TYR	3.1
1	B	305	LYS	3.0
1	B	303	GLY	2.9
1	D	327	GLN	2.9
1	D	102	LEU	2.9
1	B	302	GLY	2.9
1	C	-3	ASP	2.8
1	D	256	ARG	2.8
1	C	256	ARG	2.8
1	A	259	GLY	2.7
1	D	283	SER	2.7
1	D	301	GLU	2.7
1	B	310	ALA	2.7
1	B	197	ASP	2.6
1	A	163	GLU	2.6
1	A	196	ARG	2.6
1	B	276	GLU	2.5
1	D	-3	ASP	2.5
1	D	277	GLU	2.4
1	D	272	LYS	2.4
1	B	275	GLY	2.4
1	B	193	ASN	2.4
1	A	191	ASP	2.4
1	B	309	GLY	2.4
1	A	194	GLY	2.3
1	B	192	ARG	2.3
1	A	88	CYS	2.2
1	B	190	TYR	2.2
1	D	273	TYR	2.2
1	B	-4	ASP	2.2
1	A	89	LEU	2.2
1	A	260	GLU	2.1
1	D	-2	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	189	ASP	2.1
1	B	266	MET	2.1
1	A	91	LEU	2.0
1	B	265	ALA	2.0
1	A	180	THR	2.0
1	C	136	ARG	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, 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	BOG	C	401	20/20	0.75	0.29	4.09	81,108,113,113	0
2	BOG	A	501	20/20	0.73	0.31	2.75	88,95,98,98	0
2	BOG	D	401	20/20	0.84	0.18	1.98	61,90,95,96	0
2	BOG	B	401	20/20	0.84	0.20	1.38	73,93,95,95	0
2	BOG	A	502	20/20	0.87	0.20	1.04	67,94,100,102	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.