



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 11:42 pm BST

PDB ID : 6FNY  
Title : CRYSTAL STRUCTURE OF A CHOLINE SULFATASE FROM SINORHIZOBIUM MELLILOTI  
Authors : Valkov, E.; Van Loo, B.; Hollfelder, F.; Hyvonen, M.  
Deposited on : 2018-02-05  
Resolution : 2.79 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

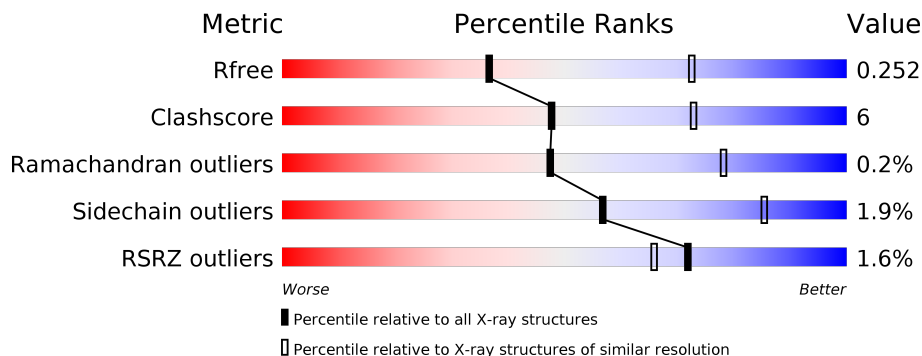
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.79 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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	516	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 85%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 14%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 1%; height: 10px; background-color: grey; margin-right: 2px;"></div> </div> <p style="margin-left: 20px;">85% 14% .</p>
1	B	516	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 84%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 16%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 1%; height: 10px; background-color: grey; margin-right: 2px;"></div> </div> <p style="margin-left: 20px;">84% 16% .</p>
1	C	516	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 86%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 13%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 1%; height: 10px; background-color: grey; margin-right: 2px;"></div> </div> <p style="margin-left: 20px;">86% 13% .</p>
1	D	516	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 82%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 16%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 1%; height: 10px; background-color: grey; margin-right: 2px;"></div> </div> <p style="margin-left: 20px;">82% 16% ..</p>
1	E	516	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 83%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 15%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 1%; height: 10px; background-color: grey; margin-right: 2px;"></div> </div> <p style="margin-left: 20px;">83% 15% ..</p>
1	F	516	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 81%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 18%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 1%; height: 10px; background-color: grey; margin-right: 2px;"></div> </div> <p style="margin-left: 20px;">81% 18% .</p>

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Mol	Chain	Length	Quality of chain
1	G	516	<p>%</p> <p>86% 13% .</p>
1	H	516	<p>%</p> <p>84% 14% ..</p>

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	CA	E	601	-	-	-	X

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 34715 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 Choline-sulfatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	515	4148	2619	723	785	21	0	1	0
1	B	515	4148	2619	723	785	21	0	1	0
1	C	513	4136	2613	721	781	21	0	1	0
1	D	510	4115	2599	718	777	21	0	1	0
1	E	510	4115	2599	718	777	21	0	1	0
1	F	509	4108	2595	717	775	21	0	1	0
1	G	509	4108	2595	717	775	21	0	1	0
1	H	510	4116	2601	718	776	21	0	1	0

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP O69787
A	-1	ASP	-	expression tag	UNP O69787
A	0	PRO	-	expression tag	UNP O69787
A	1	VAL	-	expression tag	UNP O69787
B	-2	GLY	-	expression tag	UNP O69787
B	-1	ASP	-	expression tag	UNP O69787
B	0	PRO	-	expression tag	UNP O69787
B	1	VAL	-	expression tag	UNP O69787
C	-2	GLY	-	expression tag	UNP O69787
C	-1	ASP	-	expression tag	UNP O69787
C	0	PRO	-	expression tag	UNP O69787
C	1	VAL	-	expression tag	UNP O69787
D	-2	GLY	-	expression tag	UNP O69787

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-1	ASP	-	expression tag	UNP O69787
D	0	PRO	-	expression tag	UNP O69787
D	1	VAL	-	expression tag	UNP O69787
E	-2	GLY	-	expression tag	UNP O69787
E	-1	ASP	-	expression tag	UNP O69787
E	0	PRO	-	expression tag	UNP O69787
E	1	VAL	-	expression tag	UNP O69787
F	-2	GLY	-	expression tag	UNP O69787
F	-1	ASP	-	expression tag	UNP O69787
F	0	PRO	-	expression tag	UNP O69787
F	1	VAL	-	expression tag	UNP O69787
G	-2	GLY	-	expression tag	UNP O69787
G	-1	ASP	-	expression tag	UNP O69787
G	0	PRO	-	expression tag	UNP O69787
G	1	VAL	-	expression tag	UNP O69787
H	-2	GLY	-	expression tag	UNP O69787
H	-1	ASP	-	expression tag	UNP O69787
H	0	PRO	-	expression tag	UNP O69787
H	1	VAL	-	expression tag	UNP O69787

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total Ca 1 1	0	0
2	D	1	Total Ca 1 1	0	0
2	E	1	Total Ca 1 1	0	0
2	H	1	Total Ca 1 1	0	0
2	B	1	Total Ca 1 1	0	0
2	C	1	Total Ca 1 1	0	0
2	A	1	Total Ca 1 1	0	0
2	F	1	Total Ca 1 1	0	0

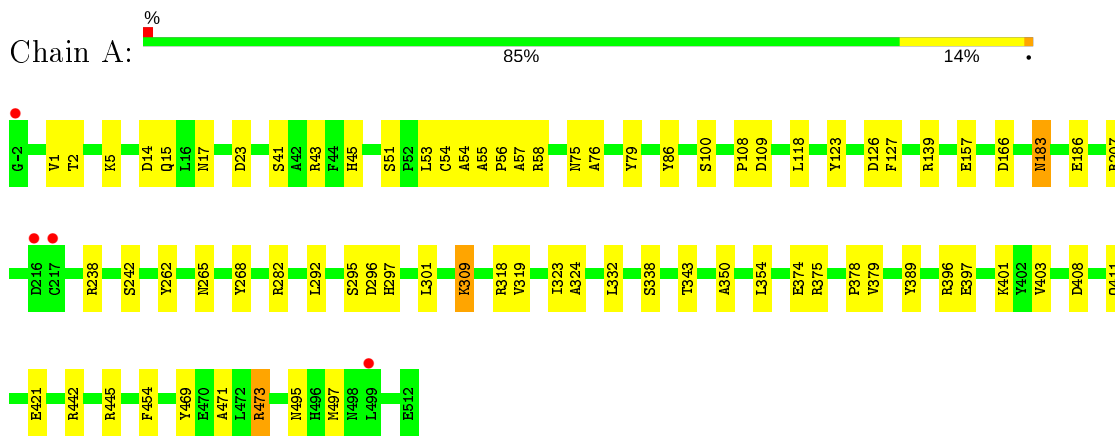
- Molecule 3 is water.

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
3	A	172	Total 172	O 172	0	0
3	B	296	Total 296	O 296	0	0
3	C	184	Total 184	O 184	0	0
3	D	218	Total 218	O 218	0	0
3	E	259	Total 259	O 259	0	0
3	F	136	Total 136	O 136	0	0
3	G	169	Total 169	O 169	0	0
3	H	279	Total 279	O 279	0	0

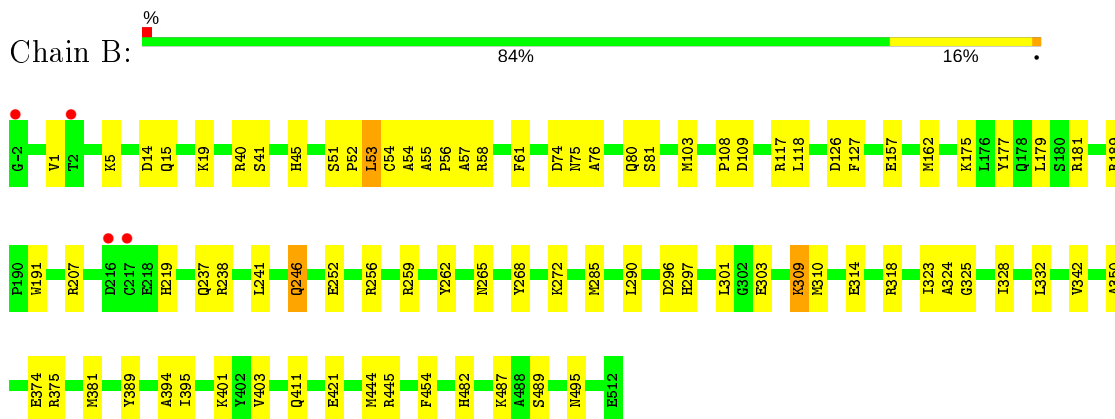
### 3 Residue-property plots [i](#)

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

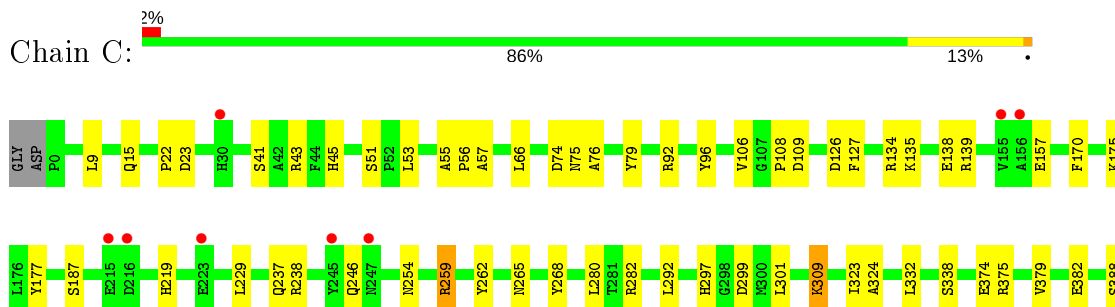
- Molecule 1: Choline-sulfatase

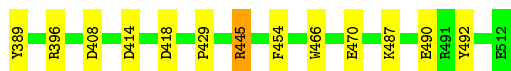


- Molecule 1: Choline-sulfatase

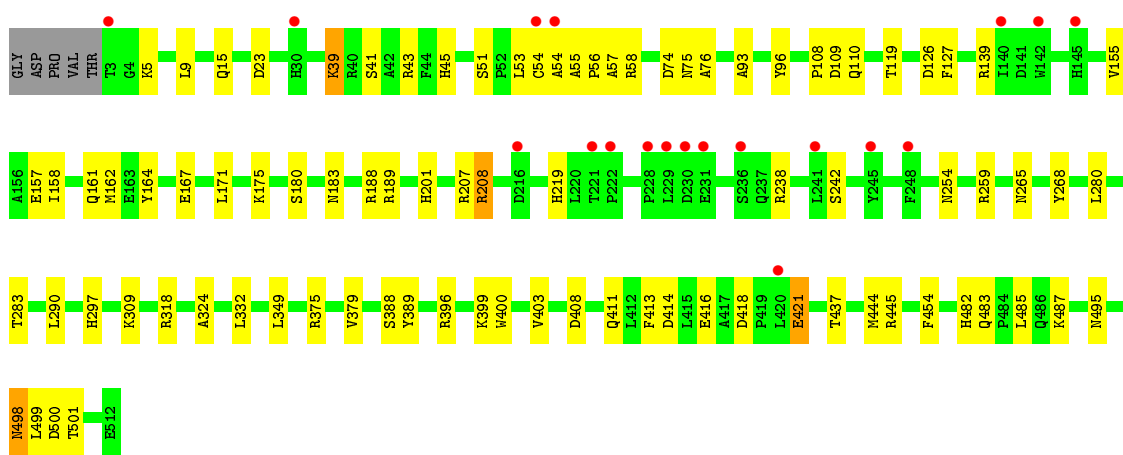
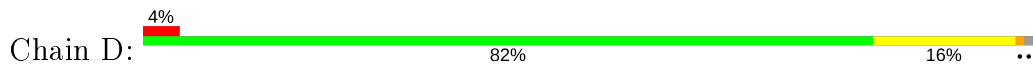


- Molecule 1: Choline-sulfatase

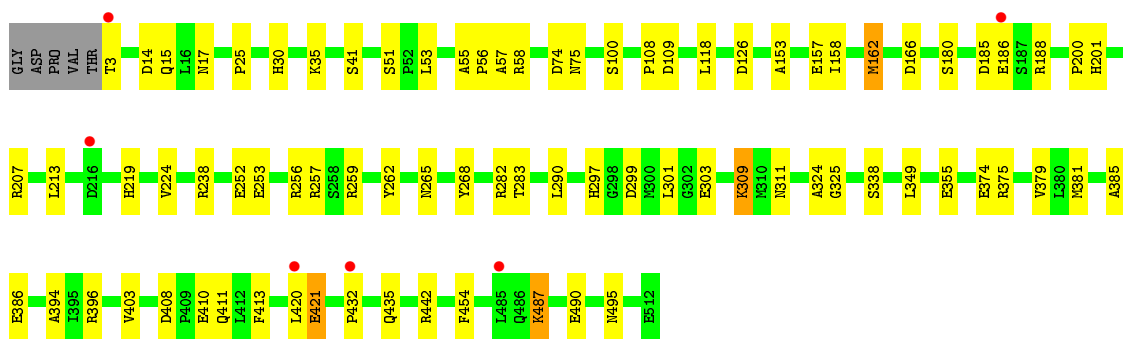
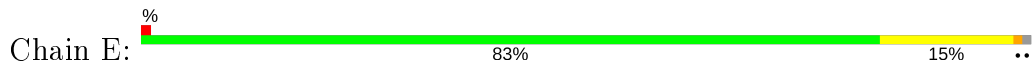




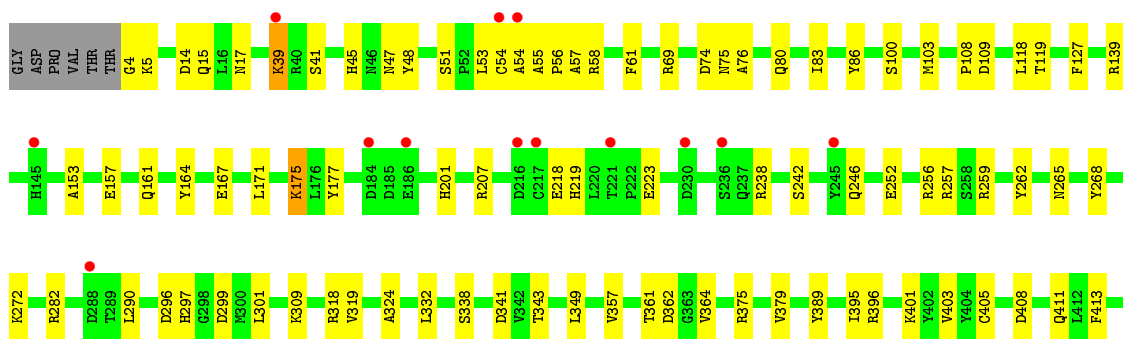
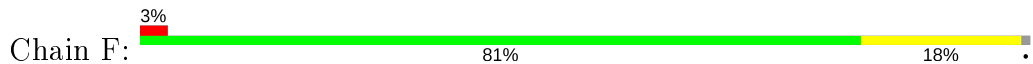
• Molecule 1: Choline-sulfatase



• Molecule 1: Choline-sulfatase



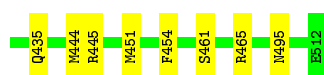
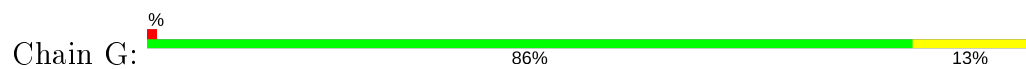
• Molecule 1: Choline-sulfatase



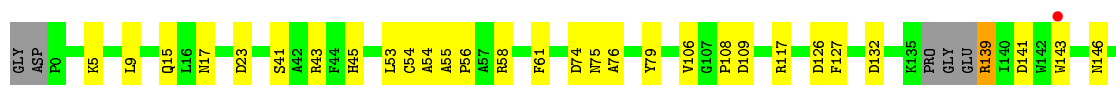
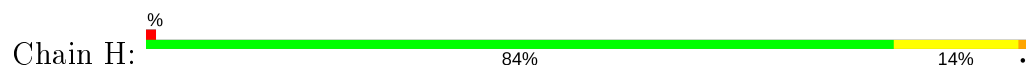




- Molecule 1: Choline-sulfatase



- Molecule 1: Choline-sulfatase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	119.56Å 163.25Å 177.62Å 90.00° 94.40° 90.00°	Depositor
Resolution (Å)	88.55 – 2.79 88.55 – 2.79	Depositor EDS
% Data completeness (in resolution range)	99.3 (88.55-2.79) 99.3 (88.55-2.79)	Depositor EDS
$R_{merge}$	0.01	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.08 (at 2.77Å)	Xtrriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, $R_{free}$	0.205 , 0.252 0.205 , 0.252	Depositor DCC
$R_{free}$ test set	8431 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.8	Xtrriage
Anisotropy	0.435	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 42.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	34715	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.16% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0/4256	0.43	0/5794
1	B	0.25	0/4256	0.43	0/5794
1	C	0.25	0/4244	0.42	0/5777
1	D	0.25	0/4222	0.43	0/5746
1	E	0.27	0/4222	0.44	0/5746
1	F	0.25	0/4215	0.42	0/5736
1	G	0.24	0/4215	0.42	0/5736
1	H	0.25	0/4222	0.43	0/5745
All	All	0.25	0/33852	0.43	0/46074

There are no bond length outliers.

There are no bond angle outliers.

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	4148	0	3952	50	0
1	B	4148	0	3951	55	0
1	C	4136	0	3947	50	0
1	D	4115	0	3920	54	0
1	E	4115	0	3921	61	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	4108	0	3912	63	0
1	G	4108	0	3911	42	0
1	H	4116	0	3928	56	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	172	0	0	3	0
3	B	296	0	0	8	0
3	C	184	0	0	4	0
3	D	218	0	0	1	0
3	E	259	0	0	4	0
3	F	136	0	0	3	0
3	G	169	0	0	2	0
3	H	279	0	0	5	0
All	All	34715	0	31442	392	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 6.

All (392) 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:E:224:VAL:HG23	1:E:420:LEU:HD22	1.45	0.99
1:D:403:VAL:HG22	1:D:411:GLN:HB2	1.56	0.85
1:E:15:GLN:HG3	1:E:297:HIS:CE1	2.13	0.82
1:B:487:LYS:HE3	1:B:489:SER:H	1.45	0.81
1:E:224:VAL:CG2	1:E:420:LEU:HD22	2.12	0.80
1:D:498:ASN:HB2	1:D:501:THR:HB	1.67	0.77
1:B:285:MET:SD	3:B:802:HOH:O	2.45	0.74
1:G:251:THR:HG22	1:G:253:GLU:H	1.51	0.74
1:B:157:GLU:O	1:B:207:ARG:NH1	2.20	0.74
1:B:445:ARG:NH1	3:B:701:HOH:O	2.21	0.73
1:D:157:GLU:HG2	1:H:282:ARG:HB3	1.71	0.71
1:C:23:ASP:OD1	1:C:43:ARG:NH1	2.24	0.70
1:H:283:THR:HG22	1:H:285:MET:HG3	1.73	0.69
1:B:15:GLN:HG3	1:B:297:HIS:HE1	1.57	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:487:LYS:HE2	1:E:490:GLU:HG3	1.74	0.69
1:D:108:PRO:HG2	1:E:108:PRO:HG2	1.73	0.69
1:A:157:GLU:O	1:A:207:ARG:NH1	2.24	0.69
1:B:109:ASP:HB2	1:H:108:PRO:HG3	1.75	0.69
1:B:15:GLN:HG3	1:B:297:HIS:CE1	2.30	0.67
1:A:15:GLN:HG2	1:A:297:HIS:HE1	1.60	0.67
1:B:41:SER:HB3	1:B:324:ALA:HB2	1.74	0.67
1:E:157:GLU:O	1:E:207:ARG:NH1	2.27	0.67
1:F:108:PRO:HG2	1:G:108:PRO:HG2	1.77	0.66
1:G:219:HIS:O	1:G:259:ARG:NH1	2.29	0.65
1:D:155:VAL:HG11	1:D:208:ARG:HG2	1.77	0.65
1:D:157:GLU:O	1:D:207:ARG:NH1	2.30	0.65
1:B:108:PRO:HG3	1:H:109:ASP:HB2	1.78	0.65
1:D:108:PRO:HG3	1:E:109:ASP:HB2	1.77	0.65
1:D:41:SER:HB3	1:D:324:ALA:HB2	1.79	0.65
1:A:126:ASP:OD1	1:G:495:ASN:ND2	2.26	0.64
1:C:41:SER:HB3	1:C:324:ALA:HB2	1.80	0.64
1:A:15:GLN:HG2	1:A:297:HIS:CE1	2.32	0.64
1:E:41:SER:HB3	1:E:324:ALA:HB2	1.80	0.64
1:C:219:HIS:O	1:C:259:ARG:NH1	2.30	0.64
1:D:109:ASP:HB2	1:E:108:PRO:HG3	1.80	0.64
1:A:108:PRO:HG2	1:C:108:PRO:HG2	1.78	0.63
1:H:23:ASP:OD1	1:H:43:ARG:NE	2.31	0.63
1:F:219:HIS:O	1:F:259:ARG:NH1	2.32	0.63
1:G:53:LEU:HD12	1:G:309:LYS:HE2	1.80	0.63
1:E:53:LEU:HB3	1:E:56:PRO:HD2	1.80	0.62
1:F:466:TRP:O	1:F:470:GLU:HG3	1.98	0.62
1:F:108:PRO:HG3	1:G:109:ASP:HB2	1.81	0.62
1:B:108:PRO:HG2	1:H:108:PRO:HG2	1.81	0.62
1:E:15:GLN:HG3	1:E:297:HIS:HE1	1.61	0.62
1:F:153:ALA:O	1:F:257:ARG:NH2	2.32	0.62
1:H:54[A]:CYS:SG	3:H:841:HOH:O	2.51	0.62
1:A:45:HIS:HB2	1:A:332:LEU:HD11	1.81	0.62
1:C:157:GLU:HG3	1:F:282:ARG:HB3	1.80	0.62
1:H:297:HIS:CE1	1:H:309:LYS:HD2	2.34	0.61
1:E:238:ARG:NH2	1:E:408:ASP:OD2	2.34	0.61
1:G:41:SER:HB3	1:G:324:ALA:HB2	1.81	0.61
1:A:55:ALA:HB3	1:A:75:ASN:HA	1.83	0.61
1:A:282:ARG:HB3	1:G:157:GLU:HG3	1.83	0.61
1:D:45:HIS:O	1:D:318:ARG:NH2	2.33	0.60
1:A:297:HIS:CE1	1:A:309:LYS:HD2	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:41:SER:HB3	1:F:324:ALA:HB2	1.84	0.60
1:C:487:LYS:HE3	1:C:490:GLU:HG3	1.84	0.60
1:A:379:VAL:HB	1:A:396:ARG:HB3	1.82	0.60
1:E:219:HIS:O	1:E:259:ARG:NH1	2.35	0.60
1:H:55:ALA:HB3	1:H:75:ASN:HA	1.84	0.60
1:D:399:LYS:HB2	1:D:416:GLU:HG3	1.84	0.59
1:G:399:LYS:HB2	1:G:416:GLU:HG3	1.84	0.59
1:D:483:GLN:NE2	1:H:488:ALA:H	2.00	0.59
1:C:374:GLU:CD	1:C:374:GLU:H	2.04	0.59
1:B:256:ARG:NH1	3:B:705:HOH:O	2.34	0.59
1:E:435:GLN:OE1	1:E:435:GLN:N	2.25	0.59
1:E:432:PRO:HA	1:E:435:GLN:NE2	2.17	0.58
1:E:55:ALA:HB3	1:E:75:ASN:HA	1.84	0.58
1:H:132:ASP:OD2	3:H:701:HOH:O	2.17	0.58
1:A:1:VAL:HG11	1:H:429:PRO:HG2	1.84	0.58
1:A:41:SER:HB3	1:A:324:ALA:HB2	1.86	0.58
1:C:177:TYR:OH	1:C:282:ARG:NH2	2.32	0.58
1:C:379:VAL:HB	1:C:396:ARG:HB3	1.84	0.58
1:E:185:ASP:HB3	1:E:188:ARG:HB3	1.85	0.58
1:B:45:HIS:O	1:B:318:ARG:NH2	2.37	0.58
1:E:53:LEU:O	1:E:297:HIS:HD2	1.86	0.57
1:F:69:ARG:NH1	1:F:362:ASP:OD1	2.36	0.57
1:B:219:HIS:O	1:B:259:ARG:NH1	2.37	0.57
1:D:53:LEU:HB3	1:D:56:PRO:HD2	1.85	0.57
1:A:108:PRO:HG3	1:C:109:ASP:HB2	1.85	0.57
1:H:45:HIS:HB2	1:H:332:LEU:HD11	1.87	0.57
1:E:153:ALA:O	1:E:257:ARG:NH1	2.37	0.57
1:E:374:GLU:OE2	3:E:701:HOH:O	2.17	0.57
1:F:109:ASP:HB2	1:G:108:PRO:HG3	1.85	0.57
1:E:303:GLU:OE2	1:E:420:LEU:HD23	2.05	0.57
1:H:487:LYS:H	1:H:487:LYS:HD2	1.71	0.56
1:C:55:ALA:HB3	1:C:75:ASN:HA	1.88	0.56
1:B:15:GLN:OE1	1:B:309:LYS:NZ	2.27	0.56
1:E:180:SER:HB2	1:E:283:THR:HG23	1.88	0.56
1:G:55:ALA:HB3	1:G:75:ASN:HA	1.88	0.56
1:E:290:LEU:HD23	1:E:325:GLY:HA3	1.87	0.56
1:H:45:HIS:O	1:H:318:ARG:NH2	2.39	0.56
1:B:55:ALA:HB3	1:B:75:ASN:HA	1.88	0.56
1:A:238:ARG:HD3	1:A:389:TYR:CE2	2.41	0.56
1:B:445:ARG:NH2	3:B:722:HOH:O	2.37	0.56
1:C:126:ASP:OD1	1:F:495:ASN:ND2	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:55:ALA:HB3	1:D:75:ASN:HA	1.89	0.55
1:H:54[A]:CYS:O	1:H:58:ARG:HG3	2.06	0.55
1:D:15:GLN:HG3	1:D:297:HIS:CE1	2.42	0.55
1:F:297:HIS:CE1	1:F:309:LYS:HD3	2.40	0.55
1:F:39:LYS:HD2	1:F:39:LYS:N	2.21	0.55
1:F:55:ALA:HB3	1:F:75:ASN:HA	1.87	0.55
1:A:109:ASP:HB2	1:C:108:PRO:HG3	1.87	0.55
1:A:157:GLU:HG3	1:G:282:ARG:HB3	1.88	0.55
1:C:238:ARG:NH2	1:C:408:ASP:OD2	2.39	0.55
1:H:180:SER:HB2	1:H:283:THR:HG23	1.88	0.55
1:H:41:SER:HB3	1:H:324:ALA:HB2	1.88	0.55
1:A:100:SER:HB2	1:A:118:LEU:HD22	1.89	0.55
1:F:53:LEU:HB3	1:F:56:PRO:HD2	1.89	0.55
1:E:3:THR:N	3:E:717:HOH:O	2.39	0.55
1:H:15:GLN:HG3	1:H:297:HIS:CE1	2.42	0.55
1:C:45:HIS:HB2	1:C:332:LEU:HD11	1.89	0.55
1:A:495:ASN:ND2	1:G:126:ASP:OD1	2.36	0.55
1:E:297:HIS:CE1	1:E:309:LYS:HD2	2.42	0.54
1:A:45:HIS:O	1:A:318:ARG:NH2	2.40	0.54
1:H:139:ARG:NH1	1:H:141:ASP:OD1	2.40	0.54
1:F:139:ARG:NH1	1:F:242:SER:O	2.40	0.54
1:E:432:PRO:HA	1:E:435:GLN:HE22	1.73	0.54
1:H:395:ILE:HD13	1:H:444:MET:HE2	1.90	0.54
1:B:381:MET:HB2	1:B:394:ALA:HB3	1.90	0.54
1:F:45:HIS:O	1:F:318:ARG:NH2	2.39	0.54
1:D:379:VAL:HB	1:D:396:ARG:HB3	1.88	0.53
1:B:53:LEU:HB3	1:B:56:PRO:HD2	1.89	0.53
1:D:119:THR:HG22	1:D:171:LEU:HD12	1.90	0.53
1:F:45:HIS:HB2	1:F:332:LEU:HD11	1.89	0.53
1:A:86:TYR:HB3	1:A:343:THR:HG23	1.89	0.53
1:E:51:SER:O	1:E:57:ALA:HB2	2.09	0.53
1:D:5:LYS:NZ	1:D:93:ALA:O	2.41	0.53
1:E:290:LEU:HD13	1:E:349:LEU:HD13	1.91	0.53
1:F:265:ASN:HA	1:F:268:TYR:HB3	1.91	0.53
1:A:2:THR:HA	1:A:5:LYS:HD2	1.91	0.52
1:D:39:LYS:HD2	1:D:39:LYS:N	2.24	0.52
1:G:100:SER:HB2	1:G:118:LEU:HD22	1.90	0.52
1:B:314:GLU:OE1	1:B:401:LYS:NZ	2.43	0.52
1:E:58:ARG:HG2	1:E:58:ARG:HH11	1.74	0.52
1:D:162:MET:SD	1:D:207:ARG:HG3	2.49	0.52
1:F:177:TYR:OH	1:F:282:ARG:NH2	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:259:ARG:NH2	3:F:713:HOH:O	2.42	0.52
1:G:338:SER:HB2	1:G:379:VAL:HG13	1.92	0.52
1:A:17:ASN:ND2	3:A:709:HOH:O	2.38	0.52
1:A:23:ASP:OD1	1:A:43:ARG:NE	2.34	0.52
1:E:265:ASN:HA	1:E:268:TYR:HB3	1.92	0.52
1:E:487:LYS:CE	1:E:490:GLU:HG3	2.39	0.52
1:F:4:GLY:N	3:F:715:HOH:O	2.43	0.52
1:C:265:ASN:HA	1:C:268:TYR:HB3	1.91	0.52
1:B:157:GLU:HA	1:B:207:ARG:HG2	1.93	0.51
1:C:187:SER:O	1:C:187:SER:OG	2.27	0.51
1:B:189:ARG:NH2	3:B:712:HOH:O	2.30	0.51
1:D:238:ARG:NH2	1:D:408:ASP:OD2	2.44	0.51
1:G:162:MET:SD	1:G:207:ARG:HG3	2.50	0.51
1:D:45:HIS:HB2	1:D:332:LEU:HD11	1.92	0.51
1:H:219:HIS:O	1:H:259:ARG:NH1	2.44	0.51
1:E:338:SER:HB2	1:E:379:VAL:HG13	1.92	0.51
1:A:295:SER:HB3	1:A:319:VAL:HB	1.93	0.50
1:B:495:ASN:ND2	1:E:126:ASP:OD1	2.44	0.50
1:C:338:SER:HB2	1:C:379:VAL:HG13	1.92	0.50
1:F:17:ASN:ND2	1:F:299:ASP:O	2.45	0.50
1:B:403:VAL:HB	1:B:411:GLN:HB2	1.93	0.50
1:B:290:LEU:HD23	1:B:325:GLY:HA3	1.94	0.50
1:C:134:ARG:NH2	3:C:707:HOH:O	2.39	0.50
1:C:238:ARG:HH11	1:C:388:SER:HA	1.77	0.50
1:D:76:ALA:HB1	1:D:127:PHE:HA	1.93	0.50
1:E:421:GLU:OE2	3:E:702:HOH:O	2.19	0.50
1:H:379:VAL:HB	1:H:396:ARG:HB3	1.94	0.50
1:C:229:LEU:O	1:C:237:GLN:NE2	2.45	0.50
1:G:290:LEU:HD23	1:G:325:GLY:HA3	1.93	0.50
1:A:15:GLN:O	1:A:262:TYR:OH	2.21	0.50
1:H:17:ASN:ND2	1:H:299:ASP:O	2.45	0.50
1:C:139:ARG:NH2	3:C:717:HOH:O	2.44	0.50
1:A:442:ARG:HG2	1:A:445:ARG:HH11	1.77	0.49
1:F:80:GLN:HB2	1:F:83:ILE:HG13	1.94	0.49
1:C:135:LYS:HB2	1:C:138:GLU:OE2	2.13	0.49
1:D:413:PHE:CD1	1:D:421:GLU:HB3	2.48	0.49
1:G:17:ASN:ND2	1:G:299:ASP:O	2.46	0.49
1:A:76:ALA:HB1	1:A:127:PHE:HA	1.95	0.49
1:B:238:ARG:HD3	1:B:389:TYR:CE2	2.47	0.49
1:E:381:MET:HB2	1:E:394:ALA:HB3	1.94	0.49
1:F:238:ARG:HD3	1:F:389:TYR:CE2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:265:ASN:HA	1:D:268:TYR:HB3	1.93	0.49
1:D:180:SER:HB2	1:D:283:THR:HG23	1.93	0.49
1:B:118:LEU:HD11	1:B:175:LYS:HD2	1.95	0.48
1:C:254:ASN:ND2	3:C:706:HOH:O	2.36	0.48
1:D:238:ARG:HD3	1:D:389:TYR:CE2	2.48	0.48
1:H:304:ARG:NH2	3:H:730:HOH:O	2.46	0.48
1:A:58:ARG:HH11	1:A:58:ARG:HG2	1.77	0.48
1:D:219:HIS:O	1:D:259:ARG:NH1	2.46	0.48
1:C:15:GLN:NE2	1:C:299:ASP:OD2	2.47	0.48
1:F:58:ARG:HD3	1:F:103:MET:HA	1.95	0.48
1:F:470:GLU:HB2	1:G:92:ARG:HD2	1.96	0.48
1:G:251:THR:HG22	1:G:253:GLU:N	2.25	0.48
1:H:9:LEU:HD22	1:H:280:LEU:HD11	1.96	0.48
1:D:126:ASP:OD1	1:H:495:ASN:ND2	2.44	0.48
1:B:297:HIS:CE1	1:B:309:LYS:HD2	2.48	0.48
1:E:379:VAL:HB	1:E:396:ARG:HB3	1.95	0.48
1:A:338:SER:HB2	1:A:379:VAL:HG13	1.95	0.48
1:E:297:HIS:HE1	1:E:309:LYS:HD2	1.78	0.48
1:F:53:LEU:HA	1:F:309:LYS:HD2	1.95	0.48
1:H:15:GLN:HG3	1:H:297:HIS:HE1	1.75	0.48
1:H:76:ALA:HB1	1:H:127:PHE:HA	1.94	0.48
1:B:76:ALA:HB1	1:B:127:PHE:HA	1.96	0.47
1:E:385:ALA:HB1	1:E:386:GLU:OE2	2.14	0.47
1:F:119:THR:HG22	1:F:171:LEU:HD12	1.94	0.47
1:H:15:GLN:HG2	1:H:299:ASP:HB2	1.95	0.47
1:B:162:MET:SD	1:B:207:ARG:HG3	2.54	0.47
1:B:246:GLN:NE2	3:B:724:HOH:O	2.39	0.47
1:B:265:ASN:HA	1:B:268:TYR:HB3	1.95	0.47
1:F:405:CYS:HB3	1:F:408:ASP:HB2	1.96	0.47
1:H:296:ASP:OD1	1:H:297:HIS:N	2.48	0.47
1:H:338:SER:HB2	1:H:379:VAL:HG13	1.95	0.47
1:A:238:ARG:NH2	1:A:408:ASP:OD2	2.46	0.47
1:C:282:ARG:HB3	1:F:157:GLU:HG3	1.95	0.47
1:D:9:LEU:HD22	1:D:280:LEU:HD11	1.96	0.47
1:D:414:ASP:O	1:D:418:ASP:N	2.47	0.47
1:D:157:GLU:HA	1:D:207:ARG:HG2	1.97	0.47
1:H:162:MET:SD	1:H:207:ARG:HG3	2.54	0.47
1:F:338:SER:HB2	1:F:379:VAL:HG13	1.97	0.47
1:D:254:ASN:ND2	3:D:715:HOH:O	2.36	0.47
1:F:395:ILE:HD13	1:F:444:MET:HE2	1.97	0.47
1:D:499:LEU:HD13	1:H:143:TRP:HA	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:ASN:ND2	1:A:183:ASN:O	2.48	0.47
1:A:354:LEU:H	1:A:354:LEU:HD12	1.80	0.47
1:C:76:ALA:HB1	1:C:127:PHE:HA	1.97	0.47
1:C:297:HIS:CE1	1:C:309:LYS:HD2	2.49	0.47
1:D:54[A]:CYS:O	1:D:58:ARG:HG3	2.13	0.47
1:B:157:GLU:HG3	1:E:282:ARG:HB3	1.96	0.47
1:H:469:TYR:OH	1:H:473:ARG:HD2	2.14	0.47
1:D:96:TYR:OH	1:D:175:LYS:HE3	2.14	0.47
1:A:108:PRO:HB2	1:C:108:PRO:HB2	1.97	0.46
1:A:5:LYS:HE3	1:A:350:ALA:O	2.14	0.46
1:E:413:PHE:CG	1:E:421:GLU:HG2	2.51	0.46
1:G:265:ASN:HA	1:G:268:TYR:HB3	1.96	0.46
1:B:252:GLU:O	1:B:256:ARG:HG3	2.15	0.46
1:E:262:TYR:CE1	1:E:301:LEU:HD11	2.50	0.46
1:F:157:GLU:HA	1:F:207:ARG:HG2	1.97	0.46
1:H:208:ARG:NH2	3:H:725:HOH:O	2.44	0.46
1:B:19:LYS:NZ	1:B:303:GLU:OE1	2.49	0.46
1:B:5:LYS:HD3	1:B:350:ALA:O	2.16	0.46
1:H:487:LYS:CD	1:H:487:LYS:H	2.28	0.46
1:D:23:ASP:OD1	1:D:43:ARG:NE	2.37	0.46
1:F:51:SER:O	1:F:57:ALA:HB2	2.16	0.46
1:G:76:ALA:HB1	1:G:127:PHE:HA	1.98	0.46
1:H:207:ARG:NH1	3:H:738:HOH:O	2.49	0.46
1:B:117:ARG:HB3	1:B:482:HIS:NE2	2.30	0.46
1:C:246:GLN:H	1:C:246:GLN:CD	2.17	0.46
1:C:238:ARG:HD3	1:C:389:TYR:CE2	2.50	0.46
1:C:66:LEU:HD22	1:C:382:GLU:HG3	1.97	0.46
1:D:238:ARG:HH11	1:D:388:SER:HA	1.80	0.46
1:D:167:GLU:HA	1:H:170:PHE:CZ	2.51	0.46
1:F:86:TYR:HB3	1:F:343:THR:HG23	1.98	0.46
1:E:15:GLN:OE1	1:E:201:HIS:CD2	2.69	0.45
1:F:15:GLN:HG3	1:F:297:HIS:CE1	2.50	0.45
1:G:395:ILE:HD13	1:G:444:MET:HE2	1.98	0.45
1:A:51:SER:O	1:A:57:ALA:HB2	2.16	0.45
1:C:22:PRO:O	1:C:45:HIS:ND1	2.39	0.45
1:C:492:TYR:CZ	1:F:164:TYR:HD1	2.35	0.45
1:G:45:HIS:O	1:G:318:ARG:NH2	2.49	0.45
1:F:15:GLN:HG2	1:F:299:ASP:HB2	1.98	0.45
1:B:40:ARG:NH1	3:B:737:HOH:O	2.49	0.45
1:E:403:VAL:HB	1:E:411:GLN:HB2	1.99	0.45
1:C:96:TYR:OH	1:C:175:LYS:HE2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:469:TYR:OH	1:A:473:ARG:NH1	2.43	0.45
1:C:262:TYR:CE1	1:C:301:LEU:HD11	2.52	0.45
1:E:410:GLU:OE1	1:E:442:ARG:NH2	2.46	0.45
1:C:374:GLU:N	1:C:374:GLU:OE2	2.42	0.44
1:D:15:GLN:HG3	1:D:297:HIS:HE1	1.82	0.44
1:B:181:ARG:HH21	1:E:158:ILE:HG13	1.81	0.44
1:F:341:ASP:HB3	1:F:364:VAL:O	2.17	0.44
1:G:378:PRO:HB3	1:G:397:GLU:HG3	1.98	0.44
1:H:132:ASP:HA	1:H:466:TRP:HZ2	1.82	0.44
1:C:76:ALA:HA	1:C:106:VAL:HG21	1.99	0.44
1:F:290:LEU:HD22	1:F:349:LEU:HD13	1.99	0.44
1:G:96:TYR:OH	1:G:116:GLU:OE1	2.27	0.44
1:G:309:LYS:HG3	1:G:310:MET:SD	2.57	0.44
1:H:76:ALA:HA	1:H:106:VAL:HG21	1.98	0.44
1:E:253:GLU:O	1:E:257:ARG:HG3	2.18	0.44
1:H:265:ASN:HA	1:H:268:TYR:HB3	1.98	0.44
1:H:216:ASP:OD1	1:H:216:ASP:N	2.49	0.44
1:B:268:TYR:OH	1:B:272:LYS:HE2	2.16	0.44
1:G:259:ARG:NH2	3:G:722:HOH:O	2.50	0.44
1:B:51:SER:O	1:B:57:ALA:HB2	2.18	0.44
1:A:43:ARG:NH2	3:A:724:HOH:O	2.51	0.44
1:A:75:ASN:ND2	3:A:708:HOH:O	2.37	0.44
1:E:15:GLN:OE1	1:E:309:LYS:NZ	2.40	0.44
1:H:139:ARG:HH22	1:H:146:ASN:HB3	1.82	0.44
1:D:485:LEU:CD1	1:D:487:LYS:HG3	2.47	0.43
1:G:404:TYR:HE2	1:G:451:MET:HG3	1.83	0.43
1:A:262:TYR:CE2	1:A:301:LEU:HD11	2.53	0.43
1:E:162:MET:HG2	1:E:207:ARG:NH2	2.33	0.43
1:G:117:ARG:NH2	1:G:121:ASP:OD2	2.48	0.43
1:A:53:LEU:HB3	1:A:56:PRO:HD2	1.99	0.43
1:B:487:LYS:HD2	1:B:487:LYS:HA	1.73	0.43
1:C:9:LEU:HD22	1:C:280:LEU:HD11	2.00	0.43
1:B:179:LEU:HD13	1:B:191:TRP:CG	2.53	0.43
1:D:158:ILE:HA	1:D:158:ILE:HD12	1.87	0.43
1:F:296:ASP:N	1:F:296:ASP:OD1	2.51	0.43
1:A:265:ASN:HA	1:A:268:TYR:HB3	1.99	0.43
1:E:166:ASP:OD2	1:E:207:ARG:NH2	2.51	0.43
1:F:252:GLU:O	1:F:256:ARG:HG3	2.18	0.43
1:F:379:VAL:HB	1:F:396:ARG:HB3	2.00	0.43
1:F:76:ALA:HB1	1:F:127:PHE:HA	2.00	0.43
1:E:311:ASN:ND2	3:E:739:HOH:O	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:262:TYR:CE1	1:F:301:LEU:HD11	2.54	0.43
1:H:268:TYR:CZ	1:H:272:LYS:HE2	2.53	0.43
1:F:403:VAL:HB	1:F:411:GLN:HB2	1.99	0.43
1:G:169:ALA:O	1:G:173:ASN:ND2	2.47	0.43
1:C:53:LEU:HB3	1:C:56:PRO:HD2	2.00	0.43
1:B:177:TYR:HB3	1:E:158:ILE:HG12	2.00	0.43
1:C:414:ASP:O	1:C:418:ASP:N	2.52	0.43
1:A:166:ASP:OD2	1:A:207:ARG:NH2	2.49	0.43
1:B:52:PRO:HB2	1:B:310:MET:H	1.82	0.43
1:C:51:SER:O	1:C:57:ALA:HB2	2.19	0.43
1:E:53:LEU:O	1:E:297:HIS:CD2	2.71	0.43
1:G:461:SER:O	1:G:465:ARG:HG3	2.19	0.43
1:D:139:ARG:NH1	1:D:242:SER:O	2.51	0.42
1:E:14:ASP:O	1:E:200:PRO:HD2	2.19	0.42
1:C:170:PHE:CZ	1:F:167:GLU:HA	2.54	0.42
1:F:14:ASP:OD2	1:F:296:ASP:OD2	2.36	0.42
1:F:396:ARG:HD3	1:F:401:LYS:HD3	2.01	0.42
1:C:15:GLN:HG2	1:C:299:ASP:HB2	2.01	0.42
1:F:357:VAL:O	1:F:361:THR:HG22	2.19	0.42
1:H:139:ARG:NH2	1:H:146:ASN:HB3	2.35	0.42
1:B:1:VAL:HG11	1:C:429:PRO:HG2	2.01	0.42
1:D:161:GLN:OE1	1:D:201:HIS:HB3	2.18	0.42
1:E:17:ASN:ND2	1:E:299:ASP:O	2.52	0.42
1:A:403:VAL:HB	1:A:411:GLN:HB2	2.01	0.42
1:C:466:TRP:O	1:C:470:GLU:HB2	2.19	0.42
1:F:268:TYR:CZ	1:F:272:LYS:HE2	2.55	0.42
1:G:57:ALA:O	1:G:61:PHE:N	2.46	0.42
1:A:378:PRO:HB3	1:A:397:GLU:HG3	2.02	0.42
1:D:180:SER:O	1:D:183:ASN:HB2	2.20	0.42
1:E:30:HIS:HD2	1:E:213:LEU:HB3	1.85	0.42
1:E:355:GLU:HG3	1:E:355:GLU:H	1.67	0.42
1:G:130:THR:HG23	1:G:465:ARG:HH21	1.84	0.42
1:H:262:TYR:CE2	1:H:301:LEU:HD11	2.54	0.42
1:F:118:LEU:HD21	1:F:175:LYS:HD2	2.02	0.42
1:E:25:PRO:HG2	1:E:35:LYS:HG3	2.02	0.42
1:F:268:TYR:OH	1:F:272:LYS:HE2	2.20	0.42
1:F:413:PHE:CD1	1:F:421:GLU:HB3	2.55	0.42
1:A:139:ARG:NH1	1:A:242:SER:O	2.53	0.42
1:H:117:ARG:HB3	1:H:482:HIS:NE2	2.34	0.42
1:B:80:GLN:HG3	3:B:772:HOH:O	2.20	0.42
1:D:51:SER:O	1:D:57:ALA:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:47:ASN:HD22	1:F:319:VAL:HG23	1.85	0.42
1:H:58:ARG:HA	1:H:61:PHE:HB3	2.01	0.42
1:B:14:ASP:OD1	1:B:296:ASP:OD2	2.37	0.41
1:F:5:LYS:NZ	3:F:719:HOH:O	2.49	0.41
1:G:297:HIS:CE1	1:G:309:LYS:HD3	2.55	0.41
1:G:404:TYR:CE2	1:G:451:MET:HG3	2.55	0.41
1:A:14:ASP:HA	1:A:296:ASP:OD1	2.19	0.41
1:B:45:HIS:HB2	1:B:332:LEU:HD11	2.01	0.41
1:B:61:PHE:CE1	1:B:342:VAL:HG11	2.55	0.41
1:C:445:ARG:NH1	3:C:701:HOH:O	2.34	0.41
1:E:252:GLU:O	1:E:256:ARG:HG3	2.20	0.41
1:G:296:ASP:OD1	1:G:296:ASP:N	2.52	0.41
1:D:164:TYR:HD1	1:H:492:TYR:CZ	2.38	0.41
1:D:290:LEU:HD13	1:D:349:LEU:HD13	2.01	0.41
1:D:110:GLN:CB	1:D:482:HIS:HB2	2.51	0.41
1:F:15:GLN:HG3	1:F:297:HIS:HE1	1.85	0.41
1:H:252:GLU:O	1:H:256:ARG:HG3	2.21	0.41
1:C:292:LEU:HG	1:C:323:ILE:HG12	2.01	0.41
1:D:444:MET:HE2	1:D:444:MET:HB3	1.98	0.41
1:F:470:GLU:OE2	1:G:92:ARG:NH1	2.53	0.41
1:G:51:SER:O	1:G:57:ALA:HB2	2.19	0.41
1:H:199:HIS:HB2	1:H:269:LEU:HD21	2.02	0.41
1:H:444:MET:HE2	1:H:444:MET:HB3	1.85	0.41
1:F:100:SER:HB2	1:F:118:LEU:HD22	2.02	0.41
1:F:57:ALA:O	1:F:61:PHE:N	2.45	0.41
1:A:123:TYR:HA	1:A:123:TYR:HD1	1.75	0.41
1:G:290:LEU:HD13	1:G:349:LEU:HD13	2.01	0.41
1:G:435:GLN:HB3	3:G:795:HOH:O	2.19	0.41
1:D:400:TRP:CD2	1:D:437:THR:HG21	2.55	0.41
1:A:396:ARG:HD3	1:A:401:LYS:HD3	2.02	0.41
1:B:58:ARG:HD3	1:B:103:MET:HA	2.01	0.41
1:B:395:ILE:HD13	1:B:444:MET:HE2	2.02	0.41
1:G:45:HIS:HB2	1:G:332:LEU:HD11	2.02	0.41
1:D:188:ARG:HG2	1:D:189:ARG:N	2.35	0.41
1:B:262:TYR:CE1	1:B:301:LEU:HD11	2.55	0.40
1:D:495:ASN:ND2	1:H:126:ASP:OD1	2.50	0.40
1:C:238:ARG:NH1	1:C:388:SER:HA	2.36	0.40
1:D:499:LEU:HD23	1:D:500:ASP:H	1.86	0.40
1:E:158:ILE:HD12	1:E:158:ILE:HA	1.94	0.40
1:H:290:LEU:HD23	1:H:325:GLY:HA3	2.03	0.40
1:B:237:GLN:O	1:B:241:LEU:HG	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:48:TYR:HB2	1:F:379:VAL:HG11	2.03	0.40
1:A:292:LEU:HG	1:A:323:ILE:HG12	2.03	0.40
1:A:471:ALA:HB2	1:C:92:ARG:HB2	2.03	0.40
1:B:126:ASP:OD1	1:E:495:ASN:ND2	2.45	0.40
1:B:323:ILE:O	1:B:328:ILE:HG21	2.21	0.40
1:E:100:SER:HB2	1:E:118:LEU:HD22	2.03	0.40
1:F:161:GLN:OE1	1:F:201:HIS:HB3	2.21	0.40
1:F:246:GLN:HG2	1:F:246:GLN:H	1.72	0.40
1:H:53:LEU:HB3	1:H:56:PRO:HD2	2.04	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	512/516 (99%)	490 (96%)	21 (4%)	1 (0%)	47	78
1	B	512/516 (99%)	494 (96%)	17 (3%)	1 (0%)	47	78
1	C	510/516 (99%)	481 (94%)	29 (6%)	0	100	100
1	D	507/516 (98%)	484 (96%)	22 (4%)	1 (0%)	47	78
1	E	507/516 (98%)	485 (96%)	21 (4%)	1 (0%)	47	78
1	F	506/516 (98%)	481 (95%)	25 (5%)	0	100	100
1	G	506/516 (98%)	491 (97%)	13 (3%)	2 (0%)	34	66
1	H	505/516 (98%)	485 (96%)	19 (4%)	1 (0%)	47	78
All	All	4065/4128 (98%)	3891 (96%)	167 (4%)	7 (0%)	47	78

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	421	GLU

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Mol	Chain	Res	Type
1	G	421	GLU
1	A	421	GLU
1	E	421	GLU
1	H	421	GLU
1	B	421	GLU
1	G	22	PRO

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	438/438 (100%)	428 (98%)	10 (2%)	50	82
1	B	438/438 (100%)	429 (98%)	9 (2%)	53	84
1	C	437/438 (100%)	430 (98%)	7 (2%)	62	88
1	D	434/438 (99%)	426 (98%)	8 (2%)	59	86
1	E	434/438 (99%)	427 (98%)	7 (2%)	62	88
1	F	433/438 (99%)	425 (98%)	8 (2%)	59	86
1	G	433/438 (99%)	426 (98%)	7 (2%)	62	88
1	H	435/438 (99%)	425 (98%)	10 (2%)	50	82
All	All	3482/3504 (99%)	3416 (98%)	66 (2%)	57	85

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54[A]	CYS
1	A	79	TYR
1	A	183	ASN
1	A	186	GLU
1	A	309	LYS
1	A	374	GLU
1	A	375	ARG
1	A	454	PHE
1	A	473	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	497	MET
1	B	53	LEU
1	B	54[A]	CYS
1	B	74	ASP
1	B	81	SER
1	B	246	GLN
1	B	309	LYS
1	B	374	GLU
1	B	375	ARG
1	B	454	PHE
1	C	74	ASP
1	C	79	TYR
1	C	259	ARG
1	C	309	LYS
1	C	375	ARG
1	C	445	ARG
1	C	454	PHE
1	D	39	LYS
1	D	74	ASP
1	D	208	ARG
1	D	309	LYS
1	D	375	ARG
1	D	445	ARG
1	D	454	PHE
1	D	498	ASN
1	E	74	ASP
1	E	162	MET
1	E	186	GLU
1	E	309	LYS
1	E	375	ARG
1	E	454	PHE
1	E	487	LYS
1	F	39	LYS
1	F	54[A]	CYS
1	F	74	ASP
1	F	175	LYS
1	F	218	GLU
1	F	223	GLU
1	F	375	ARG
1	F	454	PHE
1	G	74	ASP
1	G	230	ASP

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Mol	Chain	Res	Type
1	G	288	ASP
1	G	358	ARG
1	G	375	ARG
1	G	445	ARG
1	G	454	PHE
1	H	5	LYS
1	H	74	ASP
1	H	79	TYR
1	H	139	ARG
1	H	259	ARG
1	H	309	LYS
1	H	375	ARG
1	H	454	PHE
1	H	473	ARG
1	H	487	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	247	ASN
1	A	486	GLN
1	B	174	GLN
1	D	483	GLN
1	F	15	GLN
1	G	15	GLN
1	G	80	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues 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$
1	DDZ	B	54[B]	1,2	4,6,7	0.84	0	3,7,9	2.21	1 (33%)
1	DDZ	H	54[B]	1,2	4,6,7	0.65	0	3,7,9	2.32	1 (33%)
1	DDZ	C	54[B]	1,2	4,6,7	0.72	0	3,7,9	1.85	1 (33%)
1	DDZ	F	54[B]	1,2	4,6,7	0.77	0	3,7,9	2.36	1 (33%)
1	DDZ	G	54[B]	1,2	4,6,7	0.65	0	3,7,9	1.92	1 (33%)
1	DDZ	A	54[B]	1,2	4,6,7	0.72	0	3,7,9	2.35	1 (33%)
1	DDZ	D	54[B]	1,2	4,6,7	0.76	0	3,7,9	2.49	1 (33%)
1	DDZ	E	54[B]	1,2	4,6,7	0.86	0	3,7,9	2.24	1 (33%)

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
1	DDZ	B	54[B]	1,2	-	2/2/6/8	-
1	DDZ	H	54[B]	1,2	-	0/2/6/8	-
1	DDZ	C	54[B]	1,2	-	1/2/6/8	-
1	DDZ	F	54[B]	1,2	-	2/2/6/8	-
1	DDZ	G	54[B]	1,2	-	0/2/6/8	-
1	DDZ	A	54[B]	1,2	-	2/2/6/8	-
1	DDZ	D	54[B]	1,2	-	2/2/6/8	-
1	DDZ	E	54[B]	1,2	-	0/2/6/8	-

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	54[B]	DDZ	OG2-CB-OG1	-4.26	103.77	111.27
1	F	54[B]	DDZ	OG2-CB-OG1	-4.03	104.17	111.27
1	A	54[B]	DDZ	OG2-CB-OG1	-4.02	104.20	111.27
1	H	54[B]	DDZ	OG2-CB-OG1	-3.92	104.38	111.27
1	E	54[B]	DDZ	OG2-CB-OG1	-3.83	104.53	111.27
1	B	54[B]	DDZ	OG2-CB-OG1	-3.64	104.86	111.27
1	G	54[B]	DDZ	OG2-CB-OG1	-3.25	105.56	111.27
1	C	54[B]	DDZ	OG2-CB-OG1	-3.14	105.74	111.27

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	54[B]	DDZ	N-CA-CB-OG1
1	B	54[B]	DDZ	N-CA-CB-OG2
1	F	54[B]	DDZ	N-CA-CB-OG2
1	A	54[B]	DDZ	N-CA-CB-OG1
1	A	54[B]	DDZ	N-CA-CB-OG2
1	D	54[B]	DDZ	N-CA-CB-OG1
1	C	54[B]	DDZ	N-CA-CB-OG1
1	F	54[B]	DDZ	N-CA-CB-OG1
1	D	54[B]	DDZ	N-CA-CB-OG2

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

## 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, 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	514/516 (99%)	-0.11	4 (0%) 86 81	17, 29, 54, 83	0
1	B	514/516 (99%)	-0.24	4 (0%) 86 81	8, 17, 40, 80	0
1	C	512/516 (99%)	0.01	8 (1%) 72 66	12, 28, 52, 84	0
1	D	509/516 (98%)	0.31	17 (3%) 46 36	9, 23, 49, 100	0
1	E	509/516 (98%)	-0.25	6 (1%) 79 73	7, 18, 43, 74	0
1	F	508/516 (98%)	0.32	15 (2%) 50 40	18, 34, 56, 88	0
1	G	508/516 (98%)	-0.09	3 (0%) 89 86	15, 29, 53, 73	0
1	H	509/516 (98%)	-0.20	5 (0%) 82 77	6, 17, 45, 78	0
All	All	4083/4128 (98%)	-0.03	62 (1%) 72 68	6, 25, 51, 100	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	216	ASP	5.8
1	C	245	TYR	4.9
1	E	3	THR	4.4
1	B	216	ASP	4.1
1	D	3	THR	4.0
1	C	155	VAL	3.8
1	F	186	GLU	3.5
1	C	216	ASP	3.5
1	D	221	THR	3.4
1	D	216	ASP	3.3
1	A	216	ASP	3.3
1	F	486	GLN	3.3
1	E	432	PRO	3.2
1	D	420	LEU	3.2
1	B	-2	GLY	3.2
1	F	245	TYR	3.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	F	184	ASP	3.1
1	G	226	ALA	3.0
1	D	228	PRO	3.0
1	C	156	ALA	2.8
1	F	39	LYS	2.7
1	C	247	ASN	2.7
1	F	217	CYS	2.7
1	B	217	CYS	2.7
1	D	142	TRP	2.7
1	F	466	TRP	2.6
1	H	216	ASP	2.6
1	D	245	TYR	2.6
1	D	241	LEU	2.6
1	F	511	GLY	2.6
1	C	215	GLU	2.5
1	H	499	LEU	2.4
1	D	230	ASP	2.4
1	B	2	THR	2.4
1	E	420	LEU	2.4
1	F	420	LEU	2.4
1	A	-2	GLY	2.4
1	D	231	GLU	2.3
1	G	420	LEU	2.3
1	E	186	GLU	2.3
1	F	145	HIS	2.3
1	D	222	PRO	2.3
1	D	229	LEU	2.3
1	F	288	ASP	2.3
1	H	143	TRP	2.3
1	C	30	HIS	2.3
1	D	236	SER	2.3
1	E	485	LEU	2.2
1	H	245	TYR	2.2
1	H	215	GLU	2.2
1	A	217	CYS	2.2
1	D	140	ILE	2.2
1	A	499	LEU	2.2
1	D	30	HIS	2.2
1	C	223	GLU	2.1
1	F	236	SER	2.1
1	D	145	HIS	2.1
1	F	230	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	251	THR	2.1
1	E	216	ASP	2.1
1	F	221	THR	2.0
1	D	248	PHE	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<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	B-factors(Å <sup>2</sup> )	Q<0.9
1	DDZ	H	54[B]	7/8	0.80	0.27	38,43,62,62	7
1	DDZ	D	54[B]	7/8	0.84	0.22	25,27,34,38	7
1	DDZ	A	54[B]	7/8	0.86	0.18	25,32,34,36	7
1	DDZ	B	54[B]	7/8	0.87	0.24	21,25,32,36	7
1	DDZ	F	54[B]	7/8	0.89	0.20	32,35,37,45	7
1	DDZ	G	54[B]	7/8	0.90	0.18	31,33,33,35	7
1	DDZ	E	54[B]	7/8	0.90	0.21	25,30,44,54	7
1	DDZ	C	54[B]	7/8	0.93	0.16	28,31,34,52	7

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<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	B-factors(Å <sup>2</sup> )	Q<0.9
2	CA	D	601	1/1	0.02	0.31	48,48,48,48	1
2	CA	E	601	1/1	0.12	0.65	61,61,61,61	1
2	CA	F	601	1/1	0.21	0.21	42,42,42,42	1
2	CA	A	601	1/1	0.42	0.20	45,45,45,45	1
2	CA	B	601	1/1	0.46	0.29	48,48,48,48	1
2	CA	H	601	1/1	0.67	0.30	50,50,50,50	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CA	G	601	1/1	0.91	0.12	47,47,47,47	1
2	CA	C	601	1/1	0.97	0.05	21,21,21,21	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.