



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 03:08 am GMT

PDB ID : 3O0D  
Title : Crystal structure of Lip2 lipase from *Yarrowia lipolytica* at 1.7 Å resolution  
Authors : Bordes, F.; Tranier, S.; Mourey, L.; Marty, A.  
Deposited on : 2010-07-19  
Resolution : 1.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

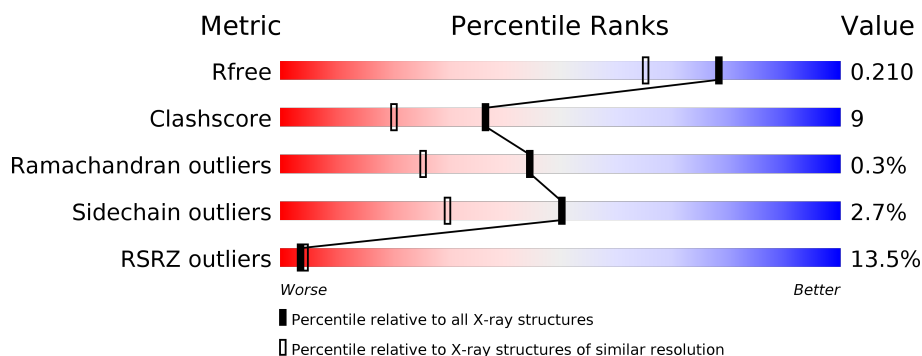
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	3453 (1.70-1.70)
Clashscore	112137	3876 (1.70-1.70)
Ramachandran outliers	110173	3815 (1.70-1.70)
Sidechain outliers	110143	3815 (1.70-1.70)
RSRZ outliers	101464	3491 (1.70-1.70)

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	301	<div> <div>4%</div> <div>81% 18% .</div> </div>
1	B	301	<div> <div>3%</div> <div>84% 15% .</div> </div>
1	C	301	<div> <div>87% 12% .</div> </div>
1	D	301	<div> <div>6%</div> <div>84% 14% ..</div> </div>
1	E	301	<div> <div>3%</div> <div>81% 18% .</div> </div>
1	F	301	<div> <div>8%</div> <div>81% 18% ..</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	301	

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	NAG	C	303	-	-	-	X
2	NAG	G	302	-	-	-	X
2	NAG	G	303	-	-	-	X
3	MPD	A	304	-	-	-	X
3	MPD	A	306	-	-	-	X
3	MPD	B	305	-	-	X	-
3	MPD	C	304	-	-	-	X
3	MPD	C	306	-	-	-	X
3	MPD	D	304	-	-	X	-
3	MPD	E	304	-	-	-	X
3	MPD	F	305	-	-	-	X
4	MRD	A	307	-	-	-	X
4	MRD	B	306	-	-	-	X
4	MRD	D	305	-	-	-	X

## 2 Entry composition [i](#)

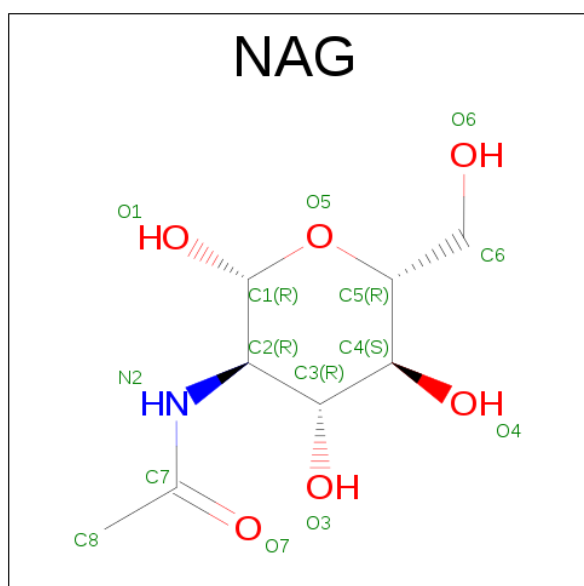
There are 6 unique types of molecules in this entry. The entry contains 18591 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Triacylglycerol lipase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	301	Total	C	N	O	S	0	10	0
			2412	1545	408	447	12			
1	B	301	Total	C	N	O	S	0	8	0
			2404	1536	401	455	12			
1	C	301	Total	C	N	O	S	0	6	0
			2372	1514	399	447	12			
1	D	297	Total	C	N	O	S	0	9	0
			2334	1489	395	440	10			
1	E	301	Total	C	N	O	S	0	13	0
			2420	1544	403	461	12			
1	F	298	Total	C	N	O	S	0	7	0
			2354	1505	400	439	10			
1	G	296	Total	C	N	O	S	0	1	0
			2289	1460	389	429	11			

- Molecule 2 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	1
			28	16	2	10		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	E	1	Total	C	N	O	0	0
			14	8	1	5		
2	E	1	Total	C	N	O	0	0
			14	8	1	5		
2	F	1	Total	C	N	O	0	0
			14	8	1	5		
2	F	1	Total	C	N	O	0	0
			14	8	1	5		
2	G	1	Total	C	N	O	0	0
			14	8	1	5		
2	G	1	Total	C	N	O	0	0
			14	8	1	5		

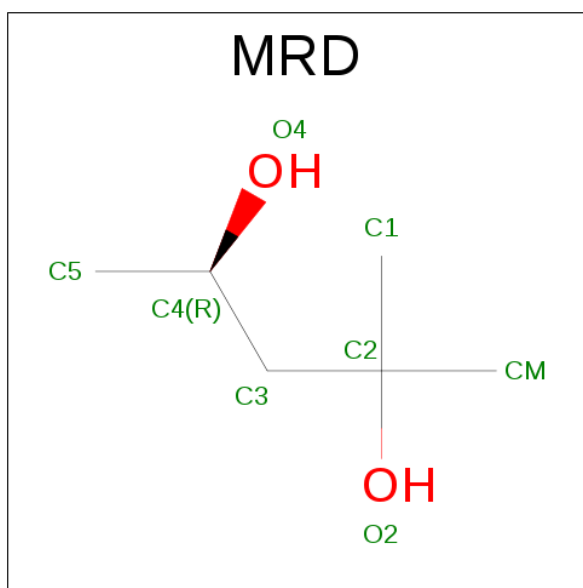
- Molecule 3 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			8	6	2		
3	A	1	Total	C	O	0	0
			8	6	2		
3	A	1	Total	C	O	0	0
			8	6	2		
3	B	1	Total	C	O	0	0
			8	6	2		
3	B	1	Total	C	O	0	0
			8	6	2		
3	C	1	Total	C	O	0	0
			8	6	2		
3	C	1	Total	C	O	0	0
			8	6	2		
3	C	1	Total	C	O	0	0
			8	6	2		
3	D	1	Total	C	O	0	0
			8	6	2		
3	D	1	Total	C	O	0	0
			8	6	2		
3	E	1	Total	C	O	0	0
			8	6	2		
3	E	1	Total	C	O	0	0
			8	6	2		
3	F	1	Total	C	O	0	0
			8	6	2		

- Molecule 4 is (4R)-2-METHYLPENTANE-2,4-DIOL (three-letter code: MRD) (formula:

C<sub>6</sub>H<sub>14</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			8	6	2		
4	B	1	Total	C	O	0	0
			8	6	2		
4	D	1	Total	C	O	0	0
			8	6	2		
4	F	1	Total	C	O	0	0
			8	6	2		

- Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	1	Total	K	0	0
			1	1		
5	D	1	Total	K	0	0
			1	1		
5	E	1	Total	K	0	0
			1	1		
5	B	1	Total	K	0	0
			1	1		
5	C	1	Total	K	0	0
			1	1		
5	A	1	Total	K	0	0
			1	1		
5	F	1	Total	K	0	0
			1	1		

- Molecule 6 is water.

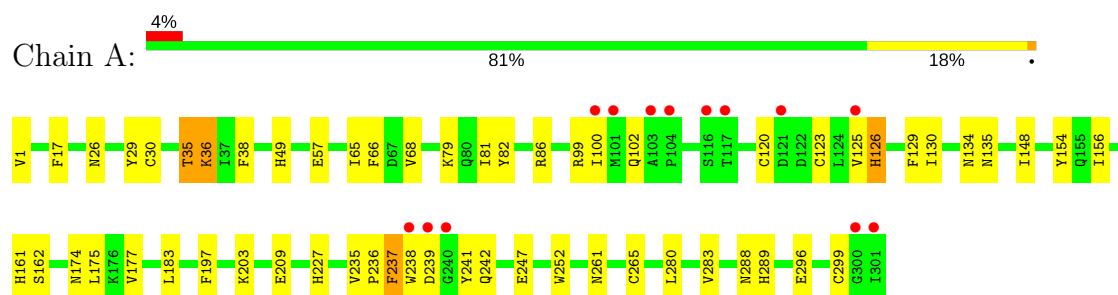
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	263	Total 263	O 263	0	0
6	B	281	Total 281	O 281	0	0
6	C	309	Total 309	O 309	0	0
6	D	222	Total 222	O 222	0	0
6	E	277	Total 277	O 277	0	0
6	F	246	Total 246	O 246	0	0
6	G	55	Total 55	O 55	0	0



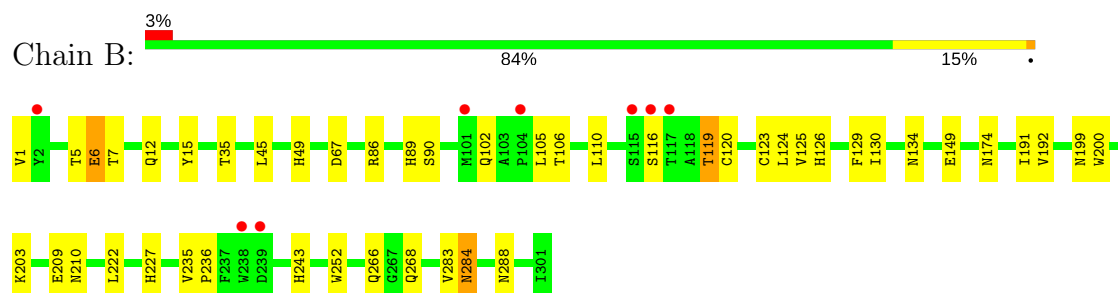
### 3 Residue-property plots

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

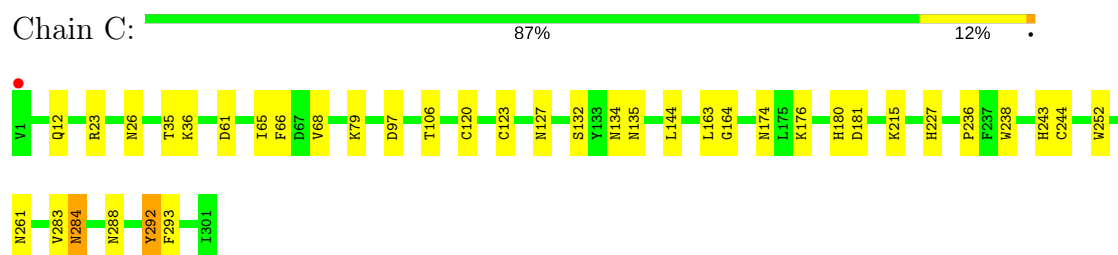
#### • Molecule 1: Triacylglycerol lipase



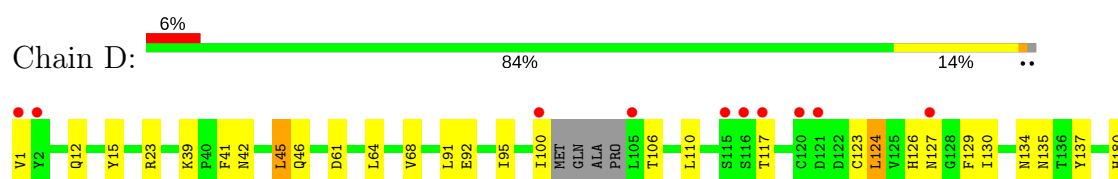
#### • Molecule 1: Triacylglycerol lipase



#### • Molecule 1: Triacylglycerol lipase

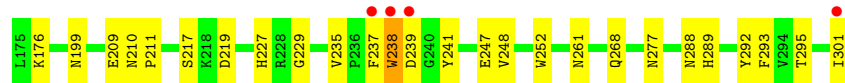
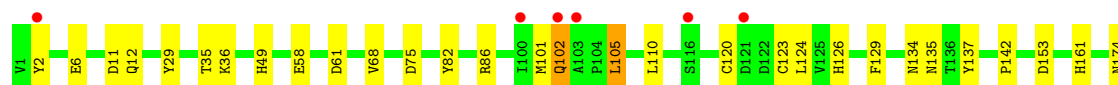
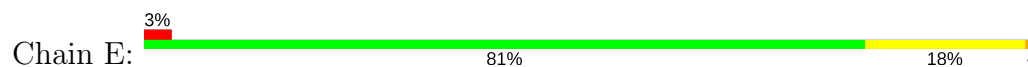


#### • Molecule 1: Triacylglycerol lipase

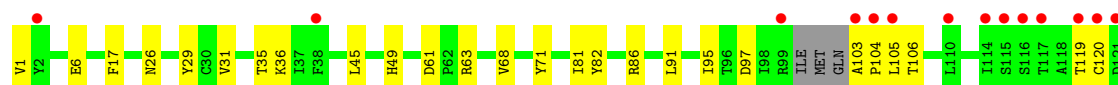
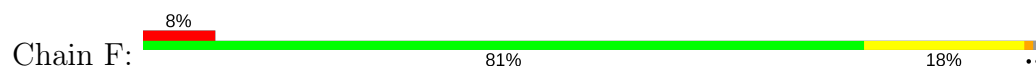




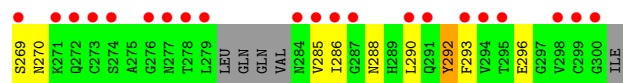
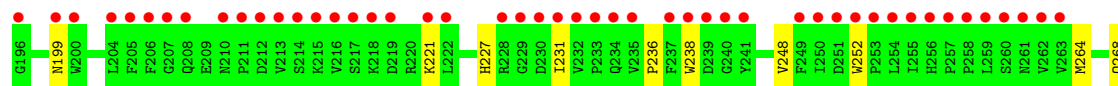
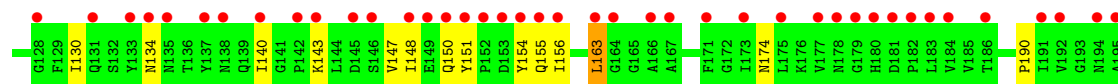
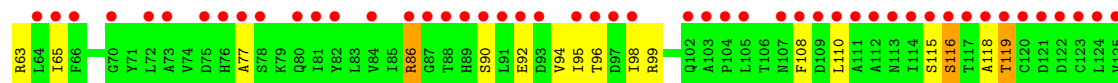
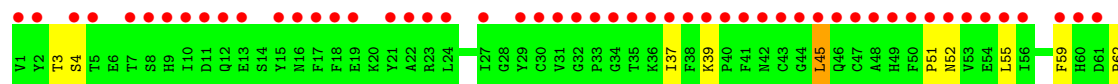
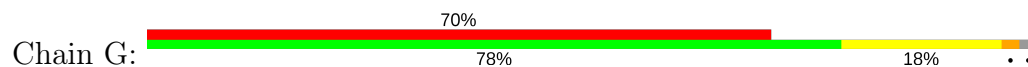
• Molecule 1: Triacylglycerol lipase



• Molecule 1: Triacylglycerol lipase



• Molecule 1: Triacylglycerol lipase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	115.35Å 132.14Å 137.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.70 19.88 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.5 (20.00-1.70) 99.5 (19.88-1.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.00 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, $R_{free}$	0.171 , 0.211 0.170 , 0.210	Depositor DCC
$R_{free}$ test set	11426 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	17.6	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 56.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.018 for -h,l,k	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	18591	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.60% 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 ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MRD, MPD, K, NAG

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	1.36	6/2488 (0.2%)	1.16	3/3389 (0.1%)
1	B	1.28	6/2480 (0.2%)	1.06	2/3379 (0.1%)
1	C	1.35	4/2445 (0.2%)	1.10	5/3332 (0.2%)
1	D	1.23	2/2405 (0.1%)	1.03	0/3276
1	E	1.35	7/2502 (0.3%)	1.06	1/3411 (0.0%)
1	F	1.23	3/2426 (0.1%)	1.02	1/3304 (0.0%)
1	G	0.94	1/2349 (0.0%)	0.73	1/3200 (0.0%)
All	All	1.26	29/17095 (0.2%)	1.03	13/23291 (0.1%)

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	238	TRP	CB-CG	-7.89	1.36	1.50
1	E	137	TYR	CD1-CE1	7.09	1.50	1.39
1	A	177	VAL	CB-CG2	-5.84	1.40	1.52
1	D	15	TYR	CD2-CE2	5.79	1.48	1.39
1	A	296	GLU	CG-CD	5.78	1.60	1.51
1	C	292	TYR	CD2-CE2	5.70	1.47	1.39
1	B	90[A]	SER	C-N	-5.68	1.21	1.34
1	B	90[B]	SER	C-N	-5.68	1.21	1.34
1	A	162	SER	CB-OG	5.66	1.49	1.42
1	F	71	TYR	CE1-CZ	5.65	1.45	1.38
1	A	197	PHE	CE1-CZ	5.59	1.48	1.37
1	E	209	GLU	CD-OE2	-5.53	1.19	1.25
1	A	82	TYR	CD2-CE2	5.50	1.47	1.39
1	B	15	TYR	CE1-CZ	5.47	1.45	1.38
1	B	86	ARG	CG-CD	-5.45	1.38	1.51
1	B	1	VAL	CB-CG1	-5.29	1.41	1.52
1	C	292	TYR	CD1-CE1	5.26	1.47	1.39
1	D	293	PHE	CD2-CE2	-5.25	1.28	1.39
1	F	82	TYR	CD2-CE2	5.23	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	292	TYR	CE1-CZ	5.18	1.45	1.38
1	E	58	GLU	CB-CG	-5.18	1.42	1.52
1	E	235	VAL	CB-CG1	5.15	1.63	1.52
1	B	149	GLU	CB-CG	5.14	1.61	1.52
1	C	164	GLY	N-CA	5.13	1.53	1.46
1	F	17	PHE	CD1-CE1	5.11	1.49	1.39
1	C	215	LYS	CE-NZ	5.09	1.61	1.49
1	E	247	GLU	CD-OE1	5.03	1.31	1.25
1	E	248	VAL	CB-CG1	5.01	1.63	1.52
1	A	154	TYR	CG-CD1	5.00	1.45	1.39

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	45	LEU	CA-CB-CG	7.17	131.78	115.30
1	A	17	PHE	CB-CG-CD2	-5.98	116.61	120.80
1	C	176	LYS	CD-CE-NZ	-5.97	97.97	111.70
1	F	212	ASP	CB-CG-OD1	5.70	123.43	118.30
1	B	67	ASP	CB-CG-OD2	-5.63	113.23	118.30
1	C	144	LEU	CB-CG-CD2	-5.51	101.64	111.00
1	C	23	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	E	11	ASP	CB-CG-OD1	5.50	123.25	118.30
1	C	181	ASP	CB-CG-OD2	-5.42	113.42	118.30
1	A	183	LEU	CB-CG-CD2	-5.31	101.98	111.00
1	C	97	ASP	CB-CG-OD1	5.30	123.08	118.30
1	B	222	LEU	CB-CG-CD2	-5.21	102.15	111.00
1	A	126	HIS	N-CA-CB	-5.09	101.44	110.60

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	2412	0	2345	51	0
1	B	2404	0	2315	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2372	0	2279	22	0
1	D	2334	0	2220	45	1
1	E	2420	0	2317	39	0
1	F	2354	0	2248	57	0
1	G	2289	0	2160	39	1
2	A	28	0	26	0	0
2	B	42	0	39	0	0
2	C	28	0	25	1	0
2	D	28	0	26	1	0
2	E	28	0	25	0	0
2	F	28	0	26	1	0
2	G	28	0	26	3	0
3	A	24	0	42	0	0
3	B	16	0	28	7	0
3	C	24	0	42	3	0
3	D	16	0	28	9	0
3	E	16	0	28	6	0
3	F	8	0	14	0	0
4	A	8	0	14	0	0
4	B	8	0	14	0	0
4	D	8	0	14	1	0
4	F	8	0	14	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
5	G	1	0	0	0	0
6	A	263	0	0	9	0
6	B	281	0	0	5	0
6	C	309	0	0	5	0
6	D	222	0	0	9	0
6	E	277	0	0	13	0
6	F	246	0	0	12	0
6	G	55	0	0	2	0
All	All	18591	0	16315	298	1

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 9.

All (298) 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:G:86:ARG:HH11	1:G:86:ARG:HG3	1.05	1.08
1:E:6[A]:GLU:HG2	6:E:1155:HOH:O	1.51	1.08
3:E:305:MPD:HM1	3:E:305:MPD:H52	1.36	1.04
1:F:103:ALA:HB1	1:F:104:PRO:HD3	1.39	1.03
1:F:127:ASN:O	1:F:130:ILE:HG22	1.66	0.95
1:A:125[A]:VAL:HG23	1:A:130:ILE:HD11	1.49	0.93
1:D:126[A]:HIS:CE1	6:D:1175:HOH:O	2.20	0.93
1:A:81:ILE:HB	1:A:156[B]:ILE:HD13	1.51	0.92
1:F:81:ILE:HD13	1:F:148[A]:ILE:HD12	1.50	0.92
3:C:305:MPD:O2	3:C:305:MPD:H52	1.69	0.92
1:A:125[A]:VAL:CG2	1:A:130:ILE:HD11	2.01	0.90
1:F:61:ASP:OD1	1:F:63[B]:ARG:HG3	1.72	0.89
1:B:5:THR:C	1:B:6[B]:GLU:CA	2.41	0.88
1:B:12:GLN:HG2	3:B:305:MPD:H12	1.59	0.85
3:E:305:MPD:H51	6:F:695:HOH:O	1.77	0.84
1:A:1[A]:VAL:HG12	1:A:242:GLN:OE1	1.78	0.83
3:E:305:MPD:H52	3:E:305:MPD:CM	2.09	0.83
1:B:6[B]:GLU:CA	1:B:7:THR:N	2.43	0.82
1:G:86:ARG:NH1	1:G:86:ARG:HG3	1.81	0.82
1:E:102:GLN:HA	1:E:238:TRP:CH2	2.15	0.81
1:F:180:HIS:HD2	6:F:610:HOH:O	1.61	0.81
1:D:68:VAL:H	1:D:135:ASN:HD22	1.29	0.81
1:B:191[A]:ILE:HD13	1:B:243:HIS:CG	2.15	0.81
1:E:176[B]:LYS:NZ	6:E:2007:HOH:O	2.12	0.80
1:G:86:ARG:CG	1:G:86:ARG:HH11	1.91	0.79
1:D:231:ILE:CG2	1:D:282:GLN:HB2	2.13	0.79
1:F:103:ALA:CB	1:F:104:PRO:HD3	2.12	0.79
1:D:45[A]:LEU:HD22	1:D:45[A]:LEU:O	1.83	0.78
3:C:305:MPD:O2	3:C:305:MPD:C5	2.32	0.77
1:B:119:THR:HG21	1:B:123[B]:CYS:SG	2.26	0.76
1:C:68:VAL:H	1:C:135:ASN:HD22	1.35	0.74
1:D:227:HIS:HD2	1:D:288:ASN:O	1.70	0.74
6:A:812:HOH:O	3:C:305:MPD:H51	1.88	0.74
1:C:227:HIS:HD2	1:C:288:ASN:O	1.70	0.73
3:E:305:MPD:HM1	3:E:305:MPD:C5	2.14	0.73
1:F:103:ALA:HB1	1:F:104:PRO:CD	2.17	0.73
6:A:1008:HOH:O	3:B:305:MPD:C1	2.36	0.72
1:F:49:HIS:HE1	6:F:850:HOH:O	1.71	0.72
3:B:305:MPD:HM3	6:C:359:HOH:O	1.90	0.71
1:E:6[A]:GLU:CG	6:E:1155:HOH:O	2.20	0.71
1:G:148:ILE:HG12	1:G:156:ILE:HD11	1.73	0.71
1:D:91:LEU:O	1:D:95:ILE:HD13	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:103:ALA:CB	1:F:104:PRO:CD	2.70	0.69
1:E:120:CYS:SG	1:E:123[A]:CYS:HB2	2.32	0.69
1:B:35[B]:THR:OG1	6:B:347:HOH:O	2.09	0.69
1:E:261:ASN:HD21	1:F:49:HIS:HA	1.57	0.69
1:A:280[A]:LEU:HD13	6:A:311:HOH:O	1.92	0.69
1:F:45:LEU:HD11	6:F:1548:HOH:O	1.92	0.69
1:F:31:VAL:O	1:F:86:ARG:NH2	2.26	0.69
1:F:91:LEU:O	1:F:95:ILE:HG12	1.91	0.69
3:D:304:MPD:H32	6:D:326:HOH:O	1.93	0.68
1:F:106:THR:HG21	1:F:127:ASN:ND2	2.08	0.68
1:F:81:ILE:HD13	1:F:148[A]:ILE:CD1	2.22	0.68
1:D:12:GLN:HG2	3:D:304:MPD:HM1	1.75	0.68
1:B:191[A]:ILE:CD1	1:B:243:HIS:CD2	2.77	0.67
1:B:191[A]:ILE:HD13	1:B:243:HIS:CD2	2.30	0.67
1:D:106:THR:HB	1:D:130:ILE:HD12	1.77	0.67
1:F:6:GLU:OE2	6:F:2111:HOH:O	2.12	0.67
1:B:227:HIS:HE1	1:B:252:TRP:O	1.78	0.66
1:D:45[A]:LEU:CD2	1:D:45[A]:LEU:O	2.44	0.66
1:E:68:VAL:H	1:E:135:ASN:HD22	1.42	0.66
1:F:1:VAL:O	1:F:1:VAL:HG13	1.96	0.66
1:B:106:THR:HG22	1:B:110:LEU:HD12	1.77	0.66
1:E:238:TRP:CD1	1:E:238:TRP:C	2.65	0.66
1:E:2[A]:TYR:HE2	6:E:1054:HOH:O	1.78	0.65
1:G:95:ILE:HD12	1:G:96:THR:HG23	1.77	0.65
1:A:125[A]:VAL:HG23	1:A:130:ILE:CD1	2.24	0.65
1:D:231:ILE:HG22	1:D:282:GLN:HE21	1.62	0.65
1:F:29:TYR:OH	1:F:161:HIS:HD2	1.80	0.65
1:C:120:CYS:SG	1:C:123[A]:CYS:HB2	2.36	0.65
1:G:130:ILE:HG21	2:G:303:NAG:H82	1.79	0.65
1:A:49:HIS:HA	1:C:261:ASN:HD21	1.61	0.64
1:E:227:HIS:HE1	1:E:252:TRP:O	1.80	0.64
3:E:304:MPD:O4	6:E:952:HOH:O	2.12	0.64
1:B:106:THR:HB	1:B:130:ILE:HD12	1.80	0.64
1:D:126[B]:HIS:HB2	1:D:241:TYR:OH	1.98	0.64
1:F:256:HIS:HE1	6:F:485:HOH:O	1.81	0.63
1:A:29:TYR:OH	1:A:161:HIS:HD2	1.81	0.63
1:F:227:HIS:HD2	1:F:288:ASN:O	1.81	0.63
1:A:261:ASN:HD21	1:B:49:HIS:HA	1.64	0.63
1:E:101:MET:O	1:E:238:TRP:HH2	1.80	0.63
1:G:116:SER:O	6:G:1994:HOH:O	2.15	0.63
1:F:144:LEU:O	1:F:148[B]:ILE:HG13	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:126[A]:HIS:HB3	1:D:129:PHE:CD2	2.34	0.63
1:E:227:HIS:HD2	1:E:288:ASN:O	1.82	0.63
1:D:91:LEU:HD12	4:D:305:MRD:H5C1	1.81	0.62
1:G:227:HIS:HE1	1:G:252:TRP:O	1.81	0.62
1:A:35[B]:THR:O	6:A:397:HOH:O	2.13	0.62
1:D:124[A]:LEU:N	1:D:124[A]:LEU:HD22	2.15	0.62
1:A:68:VAL:H	1:A:135:ASN:HD22	1.45	0.62
1:A:35[B]:THR:HG22	1:F:284:ASN:HA	1.81	0.62
3:D:306:MPD:H13	6:E:561:HOH:O	1.99	0.62
3:D:306:MPD:H11	3:D:306:MPD:O4	1.99	0.61
1:D:41:PHE:H	1:D:42:ASN:HD22	1.47	0.61
1:A:227:HIS:HD2	1:A:288:ASN:O	1.84	0.61
1:D:261:ASN:HD21	1:E:49:HIS:HA	1.66	0.61
3:E:304:MPD:HM1	3:E:304:MPD:O4	2.00	0.61
1:A:148:ILE:HG12	1:A:156[B]:ILE:HD11	1.83	0.61
1:C:79:LYS:NZ	6:C:899:HOH:O	2.34	0.61
1:A:227:HIS:HE1	1:A:252:TRP:O	1.83	0.60
1:G:227:HIS:HD2	1:G:288:ASN:O	1.84	0.60
1:A:99[B]:ARG:CZ	1:A:237:PHE:CZ	2.84	0.60
1:C:180:HIS:HE1	2:C:302:NAG:O3	1.84	0.60
1:D:61:ASP:HB3	1:D:135:ASN:HD21	1.65	0.60
1:D:68:VAL:H	1:D:135:ASN:ND2	1.97	0.60
1:F:68:VAL:H	1:F:135:ASN:HD22	1.47	0.60
1:F:227:HIS:HE1	1:F:252:TRP:O	1.84	0.60
1:A:237:PHE:O	1:A:238:TRP:C	2.40	0.60
1:D:92:GLU:HG2	6:D:1785:HOH:O	2.02	0.60
1:B:119:THR:CG2	1:B:123[B]:CYS:SG	2.90	0.59
1:F:144:LEU:O	1:F:148[A]:ILE:HD13	2.02	0.59
1:B:227:HIS:HD2	1:B:288:ASN:O	1.86	0.59
1:F:228[B]:ARG:CZ	1:F:251:ASP:OD1	2.51	0.59
1:A:49:HIS:HE1	6:A:2097:HOH:O	1.85	0.59
1:C:180:HIS:HD2	6:C:1530:HOH:O	1.86	0.59
1:G:98:ILE:HG22	6:G:2154:HOH:O	2.04	0.58
1:E:176[B]:LYS:HD2	6:E:352:HOH:O	2.04	0.58
3:D:304:MPD:HM2	1:E:12:GLN:HG2	1.84	0.58
1:A:99[B]:ARG:CZ	1:A:237:PHE:HZ	2.16	0.58
1:B:12:GLN:HG2	3:B:305:MPD:C1	2.31	0.58
1:B:191[A]:ILE:HD11	1:B:243:HIS:CD2	2.40	0.57
1:F:119:THR:HG22	1:F:120:CYS:O	2.03	0.57
1:E:105:LEU:HB3	1:E:124:LEU:HB3	1.86	0.57
1:D:124[A]:LEU:CD2	1:D:124[A]:LEU:N	2.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:227:HIS:CE1	1:B:252:TRP:O	2.58	0.57
1:F:105:LEU:HB3	1:F:124:LEU:HB3	1.86	0.57
3:D:304:MPD:H11	6:E:367:HOH:O	2.05	0.56
1:D:45[A]:LEU:HD13	6:D:1343:HOH:O	2.05	0.56
1:G:95:ILE:CD1	1:G:96:THR:HG23	2.36	0.56
1:C:68:VAL:H	1:C:135:ASN:ND2	2.01	0.56
1:D:45[A]:LEU:CD1	6:D:1343:HOH:O	2.54	0.55
1:E:68:VAL:H	1:E:135:ASN:ND2	2.04	0.55
1:B:89:HIS:CE1	1:G:62:PRO:HG2	2.42	0.55
1:G:292:TYR:O	1:G:293:PHE:HB2	2.07	0.55
1:D:180:HIS:HD2	6:D:344:HOH:O	1.89	0.55
1:G:52:ASN:HD22	1:G:77:ALA:HB2	1.70	0.55
1:B:120:CYS:SG	1:B:123[B]:CYS:HB2	2.47	0.55
1:B:119:THR:HG23	1:B:200:TRP:CH2	2.42	0.55
1:E:176[B]:LYS:HE2	6:E:1372:HOH:O	2.07	0.55
1:B:283:VAL:O	1:B:284:ASN:HB2	2.06	0.54
1:F:119:THR:CG2	1:F:123:CYS:HB2	2.37	0.54
1:G:95:ILE:HD12	1:G:96:THR:CG2	2.37	0.54
1:D:228[A]:ARG:HD2	1:D:281:GLN:CD	2.27	0.54
1:E:237:PHE:HA	6:E:1164:HOH:O	2.06	0.54
1:D:126[A]:HIS:HE1	6:D:1175:HOH:O	1.69	0.54
1:A:68:VAL:H	1:A:135:ASN:ND2	2.05	0.54
1:F:180:HIS:HE1	2:F:302:NAG:O3	1.90	0.54
1:G:227:HIS:CE1	1:G:252:TRP:O	2.61	0.54
1:D:106:THR:CG2	1:D:110:LEU:HD22	2.38	0.54
1:E:161:HIS:HE1	1:E:289:HIS:O	1.90	0.54
1:A:238:TRP:HD1	1:A:241:TYR:CE1	2.26	0.53
1:D:180:HIS:HE1	2:D:302:NAG:O3	1.92	0.53
1:D:283:VAL:O	1:D:284:ASN:CB	2.54	0.53
3:B:305:MPD:H13	1:C:12:GLN:HG2	1.91	0.53
1:G:4:SER:O	1:G:270:ASN:HA	2.08	0.53
1:A:30:CYS:HA	1:A:35[A]:THR:HG21	1.90	0.53
1:F:81:ILE:CD1	1:F:148[A]:ILE:HD12	2.32	0.53
1:F:61:ASP:HB3	1:F:135:ASN:HD21	1.74	0.53
1:F:283:VAL:CG1	1:F:284:ASN:N	2.71	0.52
1:F:68:VAL:H	1:F:135:ASN:ND2	2.07	0.52
1:B:210:ASN:OD1	6:B:2149:HOH:O	2.19	0.52
1:B:49:HIS:HE1	6:B:2041:HOH:O	1.92	0.52
1:C:283:VAL:O	1:C:284:ASN:HB2	2.09	0.52
1:D:228[B]:ARG:HD3	1:D:251:ASP:OD1	2.09	0.52
1:D:231:ILE:HG22	1:D:282:GLN:HB2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:238:TRP:HE1	1:E:241:TYR:HE2	1.57	0.52
1:A:120:CYS:SG	1:A:123[A]:CYS:HB2	2.49	0.52
1:A:57:GLU:OE2	6:A:2103:HOH:O	2.19	0.52
1:B:235:VAL:HB	1:B:236:PRO:HA	1.92	0.52
1:B:6[C]:GLU:OE2	6:B:1982:HOH:O	2.18	0.52
1:A:227:HIS:CE1	1:A:252:TRP:O	2.63	0.52
6:A:1008:HOH:O	3:B:305:MPD:H13	2.07	0.52
1:G:63:ARG:HB2	1:G:65:ILE:HG12	1.91	0.51
1:C:227:HIS:HE1	1:C:252:TRP:O	1.92	0.51
1:G:108:PHE:HD2	1:G:119:THR:HG21	1.76	0.51
1:G:130:ILE:CG2	2:G:303:NAG:H82	2.40	0.51
1:E:229:GLY:H	1:E:277:ASN:ND2	2.07	0.51
1:F:283:VAL:HG12	1:F:284:ASN:N	2.25	0.51
1:A:238:TRP:O	1:A:239:ASP:C	2.48	0.51
1:D:92:GLU:CG	6:D:1785:HOH:O	2.58	0.51
1:E:227:HIS:CE1	1:E:252:TRP:O	2.61	0.51
1:B:203:LYS:NZ	1:B:209:GLU:OE2	2.44	0.51
1:A:49:HIS:CE1	6:A:2097:HOH:O	2.63	0.50
1:D:227:HIS:CD2	1:D:288:ASN:O	2.59	0.50
1:E:295[B]:THR:HG21	6:E:1781:HOH:O	2.11	0.50
1:G:3:THR:HG22	1:G:269:SER:HB3	1.93	0.50
1:A:156[A]:ILE:HG21	1:A:175:LEU:HD13	1.94	0.50
1:B:105[B]:LEU:HB3	1:B:124:LEU:HB3	1.93	0.50
1:F:119:THR:CG2	1:F:120:CYS:N	2.74	0.50
1:A:161:HIS:HE1	1:A:289:HIS:O	1.95	0.50
1:G:286:ILE:O	1:G:290:LEU:HG	2.12	0.50
1:G:231:ILE:HG13	1:G:231:ILE:O	2.12	0.49
1:G:95:ILE:HB	1:G:285:VAL:CG1	2.42	0.49
1:E:29:TYR:OH	1:E:161:HIS:HD2	1.94	0.49
1:F:119:THR:HG23	1:F:123:CYS:HB2	1.94	0.49
1:E:238:TRP:HD1	1:E:238:TRP:C	2.15	0.49
1:G:163:LEU:HD12	1:G:190:PRO:HG3	1.95	0.49
1:A:99[B]:ARG:NH2	1:A:237:PHE:HZ	2.11	0.49
1:E:105:LEU:HD22	1:E:105:LEU:N	2.28	0.49
1:F:161:HIS:HE1	1:F:289:HIS:O	1.96	0.49
1:D:221:LYS:HE2	6:D:827:HOH:O	2.13	0.48
1:A:36:LYS:HE2	1:A:38:PHE:CE2	2.48	0.48
1:G:51:PRO:O	1:G:52:ASN:HB2	2.14	0.48
1:A:79:LYS:HD2	1:A:79:LYS:N	2.29	0.48
1:E:199:ASN:ND2	1:E:268:GLN:HE22	2.12	0.48
1:G:115:SER:OG	1:G:118:ALA:HB2	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:86:ARG:HA	1:F:164:GLY:HA3	1.96	0.48
1:A:283:VAL:HG13	1:F:36:LYS:HG2	1.95	0.47
1:F:126:HIS:HB3	1:F:129:PHE:CD2	2.49	0.47
1:G:90:SER:O	1:G:94:VAL:HG23	2.15	0.47
1:D:123:CYS:C	1:D:124[A]:LEU:HD22	2.34	0.47
1:F:227:HIS:CE1	1:F:252:TRP:O	2.67	0.47
1:F:35[B]:THR:O	6:F:345:HOH:O	2.20	0.47
1:B:6[A]:GLU:HB3	1:B:266:GLN:HG3	1.97	0.47
1:D:106:THR:HG23	1:D:110:LEU:HD22	1.97	0.47
1:E:102:GLN:HA	1:E:238:TRP:CZ2	2.49	0.47
1:A:35[A]:THR:HG22	1:A:36:LYS:N	2.28	0.47
1:A:35[A]:THR:HG21	1:A:299:CYS:SG	2.54	0.46
1:G:151:TYR:HB3	1:G:154:TYR:CD1	2.50	0.46
1:E:217:SER:OG	1:E:219[A]:ASP:OD1	2.29	0.46
1:A:99[B]:ARG:NH1	1:A:237:PHE:CZ	2.84	0.46
1:A:126:HIS:HB3	1:A:129:PHE:CD2	2.50	0.46
1:F:1:VAL:O	1:F:1:VAL:CG1	2.63	0.46
1:F:106:THR:CG2	1:F:127:ASN:ND2	2.76	0.46
1:A:238:TRP:HD1	1:A:241:TYR:HE1	1.63	0.46
1:C:106:THR:HG23	1:C:127:ASN:HD21	1.81	0.46
1:A:235:VAL:HB	1:A:236:PRO:HA	1.98	0.46
1:G:155:GLN:HE21	1:G:221:LYS:HE3	1.81	0.46
1:B:106:THR:CG2	1:B:110:LEU:HD12	2.43	0.45
1:G:37:ILE:HB	1:G:55:LEU:HD22	1.97	0.45
1:G:59:PHE:HD2	1:G:140:ILE:HD13	1.82	0.45
1:C:227:HIS:CD2	1:C:288:ASN:O	2.61	0.45
1:G:248:VAL:HG22	1:G:264:MET:SD	2.57	0.45
1:A:86[A]:ARG:NH2	6:F:2022:HOH:O	2.50	0.44
1:B:191[A]:ILE:CD1	1:B:243:HIS:CG	2.93	0.44
1:E:61:ASP:HB3	1:E:135:ASN:HD21	1.83	0.44
1:G:143:LYS:O	1:G:147:VAL:HG23	2.17	0.44
1:F:256:HIS:HD2	6:F:688:HOH:O	2.01	0.44
1:D:45[A]:LEU:HD21	1:F:252:TRP:HH2	1.81	0.44
1:G:199:ASN:ND2	1:G:268:GLN:HE22	2.15	0.44
1:C:61:ASP:HB3	1:C:135:ASN:HD21	1.83	0.44
1:F:119:THR:HG23	1:F:123:CYS:CB	2.48	0.44
1:A:99[B]:ARG:HG3	1:A:100:ILE:HD13	2.00	0.44
1:C:36:LYS:CG	6:C:2107:HOH:O	2.66	0.43
1:F:126:HIS:HD2	1:F:128:GLY:N	2.16	0.43
1:C:227:HIS:CE1	1:C:252:TRP:O	2.70	0.43
1:F:127:ASN:C	1:F:130:ILE:HG22	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:301:ILE:C	6:E:1102:HOH:O	2.57	0.43
1:D:210:ASN:N	1:D:211:PRO:CD	2.81	0.43
1:C:65:ILE:HG23	1:C:66:PHE:CD2	2.54	0.42
1:A:203:LYS:HE2	1:A:209:GLU:HG3	2.01	0.42
1:D:227:HIS:HE1	1:D:252:TRP:O	2.02	0.42
1:C:132[A]:SER:OG	1:C:163:LEU:HD11	2.19	0.42
3:D:306:MPD:C1	3:D:306:MPD:O4	2.66	0.42
1:A:35[B]:THR:HG23	6:F:343:HOH:O	2.19	0.42
1:B:126:HIS:HB3	1:B:129:PHE:CD2	2.55	0.42
1:C:236:PRO:HB2	1:C:238:TRP:CD1	2.54	0.42
1:E:75:ASP:HB2	1:E:82:TYR:CE2	2.54	0.42
1:G:236:PRO:HB3	1:G:238:TRP:CZ2	2.54	0.42
1:A:247:GLU:HB3	1:A:265:CYS:HB2	2.02	0.42
1:B:45:LEU:HD11	6:B:2042:HOH:O	2.20	0.42
1:C:243:HIS:HB3	1:C:244:CYS:O	2.20	0.42
1:F:286:ILE:HD12	6:F:343:HOH:O	2.19	0.42
1:E:292:TYR:O	1:E:293:PHE:HB2	2.19	0.41
1:F:49:HIS:CE1	6:F:850:HOH:O	2.57	0.41
1:C:292:TYR:O	1:C:293:PHE:HB2	2.20	0.41
1:D:12:GLN:HG2	3:D:304:MPD:CM	2.46	0.41
1:E:105:LEU:CD2	1:E:105:LEU:N	2.83	0.41
1:E:126:HIS:HD2	1:E:129:PHE:H	1.69	0.41
1:B:199:ASN:ND2	1:B:268:GLN:HE22	2.17	0.41
1:D:100:ILE:O	1:D:100:ILE:HG23	2.20	0.41
1:D:137:TYR:C	1:D:137:TYR:CD2	2.94	0.41
3:D:304:MPD:CM	6:E:503:HOH:O	2.68	0.41
1:G:110:LEU:O	2:G:303:NAG:H3	2.21	0.41
1:C:35:THR:O	6:C:1782:HOH:O	2.22	0.41
1:D:95:ILE:HD12	1:D:95:ILE:N	2.36	0.41
1:F:126:HIS:CD2	1:F:129:PHE:H	2.39	0.41
1:F:228[B]:ARG:NH2	1:F:251:ASP:OD1	2.54	0.41
1:B:106:THR:HB	1:B:130:ILE:CD1	2.49	0.41
1:G:95:ILE:HB	1:G:285:VAL:HG12	2.02	0.41
1:A:283:VAL:HG13	1:F:36:LYS:CG	2.51	0.41
1:A:65:ILE:HG23	1:A:66:PHE:CD2	2.56	0.41
6:A:793:HOH:O	3:B:305:MPD:H31	2.21	0.41
1:E:210[B]:ASN:N	1:E:211:PRO:CD	2.83	0.41
1:A:203:LYS:HE2	1:A:209:GLU:CG	2.51	0.40
1:A:238:TRP:CD1	1:A:241:TYR:CE1	3.09	0.40
1:B:125:VAL:HG13	1:B:192:VAL:HG12	2.04	0.40
1:D:126[A]:HIS:HB3	1:D:129:PHE:HD2	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:210:ASN:N	1:D:211:PRO:HD3	2.37	0.40
1:G:290:LEU:HD22	1:G:296:GLU:O	2.21	0.40
1:D:23:ARG:HG2	1:D:46:GLN:OE1	2.22	0.40
1:E:35[B]:THR:O	1:E:36:LYS:HG2	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:64:LEU:CD2	1:G:96:THR:CG2[4_565]	2.14	0.06

## 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	308/301 (102%)	292 (95%)	16 (5%)	0	100	100
1	B	308/301 (102%)	296 (96%)	11 (4%)	1 (0%)	44	25
1	C	305/301 (101%)	293 (96%)	11 (4%)	1 (0%)	44	25
1	D	302/301 (100%)	287 (95%)	14 (5%)	1 (0%)	44	25
1	E	312/301 (104%)	299 (96%)	12 (4%)	1 (0%)	44	25
1	F	301/301 (100%)	290 (96%)	9 (3%)	2 (1%)	25	9
1	G	293/301 (97%)	278 (95%)	15 (5%)	0	100	100
All	All	2129/2107 (101%)	2035 (96%)	88 (4%)	6 (0%)	44	25

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	284	ASN
1	E	239	ASP

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Mol	Chain	Res	Type
1	B	284	ASN
1	C	284	ASN
1	F	162	SER
1	F	283	VAL

### 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	267/260 (103%)	259 (97%)	8 (3%)	46	25
1	B	268/260 (103%)	260 (97%)	8 (3%)	46	25
1	C	263/260 (101%)	260 (99%)	3 (1%)	78	68
1	D	253/260 (97%)	244 (96%)	9 (4%)	40	18
1	E	268/260 (103%)	261 (97%)	7 (3%)	51	31
1	F	255/260 (98%)	247 (97%)	8 (3%)	45	24
1	G	246/260 (95%)	235 (96%)	11 (4%)	32	12
All	All	1820/1820 (100%)	1766 (97%)	54 (3%)	50	25

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	35[A]	THR
1	A	35[B]	THR
1	A	36	LYS
1	A	102	GLN
1	A	134	ASN
1	A	174	ASN
1	A	237	PHE
1	B	6[A]	GLU
1	B	6[C]	GLU
1	B	6[B]	GLU
1	B	102	GLN
1	B	116	SER

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Mol	Chain	Res	Type
1	B	119	THR
1	B	134	ASN
1	B	174	ASN
1	C	26	ASN
1	C	134	ASN
1	C	174	ASN
1	D	1	VAL
1	D	39	LYS
1	D	45[A]	LEU
1	D	45[B]	LEU
1	D	117	THR
1	D	124[A]	LEU
1	D	124[B]	LEU
1	D	127	ASN
1	D	134	ASN
1	E	86	ARG
1	E	102	GLN
1	E	105	LEU
1	E	110	LEU
1	E	134	ASN
1	E	142	PRO
1	E	174	ASN
1	F	26	ASN
1	F	97	ASP
1	F	134	ASN
1	F	148[A]	ILE
1	F	148[B]	ILE
1	F	174	ASN
1	F	231	ILE
1	F	242	GLN
1	G	39	LYS
1	G	45	LEU
1	G	86	ARG
1	G	92	GLU
1	G	99	ARG
1	G	116	SER
1	G	119	THR
1	G	134	ASN
1	G	150	GLN
1	G	163	LEU
1	G	174	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such



sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	HIS
1	A	60	HIS
1	A	135	ASN
1	A	138	ASN
1	A	161	HIS
1	A	174	ASN
1	A	178	ASN
1	A	199	ASN
1	A	227	HIS
1	A	261	ASN
1	A	268	GLN
1	B	49	HIS
1	B	127	ASN
1	B	178	ASN
1	B	199	ASN
1	B	227	HIS
1	C	60	HIS
1	C	127	ASN
1	C	131	GLN
1	C	135	ASN
1	C	178	ASN
1	C	180	HIS
1	C	227	HIS
1	C	261	ASN
1	D	42	ASN
1	D	131	GLN
1	D	135	ASN
1	D	178	ASN
1	D	180	HIS
1	D	227	HIS
1	D	261	ASN
1	D	282	GLN
1	E	126	HIS
1	E	135	ASN
1	E	161	HIS
1	E	178	ASN
1	E	199	ASN
1	E	227	HIS
1	E	242	GLN
1	E	261	ASN
1	E	277	ASN
1	F	49	HIS

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Mol	Chain	Res	Type
1	F	60	HIS
1	F	126	HIS
1	F	127	ASN
1	F	135	ASN
1	F	161	HIS
1	F	174	ASN
1	F	178	ASN
1	F	180	HIS
1	F	189	GLN
1	F	227	HIS
1	F	256	HIS
1	G	52	ASN
1	G	174	ASN
1	G	178	ASN
1	G	199	ASN
1	G	227	HIS
1	G	234	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](#)

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](#)

Of 39 ligands modelled in this entry, 7 are monoatomic - leaving 32 for Mogul analysis.

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	NAG	A	302	1	14,14,15	0.89	1 (7%)	15,19,21	1.12	2 (13%)
2	NAG	A	303	1	14,14,15	0.62	0	15,19,21	1.59	3 (20%)
3	MPD	A	304	-	7,7,7	0.47	0	9,10,10	0.70	0
3	MPD	A	305	-	7,7,7	0.26	0	9,10,10	0.24	0
3	MPD	A	306	-	7,7,7	0.35	0	9,10,10	0.58	0
4	MRD	A	307	-	7,7,7	1.09	0	9,10,10	1.32	1 (11%)
2	NAG	B	302[A]	1	14,14,15	0.54	0	15,19,21	1.37	1 (6%)
2	NAG	B	302[B]	1	14,14,15	0.54	0	15,19,21	1.40	2 (13%)
2	NAG	B	303	1	14,14,15	0.70	0	15,19,21	1.20	2 (13%)
3	MPD	B	304	-	7,7,7	0.50	0	9,10,10	0.57	0
3	MPD	B	305	-	7,7,7	1.42	1 (14%)	9,10,10	0.95	0
4	MRD	B	306	-	7,7,7	0.78	0	9,10,10	0.95	0
2	NAG	C	302	1	14,14,15	1.41	1 (7%)	15,19,21	2.23	5 (33%)
2	NAG	C	303	1	14,14,15	1.03	0	15,19,21	1.52	2 (13%)
3	MPD	C	304	-	7,7,7	0.57	0	9,10,10	1.44	2 (22%)
3	MPD	C	305	-	7,7,7	0.55	0	9,10,10	0.51	0
3	MPD	C	306	-	7,7,7	0.49	0	9,10,10	0.48	0
2	NAG	D	302	1	14,14,15	1.09	0	15,19,21	2.38	5 (33%)
2	NAG	D	303	1	14,14,15	0.71	0	15,19,21	1.92	5 (33%)
3	MPD	D	304	-	7,7,7	2.10	3 (42%)	9,10,10	1.76	4 (44%)
4	MRD	D	305	-	7,7,7	0.48	0	9,10,10	0.61	0
3	MPD	D	306	-	7,7,7	0.42	0	9,10,10	0.82	0
2	NAG	E	302	1	14,14,15	1.05	1 (7%)	15,19,21	2.64	4 (26%)
2	NAG	E	303	1	14,14,15	1.06	1 (7%)	15,19,21	3.09	10 (66%)
3	MPD	E	304	-	7,7,7	0.25	0	9,10,10	1.07	0
3	MPD	E	305	-	7,7,7	0.28	0	9,10,10	1.25	1 (11%)
2	NAG	F	302	1	14,14,15	0.94	0	15,19,21	1.60	4 (26%)
2	NAG	F	303	1	14,14,15	0.72	0	15,19,21	1.77	5 (33%)
4	MRD	F	304	-	7,7,7	0.20	0	9,10,10	0.57	0
3	MPD	F	305	-	7,7,7	0.41	0	9,10,10	0.87	0
2	NAG	G	302	1	14,14,15	0.61	0	15,19,21	1.11	1 (6%)
2	NAG	G	303	1	14,14,15	0.66	0	15,19,21	1.89	4 (26%)

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	NAG	A	302	1	-	0/6/23/26	0/1/1/1
2	NAG	A	303	1	-	0/6/23/26	0/1/1/1
3	MPD	A	304	-	-	0/5/5/5	0/0/0/0
3	MPD	A	305	-	-	0/5/5/5	0/0/0/0
3	MPD	A	306	-	-	0/5/5/5	0/0/0/0
4	MRD	A	307	-	-	0/5/5/5	0/0/0/0
2	NAG	B	302[A]	1	-	0/6/23/26	0/1/1/1
2	NAG	B	302[B]	1	-	0/6/23/26	0/1/1/1
2	NAG	B	303	1	-	0/6/23/26	0/1/1/1
3	MPD	B	304	-	-	0/5/5/5	0/0/0/0
3	MPD	B	305	-	-	0/5/5/5	0/0/0/0
4	MRD	B	306	-	-	0/5/5/5	0/0/0/0
2	NAG	C	302	1	-	0/6/23/26	0/1/1/1
2	NAG	C	303	1	-	0/6/23/26	0/1/1/1
3	MPD	C	304	-	-	0/5/5/5	0/0/0/0
3	MPD	C	305	-	-	0/5/5/5	0/0/0/0
3	MPD	C	306	-	-	0/5/5/5	0/0/0/0
2	NAG	D	302	1	-	0/6/23/26	0/1/1/1
2	NAG	D	303	1	-	0/6/23/26	0/1/1/1
3	MPD	D	304	-	-	0/5/5/5	0/0/0/0
4	MRD	D	305	-	-	0/5/5/5	0/0/0/0
3	MPD	D	306	-	-	0/5/5/5	0/0/0/0
2	NAG	E	302	1	-	0/6/23/26	0/1/1/1
2	NAG	E	303	1	-	0/6/23/26	0/1/1/1
3	MPD	E	304	-	-	0/5/5/5	0/0/0/0
3	MPD	E	305	-	-	0/5/5/5	0/0/0/0
2	NAG	F	302	1	-	0/6/23/26	0/1/1/1
2	NAG	F	303	1	-	0/6/23/26	0/1/1/1
4	MRD	F	304	-	-	0/5/5/5	0/0/0/0
3	MPD	F	305	-	-	0/5/5/5	0/0/0/0
2	NAG	G	302	1	-	0/6/23/26	0/1/1/1
2	NAG	G	303	1	-	0/6/23/26	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	304	MPD	CM-C2	-2.72	1.43	1.52
2	A	302	NAG	O5-C1	-2.04	1.40	1.43
2	E	303	NAG	C1-C2	-2.03	1.49	1.52
3	D	304	MPD	C3-C2	2.01	1.59	1.53
2	E	302	NAG	C1-C2	2.30	1.55	1.52
3	B	305	MPD	O2-C2	2.68	1.51	1.44
2	C	302	NAG	C1-C2	4.01	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	304	MPD	O2-C2	4.12	1.55	1.44

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	303	NAG	C1-O5-C5	-7.17	102.29	112.17
2	E	302	NAG	O5-C1-C2	-5.30	104.09	111.47
2	E	302	NAG	C3-C4-C5	-5.16	101.12	110.22
2	D	302	NAG	O5-C1-C2	-4.65	105.00	111.47
2	C	302	NAG	O6-C6-C5	-4.51	96.17	111.34
2	C	302	NAG	O5-C1-C2	-4.44	105.29	111.47
2	B	302[A]	NAG	O5-C1-C2	-4.11	105.75	111.47
2	E	303	NAG	O3-C3-C2	-4.06	100.69	109.39
2	D	302	NAG	C2-N2-C7	-3.91	117.23	122.94
2	E	303	NAG	O7-C7-C8	-3.55	115.59	122.06
4	A	307	MRD	CM-C2-C1	-3.30	103.06	110.42
2	C	303	NAG	O4-C4-C3	-3.12	103.56	110.36
2	C	303	NAG	C2-N2-C7	-2.91	118.70	122.94
3	D	304	MPD	CM-C2-C1	-2.91	103.94	110.42
2	F	302	NAG	O5-C1-C2	-2.90	107.44	111.47
3	C	304	MPD	CM-C2-C1	-2.87	104.01	110.42
3	E	305	MPD	CM-C2-C1	-2.80	104.18	110.42
2	F	302	NAG	O7-C7-C8	-2.57	117.39	122.06
2	B	303	NAG	O5-C1-C2	-2.54	107.94	111.47
2	B	302[B]	NAG	O5-C1-C2	-2.53	107.95	111.47
2	A	303	NAG	O4-C4-C3	-2.50	104.92	110.36
2	C	302	NAG	O7-C7-N2	-2.48	117.14	121.92
2	B	303	NAG	C2-N2-C7	-2.41	119.43	122.94
2	G	303	NAG	O5-C1-C2	-2.40	108.13	111.47
2	A	302	NAG	C3-C4-C5	-2.23	106.28	110.22
3	D	304	MPD	CM-C2-C3	-2.11	99.55	110.08
2	A	302	NAG	O5-C1-C2	-2.11	108.53	111.47
2	E	303	NAG	C2-N2-C7	-2.11	119.87	122.94
2	E	303	NAG	C3-C4-C5	-2.09	106.53	110.22
2	F	303	NAG	O5-C1-C2	-2.07	108.60	111.47
2	F	302	NAG	C2-N2-C7	-2.05	119.95	122.94
2	G	303	NAG	O7-C7-N2	2.02	125.80	121.92
2	E	303	NAG	C1-C2-N2	2.03	113.95	110.49
3	D	304	MPD	O2-C2-C1	2.07	115.16	108.00
2	F	303	NAG	C4-C3-C2	2.07	114.06	111.02
2	D	302	NAG	C8-C7-N2	2.09	119.89	116.11
2	D	303	NAG	O4-C4-C5	2.09	114.56	109.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	303	NAG	O7-C7-N2	2.27	126.29	121.92
2	D	303	NAG	C1-C2-N2	2.40	114.58	110.49
2	D	303	NAG	C3-C4-C5	2.40	114.44	110.22
3	C	304	MPD	O4-C4-C5	2.41	120.53	109.46
2	E	303	NAG	C8-C7-N2	2.42	120.47	116.11
2	A	303	NAG	C4-C3-C2	2.46	114.62	111.02
2	G	302	NAG	C1-O5-C5	2.48	115.59	112.17
3	D	304	MPD	O2-C2-C3	2.53	119.92	109.88
2	E	303	NAG	O6-C6-C5	2.56	119.95	111.34
2	C	302	NAG	C8-C7-N2	2.61	120.83	116.11
2	D	303	NAG	C2-N2-C7	2.77	126.98	122.94
2	C	302	NAG	C1-O5-C5	2.83	116.06	112.17
2	F	302	NAG	C1-C2-N2	2.93	115.49	110.49
2	G	303	NAG	C2-N2-C7	2.98	127.30	122.94
2	B	302[B]	NAG	C1-C2-N2	3.01	115.63	110.49
2	F	303	NAG	C3-C4-C5	3.21	115.87	110.22
2	A	303	NAG	C1-O5-C5	3.23	116.62	112.17
2	D	302	NAG	C6-C5-C4	3.32	120.78	113.00
2	F	303	NAG	C2-N2-C7	3.48	128.02	122.94
2	E	303	NAG	O4-C4-C5	3.52	118.14	109.28
2	E	302	NAG	C4-C3-C2	3.76	116.53	111.02
2	E	303	NAG	C6-C5-C4	4.06	122.50	113.00
2	E	302	NAG	C1-C2-N2	4.24	117.72	110.49
2	D	303	NAG	C4-C3-C2	4.35	117.39	111.02
2	D	302	NAG	C4-C3-C2	4.37	117.42	111.02
2	G	303	NAG	C1-O5-C5	4.77	118.74	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	305	MPD	7	0
2	C	302	NAG	1	0
3	C	305	MPD	3	0
2	D	302	NAG	1	0
3	D	304	MPD	6	0
4	D	305	MRD	1	0
3	D	306	MPD	3	0
3	E	304	MPD	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	305	MPD	4	0
2	F	302	NAG	1	0
2	G	303	NAG	3	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	301/301 (100%)	0.07	13 (4%) 36 41	8, 16, 35, 49	0
1	B	301/301 (100%)	-0.08	8 (2%) 55 60	8, 16, 30, 42	0
1	C	301/301 (100%)	-0.20	1 (0%) 93 94	8, 15, 25, 32	0
1	D	297/301 (98%)	0.18	17 (5%) 24 28	8, 19, 42, 60	0
1	E	301/301 (100%)	-0.09	10 (3%) 47 53	8, 15, 34, 52	0
1	F	298/301 (99%)	0.21	23 (7%) 14 17	8, 19, 46, 56	0
1	G	296/301 (98%)	3.15	211 (71%) 0 0	28, 42, 66, 74	0
All	All	2095/2107 (99%)	0.46	283 (13%) 3 4	8, 18, 49, 74	0

All (283) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	45	LEU	13.5
1	G	300	GLY	10.5
1	G	279	LEU	10.0
1	G	278	THR	8.5
1	G	237	PHE	8.0
1	G	105	LEU	7.8
1	G	286	ILE	7.8
1	G	77	ALA	7.7
1	D	100	ILE	7.7
1	G	255	ILE	7.5
1	G	299	CYS	7.1
1	G	238	TRP	7.1
1	G	298	VAL	6.9
1	G	252	TRP	6.9
1	G	152	PRO	6.8
1	G	35	THR	6.7
1	G	38	PHE	6.7

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Mol	Chain	Res	Type	RSRZ
1	G	48	ALA	6.7
1	G	219	ASP	6.6
1	G	1	VAL	6.1
1	G	10	ILE	5.9
1	G	88	THR	5.9
1	A	103	ALA	5.9
1	G	148	ILE	5.8
1	G	285	VAL	5.8
1	D	1	VAL	5.8
1	G	41	PHE	5.8
1	G	114	ILE	5.6
1	G	110	LEU	5.6
1	F	278	THR	5.6
1	G	149	GLU	5.6
1	G	121	ASP	5.6
1	G	95	ILE	5.5
1	F	238	TRP	5.4
1	A	104	PRO	5.4
1	G	179	GLY	5.4
1	G	258	PRO	5.4
1	G	256	HIS	5.4
1	G	150	GLN	5.4
1	G	216	VAL	5.2
1	G	211	PRO	5.2
1	G	90	SER	5.2
1	G	137	TYR	5.2
1	G	260	SER	5.1
1	G	51	PRO	5.1
1	G	30	CYS	5.1
1	G	43	CYS	5.1
1	G	151	TYR	5.0
1	E	116	SER	5.0
1	G	277	ASN	5.0
1	G	44	GLY	5.0
1	G	42	ASN	4.9
1	G	284	ASN	4.9
1	G	120	CYS	4.9
1	G	98	ILE	4.9
1	G	213	VAL	4.9
1	G	49	HIS	4.9
1	G	181	ASP	4.8
1	G	46	GLN	4.8

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Mol	Chain	Res	Type	RSRZ
1	G	33	PRO	4.8
1	G	196	GLY	4.8
1	G	206	PHE	4.7
1	G	37	ILE	4.7
1	G	123	CYS	4.6
1	G	50	PHE	4.6
1	G	239	ASP	4.6
1	A	239	ASP	4.6
1	D	280	LEU	4.5
1	G	18	PHE	4.5
1	G	192	VAL	4.5
1	F	104	PRO	4.5
1	G	29	TYR	4.5
1	G	59	PHE	4.4
1	F	239	ASP	4.4
1	G	208	GLN	4.4
1	A	100	ILE	4.4
1	F	116	SER	4.4
1	G	154	TYR	4.3
1	G	72	LEU	4.3
1	G	78	SER	4.3
1	G	66	PHE	4.3
1	G	2	TYR	4.3
1	G	109	ASP	4.3
1	G	200	TRP	4.3
1	G	140	ILE	4.3
1	F	283	VAL	4.3
1	G	207	GLY	4.2
1	A	116	SER	4.2
1	G	122	ASP	4.2
1	G	180	HIS	4.2
1	G	53	VAL	4.2
1	G	153	ASP	4.2
1	F	282	GLN	4.2
1	G	118	ALA	4.2
1	G	96	THR	4.2
1	G	272	GLN	4.1
1	G	166	ALA	4.1
1	G	64	LEU	4.1
1	G	7	THR	4.1
1	E	238	TRP	4.1
1	G	104	PRO	4.1

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Mol	Chain	Res	Type	RSRZ
1	G	257	PRO	4.1
1	G	254	LEU	4.1
1	G	89	HIS	4.0
1	G	276	GLY	4.0
1	G	173	ILE	4.0
1	G	117	THR	4.0
1	G	116	SER	4.0
1	A	300	GLY	4.0
1	G	32	GLY	3.9
1	G	91	LEU	3.9
1	F	237	PHE	3.9
1	G	17	PHE	3.8
1	G	229	GLY	3.8
1	G	259	LEU	3.8
1	E	103	ALA	3.8
1	G	39	LYS	3.8
1	G	5	THR	3.7
1	G	261	ASN	3.7
1	C	1	VAL	3.7
1	G	128	GLY	3.7
1	G	204	LEU	3.6
1	G	215	LYS	3.5
1	D	239	ASP	3.5
1	G	232	VAL	3.5
1	F	103	ALA	3.5
1	E	239	ASP	3.5
1	F	279[A]	LEU	3.4
1	G	84	VAL	3.4
1	G	177	VAL	3.4
1	D	116	SER	3.4
1	G	34	GLY	3.4
1	G	40	PRO	3.4
1	F	280	LEU	3.4
1	F	121	ASP	3.4
1	G	212	ASP	3.4
1	D	278	THR	3.4
1	A	101	MET	3.4
1	G	293	PHE	3.4
1	G	111	ALA	3.3
1	G	195	ALA	3.3
1	G	102	GLN	3.3
1	E	237	PHE	3.3

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Mol	Chain	Res	Type	RSRZ
1	E	102	GLN	3.3
1	G	82	TYR	3.3
1	G	210	ASN	3.3
1	G	23	ARG	3.3
1	G	146	SER	3.3
1	A	301	ILE	3.3
1	F	119	THR	3.2
1	G	97	ASP	3.2
1	G	235	VAL	3.2
1	G	80	GLN	3.2
1	G	115	SER	3.2
1	G	52	ASN	3.2
1	F	2	TYR	3.2
1	B	115	SER	3.2
1	G	103	ALA	3.2
1	D	121	ASP	3.2
1	E	301	ILE	3.1
1	G	76	HIS	3.1
1	G	12	GLN	3.1
1	G	287	GLY	3.1
1	G	291	GLN	3.1
1	A	238	TRP	3.1
1	G	178	ASN	3.1
1	B	116	SER	3.1
1	G	184	VAL	3.1
1	G	217	SER	3.0
1	B	238	TRP	3.0
1	F	120	CYS	3.0
1	G	218	LYS	3.0
1	G	27	ILE	3.0
1	G	22	ALA	3.0
1	D	120	CYS	3.0
1	G	73	ALA	3.0
1	G	119	THR	3.0
1	G	295	THR	3.0
1	B	239	ASP	2.9
1	G	93	ASP	2.9
1	G	230	ASP	2.9
1	G	16	ASN	2.9
1	D	117	THR	2.9
1	G	135	ASN	2.9
1	G	164	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	G	290	LEU	2.9
1	G	231	ILE	2.9
1	G	228	ARG	2.9
1	G	87	GLY	2.9
1	G	191	ILE	2.9
1	G	241	TYR	2.9
1	G	273	CYS	2.8
1	G	11	ASP	2.8
1	G	199	ASN	2.8
1	G	234	GLN	2.8
1	G	271	LYS	2.8
1	G	262	VAL	2.8
1	D	281	GLN	2.8
1	G	182	PRO	2.8
1	G	125	VAL	2.8
1	F	99	ARG	2.8
1	G	138	ASN	2.8
1	G	92	GLU	2.7
1	D	105	LEU	2.7
1	G	171	PHE	2.7
1	D	301	ILE	2.7
1	A	117	THR	2.7
1	B	2	TYR	2.7
1	D	238	TRP	2.7
1	G	214	SER	2.7
1	G	9	HIS	2.7
1	B	104	PRO	2.7
1	E	121	ASP	2.7
1	G	70	GLY	2.6
1	G	47	CYS	2.6
1	G	155	GLN	2.6
1	G	156	ILE	2.6
1	G	8	SER	2.6
1	G	24	LEU	2.6
1	G	205	PHE	2.6
1	G	142	PRO	2.6
1	G	31	VAL	2.6
1	G	131	GLN	2.6
1	G	113	ASN	2.6
1	E	100	ILE	2.6
1	G	167	ALA	2.6
1	G	145	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	G	81	ILE	2.5
1	G	36	LYS	2.5
1	G	143	LYS	2.5
1	G	13	GLU	2.5
1	D	115	SER	2.5
1	G	107	ASN	2.4
1	F	114	ILE	2.4
1	G	56	ILE	2.4
1	F	110	LEU	2.4
1	G	55	LEU	2.4
1	G	163	LEU	2.4
1	G	133	TYR	2.4
1	G	134	ASN	2.4
1	A	121	ASP	2.4
1	G	294	VAL	2.4
1	F	117	THR	2.4
1	G	240	GLY	2.4
1	G	183	LEU	2.3
1	G	250	ILE	2.3
1	G	60	HIS	2.3
1	G	253	PRO	2.3
1	D	127	ASN	2.3
1	G	175	LEU	2.3
1	B	117	THR	2.3
1	F	115	SER	2.2
1	G	75	ASP	2.2
1	G	233	PRO	2.2
1	G	61	ASP	2.2
1	D	2[A]	TYR	2.2
1	G	21	TYR	2.2
1	G	263	VAL	2.2
1	G	19	GLU	2.2
1	G	274[A]	SER	2.2
1	G	65	ILE	2.2
1	G	194	ASN	2.2
1	G	108	PHE	2.2
1	G	222	LEU	2.2
1	B	101	MET	2.1
1	E	2[A]	TYR	2.1
1	F	123	CYS	2.1
1	F	105	LEU	2.1
1	G	112	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	54	GLU	2.1
1	G	4	SER	2.1
1	G	186	THR	2.1
1	D	283	VAL	2.1
1	G	251	ASP	2.1
1	G	269	SER	2.1
1	G	15	TYR	2.1
1	G	124	LEU	2.1
1	G	221	LYS	2.0
1	A	240	GLY	2.0
1	A	125[A]	VAL	2.0
1	F	38	PHE	2.0
1	G	249	PHE	2.0
1	G	86	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(Å <sup>2</sup> )	Q<0.9
4	MRD	B	306	8/8	0.80	0.22	9.53	19,29,34,34	0
3	MPD	E	304	8/8	0.93	0.18	6.61	38,42,44,45	0
3	MPD	C	304	8/8	0.84	0.17	5.17	21,27,30,31	0
4	MRD	A	307	8/8	0.85	0.17	5.05	20,28,30,33	0
2	NAG	C	303	14/15	0.91	0.12	5.01	19,24,28,28	0
4	MRD	D	305	8/8	0.92	0.15	3.38	39,42,42,43	0
3	MPD	A	304	8/8	0.82	0.17	3.26	31,34,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAG	G	303	14/15	0.67	0.41	3.17	67,73,74,75	0
3	MPD	F	305	8/8	0.94	0.14	2.76	34,38,46,49	0
3	MPD	A	306	8/8	0.90	0.16	2.45	43,46,54,54	0
3	MPD	C	306	8/8	0.79	0.15	2.28	56,58,60,60	0
2	NAG	G	302	14/15	0.54	0.36	2.13	58,60,63,63	0
2	NAG	E	303	14/15	0.70	0.24	1.79	30,39,41,46	0
2	NAG	D	303	14/15	0.81	0.17	1.62	41,45,48,48	0
2	NAG	B	303	14/15	0.93	0.13	1.32	22,26,30,32	0
2	NAG	F	303	14/15	0.84	0.16	1.13	32,39,43,46	0
2	NAG	B	302[A]	14/15	0.95	0.09	0.52	20,22,25,25	14
2	NAG	A	302	14/15	0.92	0.10	0.45	21,24,26,29	0
2	NAG	B	302[B]	14/15	0.95	0.09	0.44	19,22,24,26	14
2	NAG	F	302	14/15	0.93	0.09	-0.13	22,26,32,40	0
2	NAG	C	302	14/15	0.94	0.08	-0.48	15,20,24,24	0
2	NAG	A	303	14/15	0.94	0.10	-0.55	26,32,36,36	0
2	NAG	D	302	14/15	0.95	0.08	-1.03	16,22,26,28	0
2	NAG	E	302	14/15	0.97	0.06	-1.22	14,17,23,25	0
5	K	F	306	1/1	0.98	0.07	-1.41	25,25,25,25	0
5	K	D	307	1/1	0.99	0.07	-1.46	25,25,25,25	0
5	K	A	308	1/1	0.99	0.05	-1.99	21,21,21,21	0
5	K	E	306	1/1	0.98	0.06	-2.22	20,20,20,20	0
5	K	C	307	1/1	0.99	0.04	-2.84	18,18,18,18	0
5	K	B	307	1/1	0.99	0.06	-3.04	20,20,20,20	0
5	K	G	304	1/1	0.99	0.04	-3.59	42,42,42,42	0
4	MRD	F	304	8/8	0.91	0.12	-	26,28,32,33	0
3	MPD	D	304	8/8	0.87	0.19	-	16,22,40,42	0
3	MPD	E	305	8/8	0.95	0.09	-	27,33,36,37	0
3	MPD	D	306	8/8	0.94	0.11	-	26,27,32,34	0
3	MPD	C	305	8/8	0.93	0.11	-	27,34,39,39	0
3	MPD	B	305	8/8	0.81	0.21	-	17,26,37,45	0
3	MPD	B	304	8/8	0.90	0.12	-	28,30,32,33	0
3	MPD	A	305	8/8	0.92	0.16	-	28,32,34,36	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.