



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 04:19 PM UTC

PDB ID : 3O0D / pdb_00003o0d
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

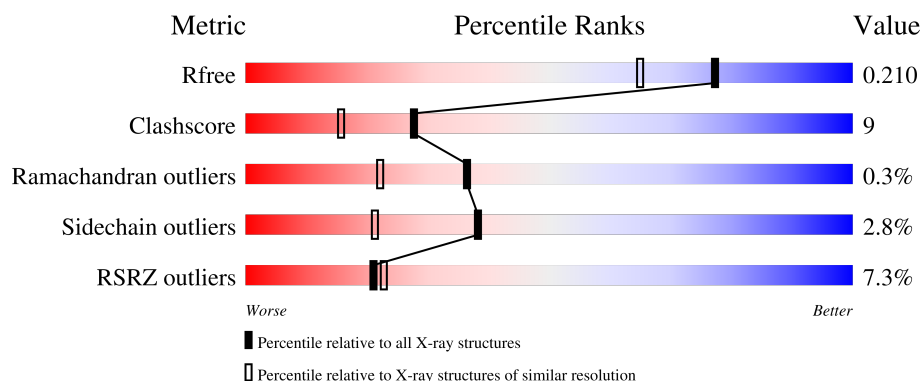
1 Overall quality at a glance

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}	180053	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	301	3% 72% 26% .
1	B	301	2% 82% 17% .
1	C	301	83% 16% .
1	D	301	6% 78% 18% ...
1	E	301	3% 79% 18% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	301	
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
3	MPD	B	305	-	-	X	-
3	MPD	D	304	-	-	X	-

2 Entry composition [i](#)

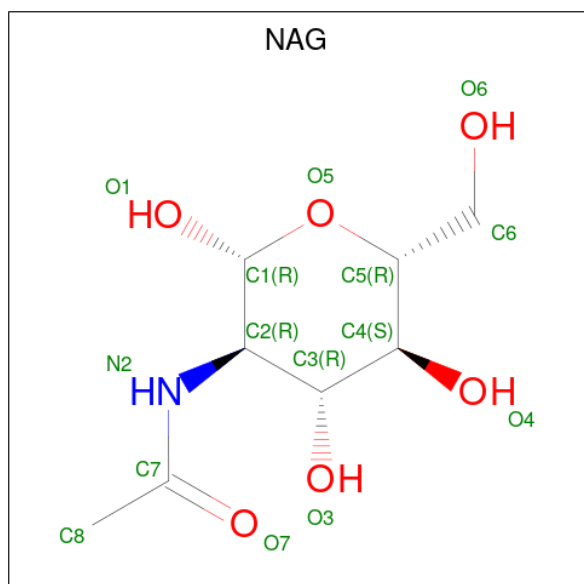
There are 6 unique types of molecules in this entry. The entry contains 18591 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

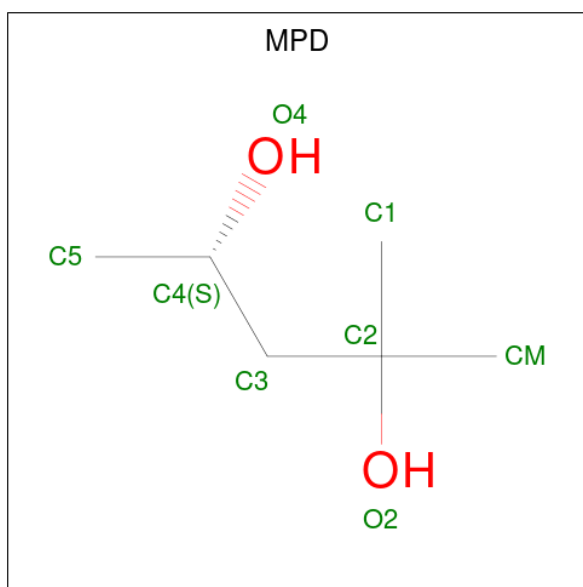
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	301	Total	C	N	O	S	0	10	0
			2412	1545	408	447	12			
1	B	301	Total	C	N	O	S	0	8	0
			2404	1536	401	455	12			
1	C	301	Total	C	N	O	S	0	6	0
			2372	1514	399	447	12			
1	D	297	Total	C	N	O	S	0	9	0
			2334	1489	395	440	10			
1	E	301	Total	C	N	O	S	0	13	0
			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 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



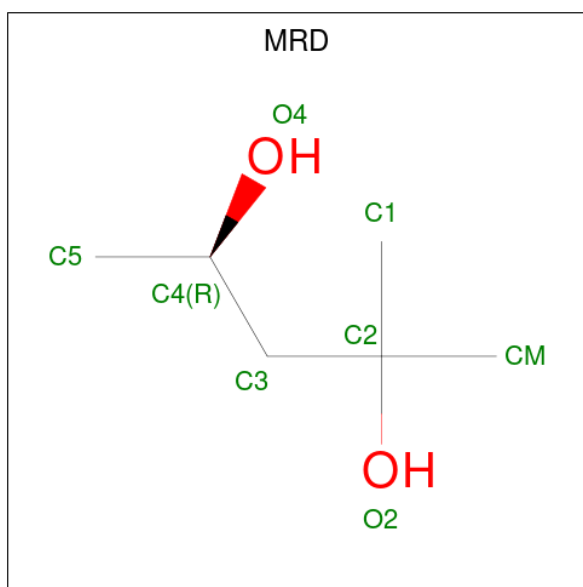
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	1
			28	16	2	10		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	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 (CCD ID: MPD) (formula: C₆H₁₄O₂).



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 (CCD ID: MRD) (formula: C₆H₁₄O₂).



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 (CCD ID: K) (formula: K).

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

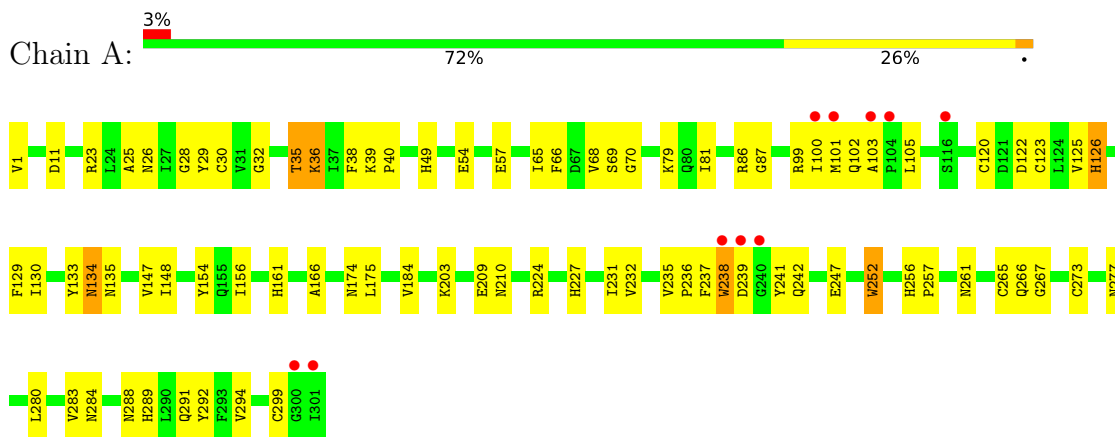
- Molecule 6 is water.

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

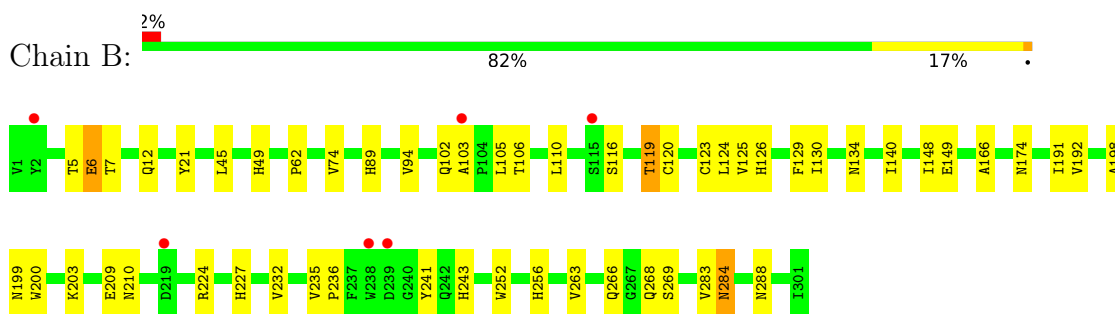
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

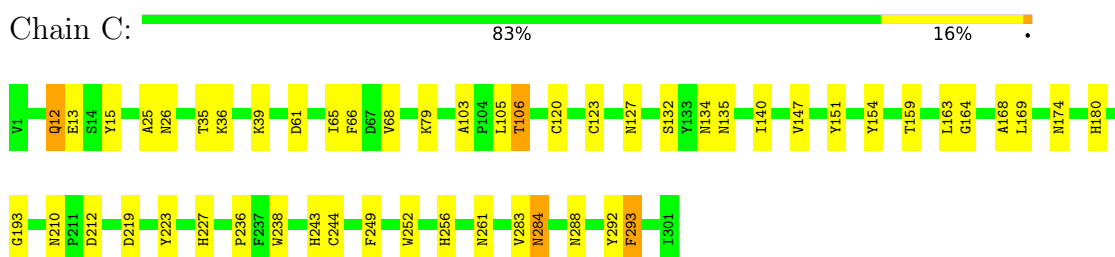
- Molecule 1: Triacylglycerol lipase



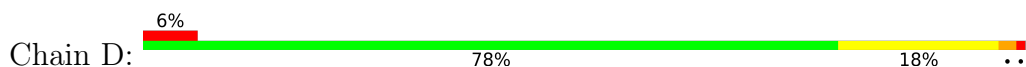
- Molecule 1: Triacylglycerol lipase

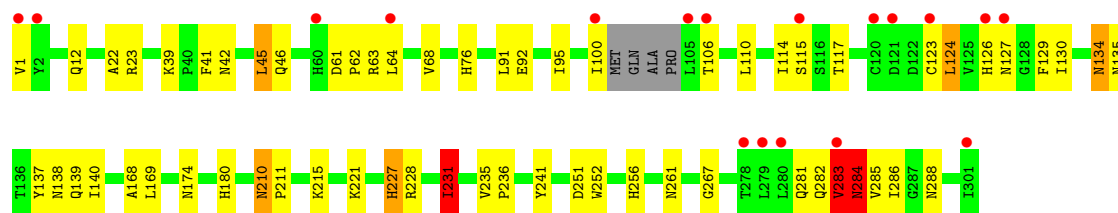


- Molecule 1: Triacylglycerol lipase

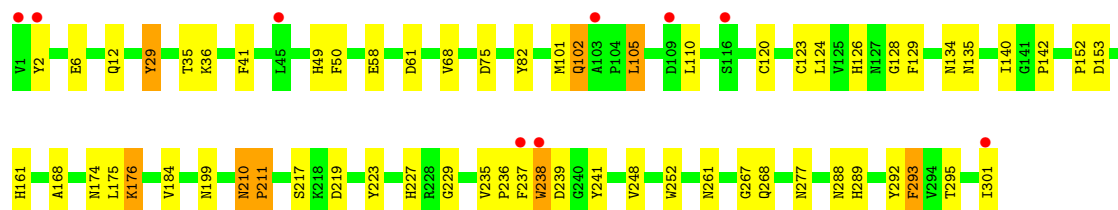
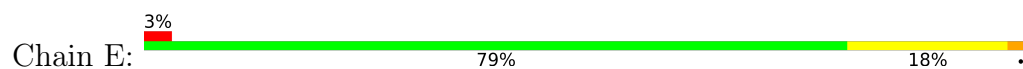


- Molecule 1: Triacylglycerol lipase

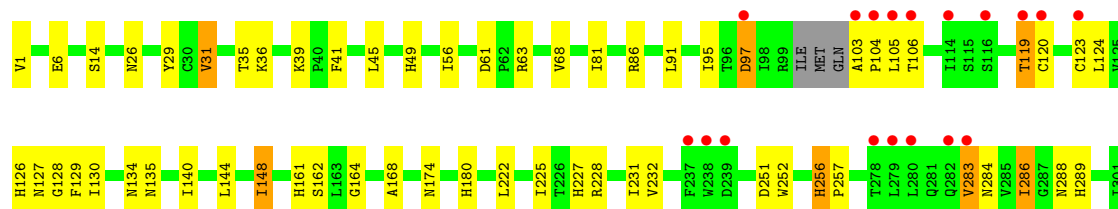
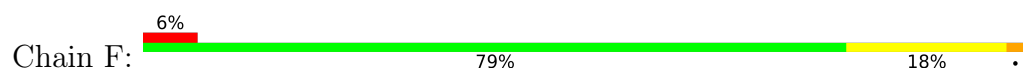




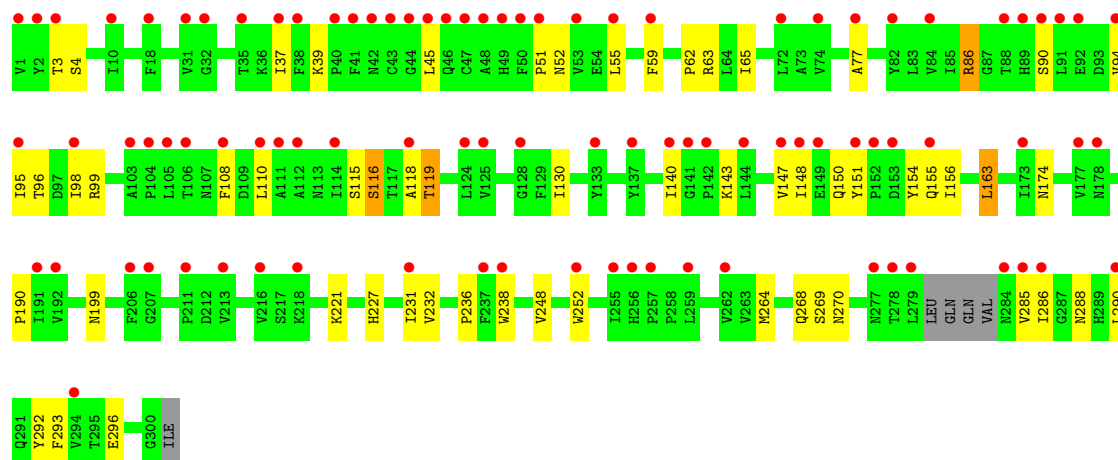
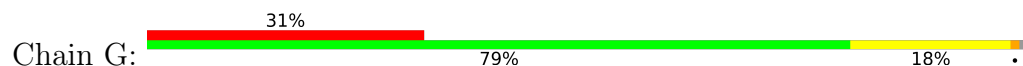
• Molecule 1: Triacylglycerol lipase



• 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, α , β , γ	115.35Å 132.14Å 137.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.70 20.00 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.5 (20.00-1.70) 99.4 (20.00-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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 (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	17.6	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 46.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	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 ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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: NAG, MRD, MPD, K

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	1.67	27/2488 (1.1%)	1.39	10/3389 (0.3%)
1	B	1.53	13/2480 (0.5%)	1.24	6/3379 (0.2%)
1	C	1.62	23/2445 (0.9%)	1.31	1/3332 (0.0%)
1	D	1.50	14/2405 (0.6%)	1.27	9/3276 (0.3%)
1	E	1.61	16/2502 (0.6%)	1.26	7/3411 (0.2%)
1	F	1.48	10/2426 (0.4%)	1.24	5/3304 (0.2%)
1	G	1.15	1/2349 (0.0%)	0.99	1/3200 (0.0%)
All	All	1.52	104/17095 (0.6%)	1.25	39/23291 (0.2%)

All (104) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	210[A]	ASN	C-O	-16.09	1.16	1.23
1	E	210[B]	ASN	C-O	-16.09	1.16	1.23
1	B	256	HIS	C-O	11.20	1.29	1.23
1	A	70	GLY	N-CA	8.87	1.53	1.45
1	C	169	LEU	C-O	-8.43	1.14	1.24
1	G	232	VAL	CA-CB	8.29	1.58	1.54
1	D	231	ILE	CA-CB	8.20	1.64	1.54
1	C	140	ILE	CA-CB	7.52	1.64	1.54
1	D	210	ASN	C-O	-7.25	1.20	1.23
1	D	256	HIS	CA-CB	7.23	1.57	1.52
1	F	56	ILE	CA-CB	-7.19	1.45	1.54
1	F	140	ILE	CA-CB	7.18	1.64	1.54
1	D	115	SER	N-CA	7.17	1.54	1.45
1	E	211	PRO	C-O	-6.99	1.15	1.23
1	A	266	GLN	N-CA	6.88	1.54	1.45
1	C	15	TYR	C-O	-6.68	1.16	1.24
1	A	23	ARG	C-O	-6.67	1.16	1.24
1	B	256	HIS	N-CA	6.66	1.51	1.46
1	B	74	VAL	CA-CB	6.65	1.62	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	41	PHE	C-O	-6.39	1.16	1.24
1	F	225	ILE	C-O	6.39	1.31	1.24
1	C	293	PHE	C-O	-6.39	1.16	1.24
1	E	128	GLY	CA-C	6.35	1.58	1.52
1	A	256	HIS	CA-CB	6.33	1.58	1.52
1	C	256	HIS	C-O	6.23	1.26	1.23
1	B	198	ALA	N-CA	6.20	1.53	1.46
1	E	50	PHE	C-O	-6.19	1.17	1.24
1	A	87	GLY	N-CA	6.12	1.52	1.45
1	A	232	VAL	CA-CB	-6.12	1.51	1.54
1	C	13	GLU	N-CA	6.10	1.53	1.46
1	E	29	TYR	C-O	-6.06	1.15	1.24
1	C	159	THR	CA-C	-6.04	1.45	1.52
1	C	164	GLY	N-CA	6.01	1.53	1.45
1	A	103	ALA	CA-C	6.01	1.59	1.53
1	A	154	TYR	N-CA	5.92	1.53	1.45
1	F	256	HIS	N-CA	5.91	1.50	1.46
1	A	231	ILE	CA-CB	5.90	1.61	1.54
1	A	292	TYR	C-O	-5.89	1.15	1.23
1	C	223	TYR	N-CA	5.89	1.53	1.46
1	E	176[A]	LYS	N-CA	-5.88	1.39	1.46
1	E	176[B]	LYS	N-CA	-5.88	1.39	1.46
1	C	151	TYR	CA-CB	5.87	1.60	1.53
1	D	284	ASN	C-O	-5.81	1.16	1.24
1	A	133	TYR	N-CA	5.79	1.53	1.46
1	A	54	GLU	N-CA	5.79	1.53	1.46
1	C	212	ASP	C-O	5.79	1.31	1.24
1	D	285	VAL	C-O	-5.78	1.17	1.24
1	A	210	ASN	C-O	5.77	1.26	1.23
1	B	263	VAL	N-CA	5.76	1.52	1.46
1	C	249	PHE	C-O	-5.72	1.17	1.24
1	C	106	THR	CA-C	-5.72	1.45	1.52
1	F	222	LEU	C-O	5.71	1.30	1.23
1	A	134	ASN	CA-C	-5.70	1.45	1.52
1	E	223	TYR	C-O	5.67	1.30	1.23
1	A	147	VAL	CA-CB	5.67	1.61	1.54
1	A	166	ALA	CA-CB	5.66	1.62	1.53
1	F	256	HIS	C-O	5.65	1.26	1.23
1	E	168	ALA	CA-CB	5.61	1.62	1.53
1	C	147	VAL	CA-CB	5.59	1.61	1.54
1	D	139	GLN	N-CA	-5.59	1.39	1.46
1	D	140	ILE	CA-CB	5.58	1.62	1.55

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	140	ILE	CA-CB	5.56	1.62	1.54
1	C	39	LYS	CA-C	-5.56	1.46	1.53
1	B	224	ARG	N-CA	5.54	1.54	1.46
1	D	286	ILE	C-O	-5.52	1.17	1.24
1	F	168	ALA	CA-CB	5.52	1.62	1.53
1	D	215	LYS	N-CA	5.49	1.52	1.46
1	B	94	VAL	CA-CB	5.48	1.61	1.54
1	B	256	HIS	CA-CB	5.48	1.57	1.52
1	A	25	ALA	N-CA	5.48	1.52	1.46
1	B	140	ILE	CA-CB	5.47	1.61	1.54
1	F	31	VAL	N-CA	5.46	1.53	1.46
1	E	293	PHE	C-O	-5.46	1.17	1.24
1	C	154	TYR	C-O	-5.45	1.17	1.23
1	E	184	VAL	CA-CB	5.45	1.61	1.54
1	A	277	ASN	N-CA	5.44	1.53	1.46
1	A	11	ASP	C-O	-5.43	1.16	1.23
1	D	227	HIS	ND1-CE1	5.41	1.38	1.32
1	A	257	PRO	CA-C	5.40	1.55	1.52
1	C	25	ALA	CA-CB	5.40	1.61	1.53
1	A	284	ASN	C-O	5.38	1.30	1.23
1	C	103	ALA	CA-CB	5.34	1.60	1.54
1	B	269	SER	C-O	-5.33	1.17	1.23
1	A	252	TRP	N-CA	5.31	1.51	1.46
1	A	273	CYS	C-O	-5.29	1.17	1.24
1	A	294	VAL	C-O	-5.26	1.17	1.23
1	C	193	GLY	N-CA	5.25	1.52	1.45
1	F	41	PHE	C-O	-5.21	1.17	1.24
1	D	22	ALA	CA-CB	5.20	1.61	1.53
1	B	62	PRO	N-CA	-5.17	1.43	1.47
1	B	241	TYR	C-O	5.16	1.30	1.23
1	A	224	ARG	N-CA	5.15	1.53	1.46
1	C	219	ASP	C-O	-5.15	1.17	1.24
1	E	152	PRO	C-O	-5.14	1.17	1.24
1	A	291	GLN	C-O	-5.11	1.17	1.23
1	C	12	GLN	CA-C	5.11	1.59	1.52
1	E	223	TYR	N-CA	5.11	1.52	1.46
1	D	174	ASN	N-CA	5.11	1.52	1.46
1	C	159	THR	N-CA	5.10	1.52	1.45
1	D	76	HIS	N-CA	-5.08	1.39	1.46
1	C	210	ASN	C-O	5.05	1.26	1.23
1	B	149	GLU	N-CA	5.05	1.52	1.46
1	A	122	ASP	CA-C	5.04	1.59	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	256	HIS	CA-CB	5.01	1.56	1.52

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	103	ALA	CA-C-N	-7.72	112.06	119.85
1	B	103	ALA	C-N-CA	-7.72	112.06	119.85
1	D	134	ASN	N-CA-C	7.42	120.02	111.11
1	F	232	VAL	N-CA-CB	7.38	115.15	110.50
1	D	138	ASN	N-CA-C	7.38	121.38	112.38
1	F	97	ASP	N-CA-C	7.23	120.03	111.71
1	E	267	GLY	N-CA-C	6.74	119.83	112.29
1	E	176[A]	LYS	CA-C-O	-6.68	113.82	120.70
1	E	176[B]	LYS	CA-C-O	-6.68	113.82	120.70
1	E	238	TRP	N-CA-C	6.41	117.03	108.38
1	A	32	GLY	CA-C-N	-6.23	111.84	120.25
1	A	32	GLY	C-N-CA	-6.23	111.84	120.25
1	D	115	SER	N-CA-C	6.09	119.97	110.17
1	F	39	LYS	CB-CA-C	5.92	117.99	109.11
1	D	267	GLY	N-CA-C	5.83	121.44	112.81
1	A	238	TRP	N-CA-C	-5.76	102.12	110.64
1	D	168	ALA	N-CA-C	5.72	117.52	111.28
1	B	148	ILE	N-CA-C	-5.69	104.97	110.72
1	F	14	SER	N-CA-C	5.63	117.41	111.28
1	D	140	ILE	N-CA-C	5.61	119.04	113.71
1	E	175	LEU	N-CA-C	5.60	117.38	111.28
1	B	166	ALA	N-CA-C	-5.53	105.34	111.36
1	D	283	VAL	N-CA-CB	5.37	117.61	110.26
1	B	232	VAL	N-CA-CB	5.34	113.86	110.50
1	A	126	HIS	N-CA-CB	-5.32	101.44	109.59
1	C	168	ALA	N-CA-C	5.28	117.03	111.28
1	D	169	LEU	O-C-N	5.27	127.71	122.12
1	A	28	GLY	N-CA-C	-5.22	107.31	113.99
1	D	114	ILE	CB-CA-C	-5.16	103.71	110.98
1	E	248	VAL	N-CA-C	-5.15	100.14	107.77
1	A	69	SER	CA-C-N	-5.15	114.33	121.23
1	A	69	SER	C-N-CA	-5.15	114.33	121.23
1	F	257	PRO	CB-CA-C	-5.09	104.71	110.92
1	A	267	GLY	N-CA-C	5.07	120.31	112.81
1	B	21	TYR	CA-CB-CG	-5.07	104.77	113.90
1	E	58	GLU	CB-CG-CD	-5.01	104.08	112.60
1	G	232	VAL	N-CA-CB	5.01	114.36	110.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	184	VAL	CA-C-N	-5.01	116.03	122.99
1	A	184	VAL	C-N-CA	-5.01	116.03	122.99

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2412	0	2345	53	0
1	B	2404	0	2315	34	0
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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	8	0
6	B	281	0	0	4	0
6	C	309	0	0	5	0
6	D	222	0	0	7	0
6	E	277	0	0	12	0
6	F	246	0	0	12	0
6	G	55	0	0	2	0
All	All	18591	0	16315	299	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 (299) 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:HG3	1:G:86:ARG:HH11	1.05	1.08
1:E:6[A]:GLU:HG2	6:E:1155:HOH:O	1.51	1.08
3:E:305:MPD:H52	3:E:305:MPD:HM1	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:B:5:THR:C	1:B:6[B]:GLU:CA	2.41	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:H52	3:C:305:MPD:O2	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: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:HG3	1:G:86:ARG:NH1	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:86:ARG:HH11	1:G:86:ARG:CG	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:E:238:TRP:CD1	1:E:238:TRP:C	2.65	0.70
1:D:91:LEU:O	1:D:95:ILE:HD13	1.91	0.70
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: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:31:VAL:O	1:F:86:ARG:NH2	2.26	0.69
1:F:45:LEU:HD11	6:F:1548:HOH:O	1.92	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:81:ILE:HD13	1:F:148[A]:ILE:CD1	2.22	0.68
1:F:106:THR:HG21	1:F:127:ASN:ND2	2.08	0.68
1:D:12:GLN:HG2	3:D:304:MPD:HM1	1.75	0.68
1:B:191[A]:ILE:HD13	1:B:243:HIS:CD2	2.30	0.67
1:B:191[A]:ILE:CD1	1:B:243:HIS:CD2	2.77	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:O	1:D:45[A]:LEU:CD2	2.44	0.66
1:E:68:VAL:H	1:E:135:ASN:HD22	1.42	0.66
1:F:1:VAL:HG13	1:F:1:VAL:O	1.96	0.66
1:B:106:THR:HG22	1:B:110:LEU:HD12	1.77	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:237:PHE:O	1:A:238:TRP:C	2.40	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
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:D:124[A]:LEU:HD22	1:D:124[A]:LEU:N	2.15	0.62
1:A:35[B]:THR:HG22	1:F:284:ASN:HA	1.81	0.62
1:A:68:VAL:H	1:A:135:ASN:HD22	1.45	0.62
3:D:306:MPD:H13	6:E:561:HOH:O	1.99	0.62
3:D:306:MPD:O4	3:D:306:MPD:H11	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:O4	3:E:304:MPD:HM1	2.00	0.61
1:A:148:ILE:HG12	1:A:156[B]:ILE:HD11	1.83	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:D:92:GLU:HG2	6:D:1785:HOH:O	2.02	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:228[A]:ARG:HD2	1:D:281:GLN:CD	2.27	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:N	1:D:124[A]:LEU:CD2	2.68	0.57
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
1:D:45[A]:LEU:HD13	6:D:1343:HOH:O	2.05	0.56
3:D:304:MPD:H11	6:E:367: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:A:238:TRP:O	1:A:239:ASP:C	2.48	0.55
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: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:119:THR:HG23	1:B:200:TRP:CH2	2.42	0.55
1:B:120:CYS:SG	1:B:123[B]:CYS:HB2	2.47	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:G:292:TYR:O	1:G:293:PHE:HB2	2.07	0.54
1:E:237:PHE:HA	6:E:1164:HOH:O	2.06	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:238:TRP:C	1:E:238:TRP:HD1	2.15	0.53
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:68:VAL:H	1:F:135:ASN:ND2	2.07	0.52
1:F:283:VAL:CG1	1:F:284:ASN:N	2.71	0.52
1:B:210:ASN:OD1	6:B:2149:HOH:O	2.19	0.52
1:D:123:CYS:C	1:D:124[A]:LEU:HD22	2.34	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
1:E:238:TRP:HE1	1:E:241:TYR:HE2	1.57	0.52
1:C:79:LYS:NZ	6:C:899:HOH:O	2.34	0.52
1:A:57:GLU:OE2	6:A:2103:HOH:O	2.19	0.52
1:A:120:CYS:SG	1:A:123[A]:CYS:HB2	2.49	0.52
1:B:6[C]:GLU:OE2	6:B:1982:HOH:O	2.18	0.52
1:B:235:VAL:HB	1:B:236:PRO:HA	1.92	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:101:MET:HE2	1:A:101:MET:HA	1.94	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: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:N	1:E:105:LEU:HD22	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:A:79:LYS:N	1:A:79:LYS:HD2	2.29	0.48
1:E:199:ASN:ND2	1:E:268:GLN:HE22	2.12	0.48
1:G:51:PRO:O	1:G:52:ASN:HB2	2.14	0.48
1:G:115:SER:OG	1:G:118:ALA:HB2	2.12	0.48
1:F:86:ARG:HA	1:F:164:GLY:HA3	1.96	0.48
1:F:127:ASN:C	1:F:130:ILE:HG22	2.36	0.48
1:E:301:ILE:C	6:E:1102:HOH:O	2.57	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:F:227:HIS:CE1	1:F:252:TRP:O	2.67	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:F:35[B]:THR:O	6:F:345:HOH:O	2.20	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:D:137:TYR:C	1:D:137:TYR:CD2	2.94	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:39:LYS:HA	1:A:40:PRO:C	2.41	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:A:239:ASP:C	1:A:239:ASP:OD1	2.62	0.43
1:C:227:HIS:CE1	1:C:252:TRP:O	2.70	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:62:PRO:O	1:D:63:ARG:C	2.61	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:O4	3:D:306:MPD:C1	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:N	1:E:105:LEU:CD2	2.83	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HG23	1:D:100:ILE:O	2.20	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:N	1:D:95:ILE:HD12	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:A:283:VAL:HG13	1:F:36:LYS:CG	2.51	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: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:E:235:VAL:HA	1:E:236:PRO:C	2.46	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
1:D:210:ASN:N	1:D:211:PRO:HD3	2.37	0.40
1:D:235:VAL:HA	1:D:236:PRO:C	2.46	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%)	36	22
1	C	305/301 (101%)	293 (96%)	11 (4%)	1 (0%)	36	22
1	D	302/301 (100%)	287 (95%)	14 (5%)	1 (0%)	36	22
1	E	312/301 (104%)	299 (96%)	12 (4%)	1 (0%)	36	22
1	F	301/301 (100%)	290 (96%)	9 (3%)	2 (1%)	18	7
1	G	293/301 (97%)	278 (95%)	15 (5%)	0	100	100
All	All	2129/2107 (101%)	2035 (96%)	88 (4%)	6 (0%)	36	22

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	284	ASN
1	E	239	ASP
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%)	36	19
1	B	268/260 (103%)	260 (97%)	8 (3%)	36	19
1	C	263/260 (101%)	259 (98%)	4 (2%)	57	43
1	D	253/260 (97%)	242 (96%)	11 (4%)	26	10
1	E	268/260 (103%)	262 (98%)	6 (2%)	45	29
1	F	255/260 (98%)	246 (96%)	9 (4%)	32	15

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	246/260 (95%)	237 (96%)	9 (4%)	30	14
All	All	1820/1820 (100%)	1765 (97%)	55 (3%)	38	19

All (55) 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	105	LEU
1	A	134	ASN
1	A	174	ASN
1	B	6[A]	GLU
1	B	6[C]	GLU
1	B	6[B]	GLU
1	B	102	GLN
1	B	116	SER
1	B	119	THR
1	B	134	ASN
1	B	174	ASN
1	C	26	ASN
1	C	105	LEU
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	D	231	ILE
1	D	283	VAL
1	E	102	GLN
1	E	105	LEU
1	E	110	LEU
1	E	134	ASN
1	E	142	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	174	ASN
1	F	26	ASN
1	F	97	ASP
1	F	119	THR
1	F	134	ASN
1	F	148[A]	ILE
1	F	148[B]	ILE
1	F	174	ASN
1	F	231	ILE
1	F	286	ILE
1	G	39	LYS
1	G	45	LEU
1	G	86	ARG
1	G	99	ARG
1	G	116	SER
1	G	119	THR
1	G	150	GLN
1	G	163	LEU
1	G	174	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (77) 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	189	GLN
1	A	199	ASN
1	A	227	HIS
1	A	261	ASN
1	A	268	GLN
1	A	272	GLN
1	B	12	GLN
1	B	49	HIS
1	B	127	ASN
1	B	178	ASN
1	B	199	ASN
1	B	208	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	227	HIS
1	B	242	GLN
1	C	12	GLN
1	C	60	HIS
1	C	127	ASN
1	C	131	GLN
1	C	135	ASN
1	C	180	HIS
1	C	189	GLN
1	C	227	HIS
1	C	261	ASN
1	D	42	ASN
1	D	127	ASN
1	D	131	GLN
1	D	135	ASN
1	D	178	ASN
1	D	180	HIS
1	D	189	GLN
1	D	227	HIS
1	D	261	ASN
1	D	282	GLN
1	E	12	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	E	282	GLN
1	F	12	GLN
1	F	49	HIS
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	208	GLN
1	F	227	HIS
1	F	242	GLN
1	F	256	HIS
1	G	12	GLN
1	G	16	ASN
1	G	52	ASN
1	G	89	HIS
1	G	135	ASN
1	G	139	GLN
1	G	174	ASN
1	G	178	ASN
1	G	199	ASN
1	G	227	HIS
1	G	234	GLN
1	G	242	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 oligosaccharides 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
4	MRD	A	307	-	7,7,7	1.16	0	9,10,10	1.38	1 (11%)
2	NAG	F	303	1	14,14,15	0.73	0	17,19,21	1.71	5 (29%)
3	MPD	A	306	-	7,7,7	0.40	0	9,10,10	0.63	0
2	NAG	C	302	1	14,14,15	1.44	1 (7%)	17,19,21	2.10	5 (29%)
3	MPD	D	306	-	7,7,7	0.48	0	9,10,10	0.94	0
4	MRD	B	306	-	7,7,7	0.86	0	9,10,10	1.03	1 (11%)
2	NAG	B	303	1	14,14,15	0.70	0	17,19,21	1.24	3 (17%)
3	MPD	D	304	-	7,7,7	2.24	2 (28%)	9,10,10	1.94	4 (44%)
2	NAG	D	303	1	14,14,15	0.72	0	17,19,21	1.86	5 (29%)
3	MPD	C	305	-	7,7,7	0.61	0	9,10,10	0.61	0
2	NAG	A	303	1	14,14,15	0.63	0	17,19,21	1.61	4 (23%)
3	MPD	E	305	-	7,7,7	0.32	0	9,10,10	1.34	2 (22%)
3	MPD	A	305	-	7,7,7	0.31	0	9,10,10	0.26	0
2	NAG	G	303	1	14,14,15	0.68	0	17,19,21	1.83	4 (23%)
3	MPD	B	304	-	7,7,7	0.56	0	9,10,10	0.65	0
3	MPD	F	305	-	7,7,7	0.47	0	9,10,10	0.96	0
3	MPD	B	305	-	7,7,7	1.50	1 (14%)	9,10,10	1.08	0
2	NAG	D	302	1	14,14,15	1.12	0	17,19,21	2.26	5 (29%)
2	NAG	C	303	1	14,14,15	1.04	1 (7%)	17,19,21	1.47	2 (11%)
4	MRD	D	305	-	7,7,7	0.53	0	9,10,10	0.66	0
2	NAG	E	303	1	14,14,15	1.07	0	17,19,21	3.38	12 (70%)
3	MPD	C	304	-	7,7,7	0.65	0	9,10,10	1.54	2 (22%)
2	NAG	E	302	1	14,14,15	1.07	1 (7%)	17,19,21	2.44	5 (29%)
2	NAG	A	302	1	14,14,15	0.90	0	17,19,21	1.16	1 (5%)
2	NAG	F	302	1	14,14,15	0.97	0	17,19,21	1.79	5 (29%)
3	MPD	C	306	-	7,7,7	0.53	0	9,10,10	0.57	0
3	MPD	E	304	-	7,7,7	0.29	0	9,10,10	1.15	0
4	MRD	F	304	-	7,7,7	0.24	0	9,10,10	0.65	0
3	MPD	A	304	-	7,7,7	0.51	0	9,10,10	0.78	0
2	NAG	B	302[B]	1	14,14,15	0.55	0	17,19,21	1.52	3 (17%)
2	NAG	B	302[A]	1	14,14,15	0.57	0	17,19,21	1.26	1 (5%)
2	NAG	G	302	1	14,14,15	0.63	0	17,19,21	1.19	2 (11%)

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

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	304	MPD	O2-C2	4.44	1.55	1.44
2	C	302	NAG	C1-C2	4.14	1.58	1.52
3	D	304	MPD	CM-C2	-3.03	1.43	1.52
3	B	305	MPD	O2-C2	2.89	1.51	1.44
2	E	302	NAG	C1-C2	2.40	1.55	1.52
2	C	303	NAG	C3-C2	2.04	1.56	1.52

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	303	NAG	C1-O5-C5	-7.39	102.29	112.19
2	E	303	NAG	O5-C5-C6	6.06	119.46	107.66
2	E	302	NAG	C3-C4-C5	-5.02	101.12	110.23
2	G	303	NAG	C1-O5-C5	4.89	118.74	112.19
2	E	302	NAG	O5-C1-C2	-4.65	104.09	111.29
2	E	302	NAG	C1-C2-N2	4.63	117.72	110.43
2	C	302	NAG	O6-C6-C5	-4.45	96.17	111.33
2	D	302	NAG	C4-C3-C2	4.37	117.42	111.02
2	D	303	NAG	C4-C3-C2	4.35	117.39	111.02
2	D	302	NAG	C2-N2-C7	-4.23	117.23	122.90
2	E	303	NAG	O3-C3-C2	-4.19	100.69	109.40
2	D	302	NAG	O5-C1-C2	-4.07	105.00	111.29
2	C	302	NAG	O5-C1-C2	-3.88	105.29	111.29
2	E	303	NAG	C6-C5-C4	3.86	122.50	113.02
2	F	303	NAG	C2-N2-C7	3.82	128.02	122.90
2	E	302	NAG	C4-C3-C2	3.76	116.53	111.02
2	E	303	NAG	O7-C7-C8	-3.63	115.59	122.05
2	F	302	NAG	O5-C5-C6	3.62	114.71	107.66
2	E	303	NAG	O4-C4-C5	3.58	118.14	109.32
2	B	302[A]	NAG	O5-C1-C2	-3.58	105.75	111.29
4	A	307	MRD	CM-C2-C1	-3.38	103.06	110.63
2	A	303	NAG	C1-O5-C5	3.31	116.62	112.19
2	B	302[B]	NAG	C1-C2-N2	3.30	115.63	110.43
2	G	303	NAG	C2-N2-C7	3.28	127.30	122.90
2	F	302	NAG	C1-C2-N2	3.21	115.49	110.43
2	D	302	NAG	C6-C5-C4	3.16	120.78	113.02
2	C	303	NAG	C2-N2-C7	-3.14	118.70	122.90
2	F	303	NAG	C3-C4-C5	3.11	115.87	110.23
2	E	303	NAG	O5-C5-C4	-3.09	103.30	110.83
2	D	303	NAG	C2-N2-C7	3.05	126.98	122.90
3	D	304	MPD	CM-C2-C1	-2.99	103.94	110.63
3	C	304	MPD	CM-C2-C1	-2.95	104.01	110.63
2	C	302	NAG	C1-O5-C5	2.89	116.06	112.19
2	C	303	NAG	O4-C4-C3	-2.89	103.56	110.38
3	E	305	MPD	CM-C2-C1	-2.88	104.18	110.63
3	D	304	MPD	O2-C2-C3	2.85	119.92	109.27
2	C	302	NAG	C8-C7-N2	2.84	120.83	116.12
2	C	302	NAG	O7-C7-N2	-2.74	117.14	121.98
2	B	302[B]	NAG	O5-C5-C6	2.63	112.79	107.66
2	D	303	NAG	C1-C2-N2	2.63	114.58	110.43
2	E	303	NAG	C8-C7-N2	2.63	120.47	116.12
2	F	302	NAG	O7-C7-C8	-2.62	117.39	122.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	303	NAG	C2-N2-C7	-2.59	119.43	122.90
3	C	304	MPD	O4-C4-C5	2.57	120.53	109.45
2	G	302	NAG	C1-O5-C5	2.54	115.59	112.19
2	E	303	NAG	O6-C6-C5	2.53	119.95	111.33
2	F	302	NAG	O5-C1-C2	-2.49	107.44	111.29
3	D	304	MPD	CM-C2-C3	-2.47	99.55	110.20
2	A	303	NAG	C4-C3-C2	2.46	114.62	111.02
2	F	303	NAG	O7-C7-N2	2.44	126.29	121.98
2	A	303	NAG	O5-C5-C6	-2.32	103.14	107.66
2	D	303	NAG	C3-C4-C5	2.32	114.44	110.23
2	A	303	NAG	O4-C4-C3	-2.31	104.92	110.38
3	D	304	MPD	O2-C2-C1	2.30	115.16	107.99
2	D	302	NAG	C8-C7-N2	2.27	119.89	116.12
2	E	303	NAG	C2-N2-C7	-2.26	119.87	122.90
2	E	303	NAG	C1-C2-N2	2.23	113.95	110.43
2	G	302	NAG	O5-C5-C6	2.22	111.98	107.66
2	F	302	NAG	C2-N2-C7	-2.20	119.95	122.90
2	A	302	NAG	C3-C4-C5	-2.18	106.28	110.23
2	B	303	NAG	O5-C5-C6	2.17	111.89	107.66
2	B	303	NAG	O5-C1-C2	-2.16	107.94	111.29
2	G	303	NAG	O7-C7-N2	2.16	125.80	121.98
2	B	302[B]	NAG	O5-C1-C2	-2.16	107.95	111.29
2	D	303	NAG	O4-C4-C5	2.13	114.56	109.32
2	E	302	NAG	C8-C7-N2	2.10	119.61	116.12
2	F	303	NAG	C8-C7-N2	-2.09	112.64	116.12
2	F	303	NAG	C4-C3-C2	2.07	114.06	111.02
4	B	306	MRD	O4-C4-C5	2.07	118.37	109.45
3	E	305	MPD	CM-C2-C3	2.04	119.01	110.20
2	G	303	NAG	O5-C1-C2	-2.04	108.13	111.29
2	E	303	NAG	C3-C4-C5	-2.04	106.53	110.23

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	305	MPD	C2-C3-C4-O4
3	C	304	MPD	C2-C3-C4-O4
3	C	305	MPD	C2-C3-C4-C5
3	E	305	MPD	CM-C2-C3-C4
3	E	305	MPD	C2-C3-C4-O4
3	E	305	MPD	C2-C3-C4-C5
2	E	303	NAG	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	E	303	NAG	C4-C5-C6-O6
3	E	305	MPD	O2-C2-C3-C4
3	A	304	MPD	CM-C2-C3-C4
3	B	305	MPD	CM-C2-C3-C4
3	C	305	MPD	C1-C2-C3-C4
3	F	305	MPD	CM-C2-C3-C4
2	F	302	NAG	C4-C5-C6-O6
3	E	304	MPD	C2-C3-C4-C5
2	A	303	NAG	C4-C5-C6-O6
3	B	305	MPD	O2-C2-C3-C4
3	C	304	MPD	O2-C2-C3-C4
3	C	306	MPD	O2-C2-C3-C4
3	D	306	MPD	O2-C2-C3-C4
3	F	305	MPD	O2-C2-C3-C4
4	F	304	MRD	O2-C2-C3-C4
3	C	305	MPD	C2-C3-C4-O4
3	E	304	MPD	C2-C3-C4-O4
4	F	304	MRD	C2-C3-C4-O4
3	A	306	MPD	CM-C2-C3-C4
3	B	305	MPD	C1-C2-C3-C4
3	C	305	MPD	CM-C2-C3-C4
3	E	304	MPD	CM-C2-C3-C4
3	E	305	MPD	C1-C2-C3-C4
3	F	305	MPD	C1-C2-C3-C4
4	F	304	MRD	C1-C2-C3-C4
4	F	304	MRD	CM-C2-C3-C4
2	D	303	NAG	C4-C5-C6-O6

There are no ring outliers.

11 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	302	NAG	1	0
3	D	306	MPD	3	0
3	D	304	MPD	6	0
3	C	305	MPD	3	0
3	E	305	MPD	4	0
2	G	303	NAG	3	0
3	B	305	MPD	7	0
2	D	302	NAG	1	0
4	D	305	MRD	1	0
2	F	302	NAG	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	304	MPD	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	301/301 (100%)	-0.23	10 (3%) 49 53	7, 15, 35, 49	10 (3%)
1	B	301/301 (100%)	-0.40	6 (1%) 65 69	6, 15, 30, 42	8 (2%)
1	C	301/301 (100%)	-0.51	0 100 100	6, 14, 25, 32	6 (1%)
1	D	297/301 (98%)	0.01	18 (6%) 27 29	8, 19, 42, 60	9 (3%)
1	E	301/301 (100%)	-0.36	9 (2%) 52 56	6, 15, 34, 52	13 (4%)
1	F	298/301 (99%)	-0.04	18 (6%) 27 30	8, 19, 46, 56	7 (2%)
1	G	296/301 (98%)	1.61	92 (31%) 1 1	19, 42, 66, 74	1 (0%)
All	All	2095/2107 (99%)	0.01	153 (7%) 21 23	6, 18, 49, 74	54 (2%)

All (153) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	103	ALA	5.5
1	G	114	ILE	4.9
1	F	283	VAL	4.8
1	G	148	ILE	4.7
1	G	279	LEU	4.7
1	F	238	TRP	4.6
1	A	103	ALA	4.6
1	A	238	TRP	4.5
1	F	279[A]	LEU	4.4
1	D	1	VAL	4.4
1	F	278	THR	4.3
1	A	300	GLY	4.2
1	G	53	VAL	4.1
1	F	104	PRO	4.1
1	D	105	LEU	3.7
1	G	105	LEU	3.7
1	G	110	LEU	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	48	ALA	3.6
1	D	115	SER	3.6
1	G	40	PRO	3.5
1	A	100	ILE	3.5
1	G	10	ILE	3.5
1	E	301	ILE	3.5
1	G	177	VAL	3.5
1	G	140	ILE	3.4
1	D	120	CYS	3.4
1	A	116	SER	3.4
1	E	116	SER	3.3
1	A	301	ILE	3.3
1	G	149	GLU	3.3
1	D	283	VAL	3.3
1	G	35	THR	3.2
1	B	238	TRP	3.2
1	E	238	TRP	3.2
1	B	115	SER	3.2
1	A	101	MET	3.1
1	G	59	PHE	3.1
1	A	104	PRO	3.0
1	F	123	CYS	3.0
1	G	84	VAL	3.0
1	G	147	VAL	3.0
1	G	51	PRO	3.0
1	G	1	VAL	3.0
1	D	2[A]	TYR	3.0
1	E	2[A]	TYR	3.0
1	F	282	GLN	3.0
1	G	191	ILE	3.0
1	A	239	ASP	2.9
1	E	1	VAL	2.9
1	G	46	GLN	2.9
1	G	151	TYR	2.9
1	G	111	ALA	2.9
1	G	55	LEU	2.9
1	F	280	LEU	2.9
1	G	45	LEU	2.9
1	D	278	THR	2.9
1	G	277	ASN	2.9
1	G	112	ALA	2.9
1	F	120	CYS	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	239	ASP	2.9
1	G	152	PRO	2.9
1	G	153	ASP	2.9
1	G	38	PHE	2.8
1	G	237	PHE	2.8
1	G	103	ALA	2.8
1	F	106	THR	2.8
1	G	262	VAL	2.8
1	G	211	PRO	2.7
1	G	43	CYS	2.7
1	G	286	ILE	2.7
1	G	238	TRP	2.7
1	D	64	LEU	2.7
1	D	280	LEU	2.7
1	G	173	ILE	2.7
1	F	103	ALA	2.7
1	D	123	CYS	2.7
1	G	44	GLY	2.7
1	D	301	ILE	2.7
1	G	37	ILE	2.7
1	D	100	ILE	2.6
1	G	47	CYS	2.6
1	D	60	HIS	2.6
1	G	252	TRP	2.6
1	G	77	ALA	2.6
1	G	41	PHE	2.6
1	G	137	TYR	2.6
1	G	95	ILE	2.6
1	G	216	VAL	2.5
1	G	118	ALA	2.5
1	F	97	ASP	2.5
1	G	88	THR	2.5
1	B	2	TYR	2.5
1	E	237	PHE	2.5
1	G	259	LEU	2.5
1	F	105	LEU	2.4
1	G	257	PRO	2.4
1	B	103	ALA	2.4
1	G	82	TYR	2.4
1	F	116	SER	2.4
1	G	98	ILE	2.4
1	G	213	VAL	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	72	LEU	2.4
1	G	18	PHE	2.4
1	G	206	PHE	2.4
1	D	121	ASP	2.4
1	D	126[A]	HIS	2.4
1	G	3	THR	2.4
1	G	285	VAL	2.4
1	F	119	THR	2.3
1	G	133	TYR	2.3
1	D	279	LEU	2.3
1	F	237	PHE	2.3
1	G	108	PHE	2.3
1	G	256	HIS	2.2
1	G	42	ASN	2.2
1	E	45	LEU	2.2
1	G	124	LEU	2.2
1	B	239	ASP	2.2
1	G	32	GLY	2.2
1	G	31	VAL	2.2
1	D	127	ASN	2.2
1	G	284	ASN	2.2
1	G	50	PHE	2.2
1	G	2	TYR	2.2
1	G	144	LEU	2.2
1	G	290	LEU	2.2
1	F	114	ILE	2.2
1	D	106	THR	2.2
1	G	106	THR	2.2
1	G	128	GLY	2.1
1	G	218	LYS	2.1
1	G	142	PRO	2.1
1	G	231	ILE	2.1
1	G	255	ILE	2.1
1	G	74	VAL	2.1
1	G	89	HIS	2.1
1	A	240	GLY	2.1
1	G	141	GLY	2.1
1	G	207	GLY	2.1
1	G	92	GLU	2.1
1	G	49	HIS	2.1
1	G	125	VAL	2.1
1	G	192	VAL	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	294	VAL	2.1
1	E	109	ASP	2.1
1	G	155	GLN	2.1
1	G	90	SER	2.1
1	G	91	LEU	2.1
1	G	278	THR	2.1
1	G	104	PRO	2.1
1	G	178	ASN	2.0
1	B	219	ASP	2.0
1	G	94	VAL	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 oligosaccharides 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	G	303	14/15	0.66	0.14	67,73,74,75	0
2	NAG	G	302	14/15	0.69	0.13	58,60,63,63	0
2	NAG	E	303	14/15	0.73	0.16	30,39,41,46	0
3	MPD	C	306	8/8	0.73	0.15	56,58,60,60	0
3	MPD	A	306	8/8	0.78	0.13	43,46,54,54	0
2	NAG	D	303	14/15	0.80	0.13	41,45,48,48	0
3	MPD	B	305	8/8	0.83	0.14	17,26,37,45	0
2	NAG	F	303	14/15	0.83	0.11	32,39,43,46	0
3	MPD	C	304	8/8	0.84	0.12	21,27,30,31	0
4	MRD	B	306	8/8	0.84	0.11	19,29,34,34	0
3	MPD	A	305	8/8	0.87	0.09	28,32,34,36	0
3	MPD	A	304	8/8	0.88	0.10	31,34,36,36	0
4	MRD	D	305	8/8	0.88	0.11	39,42,42,43	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	A	303	14/15	0.89	0.09	26,32,36,36	0
4	MRD	F	304	8/8	0.89	0.09	26,28,32,33	0
2	NAG	C	303	14/15	0.90	0.09	19,24,28,28	0
3	MPD	B	304	8/8	0.90	0.09	28,30,32,33	0
3	MPD	E	305	8/8	0.91	0.09	27,33,36,37	0
4	MRD	A	307	8/8	0.91	0.08	20,28,30,33	0
3	MPD	C	305	8/8	0.91	0.09	27,34,39,39	0
3	MPD	D	304	8/8	0.91	0.12	16,22,40,42	0
3	MPD	E	304	8/8	0.91	0.10	38,42,44,45	0
2	NAG	B	302[A]	14/15	0.92	0.07	20,22,25,25	14
3	MPD	F	305	8/8	0.92	0.10	34,38,46,49	0
2	NAG	B	302[B]	14/15	0.92	0.07	19,22,24,26	14
2	NAG	A	302	14/15	0.93	0.07	21,24,26,29	0
3	MPD	D	306	8/8	0.93	0.10	26,27,32,34	0
2	NAG	B	303	14/15	0.93	0.07	22,26,30,32	0
2	NAG	C	302	14/15	0.94	0.06	15,20,24,24	0
2	NAG	F	302	14/15	0.94	0.07	22,26,32,40	0
5	K	D	307	1/1	0.95	0.05	25,25,25,25	0
2	NAG	D	302	14/15	0.96	0.06	16,22,26,28	0
2	NAG	E	302	14/15	0.97	0.05	14,17,23,25	0
5	K	F	306	1/1	0.97	0.05	25,25,25,25	0
5	K	E	306	1/1	0.98	0.04	20,20,20,20	0
5	K	B	307	1/1	0.98	0.03	20,20,20,20	0
5	K	G	304	1/1	0.98	0.14	42,42,42,42	0
5	K	A	308	1/1	0.99	0.04	21,21,21,21	0
5	K	C	307	1/1	0.99	0.05	18,18,18,18	0

6.5 Other polymers [i](#)

There are no such residues in this entry.