



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 01:01 PM UTC

PDB ID : 5EBB / pdb_00005ebb
Title : Structure of human sphingomyelinase phosphodiesterase like 3A (SMPDL3A) with Zn²⁺
Authors : Lim, S.M.; Yeung, K.; Tresaugues, L.; Teo, H.L.; Nordlund, P.
Deposited on : 2015-10-19
Resolution : 2.60 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

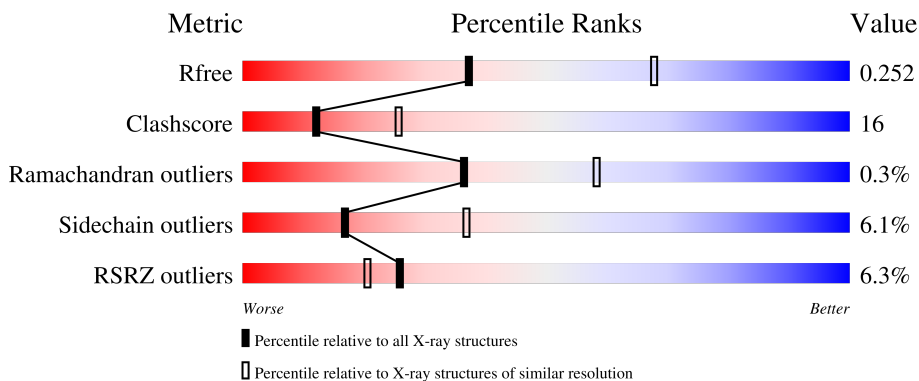
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION




The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	410	
1	B	410	
1	C	410	

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	NAG	C	704	X	-	-	-
4	MLI	B	706	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10414 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 Acid sphingomyelinase-like phosphodiesterase 3a.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	410	3302	2127	529	633	13	0	3	0
1	B	410	3327	2143	532	639	13	0	7	0
1	C	410	3319	2139	532	635	13	0	5	0

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

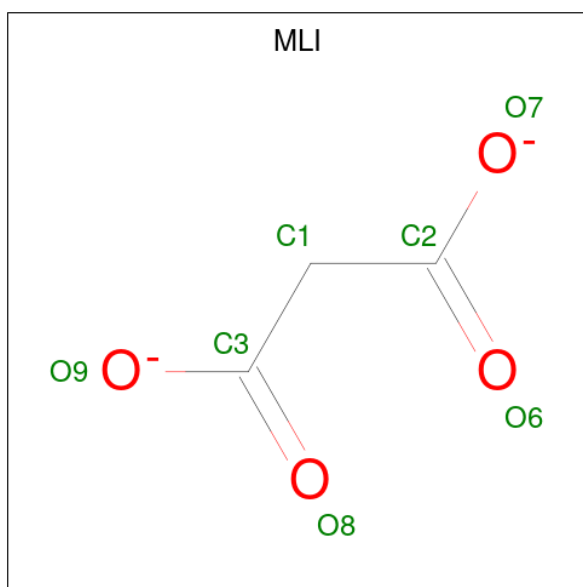
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total 2	Zn 2	0	0
2	B	2	Total 2	Zn 2	0	0
2	C	2	Total 2	Zn 2	0	0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	Total 14	8	1	5	0	0
3	A	1	Total 14	8	1	5	0	0
3	A	1	Total 14	8	1	5	0	0
3	B	1	Total 14	8	1	5	0	0
3	B	1	Total 14	8	1	5	0	0
3	B	1	Total 14	8	1	5	0	0
3	C	1	Total 14	8	1	5	0	0
3	C	1	Total 14	8	1	5	0	0
3	C	1	Total 14	8	1	5	0	0

- Molecule 4 is MALONATE ION (CCD ID: MLI) (formula: $C_3H_2O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	3	4		
4	B	1	Total	C	O	0	0
			7	3	4		
4	C	1	Total	C	O	0	0
			7	3	4		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			6	3	3		

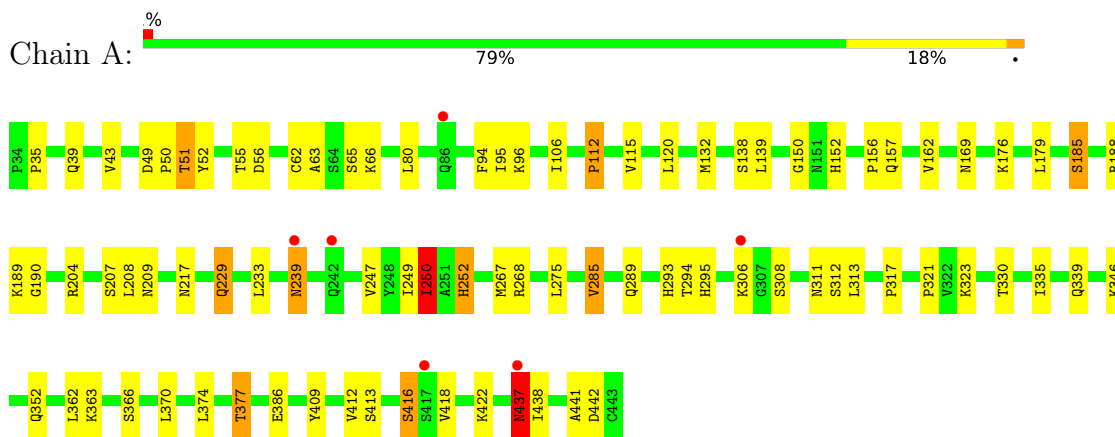
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	56	Total	O	0	0
			56	56		
6	B	126	Total	O	0	0
			126	126		
6	C	119	Total	O	0	0
			119	119		

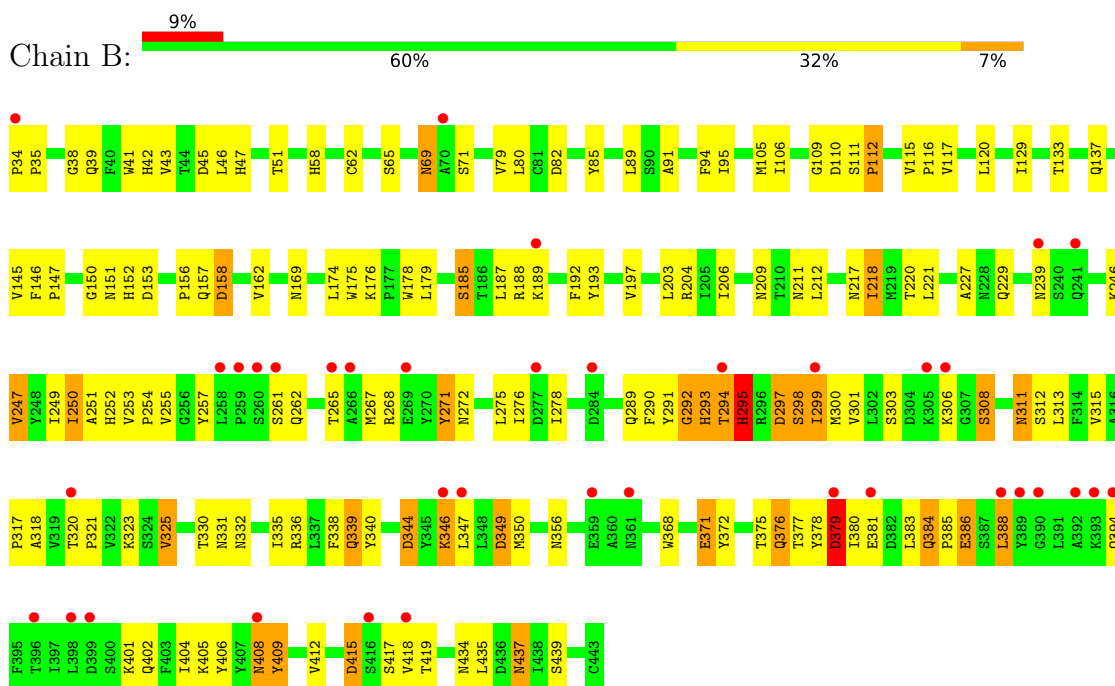
3 Residue-property plots [i](#)

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.

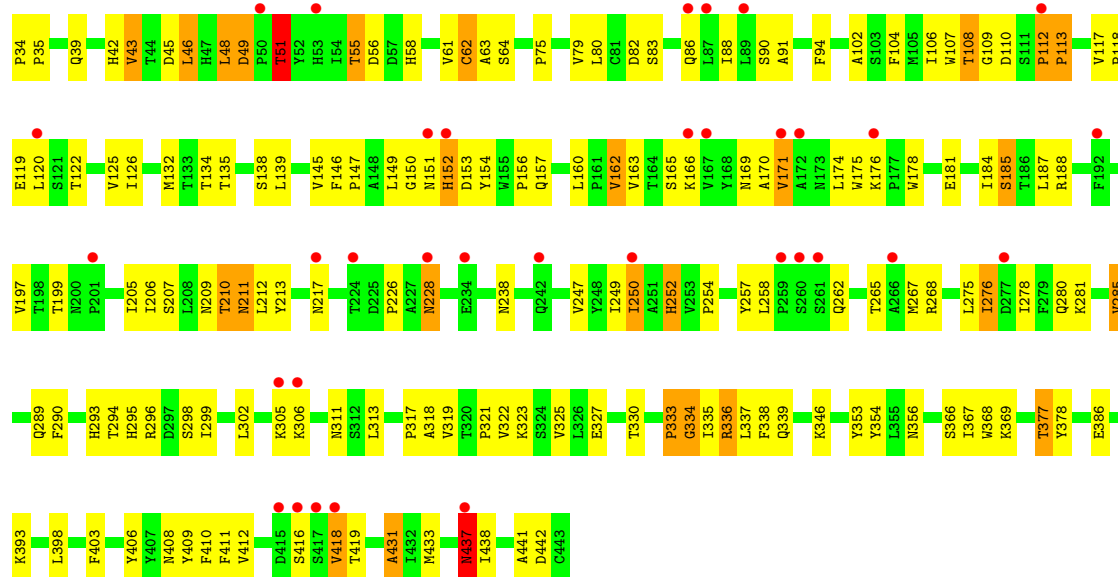
- Molecule 1: Acid sphingomyelinase-like phosphodiesterase 3a



- Molecule 1: Acid sphingomyelinase-like phosphodiesterase 3a



- Molecule 1: Acid sphingomyelinase-like phosphodiesterase 3a



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	147.79Å 147.79Å 139.90Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.38 – 2.60 48.38 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.3 (48.38-2.60) 99.4 (48.38-2.60)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.61 (at 2.61Å)	Xtrriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.237 , 0.255 0.246 , 0.252	Depositor DCC
R_{free} test set	2658 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	22.8	Xtrriage
Anisotropy	0.108	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 53.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtrriage
Estimated twinning fraction	0.000 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10414	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 77.32 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.7055e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, GOL, ZN, MLI

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	1.28	9/3399 (0.3%)	1.16	9/4641 (0.2%)
1	B	1.49	31/3430 (0.9%)	1.37	23/4684 (0.5%)
1	C	1.52	35/3416 (1.0%)	1.51	39/4663 (0.8%)
All	All	1.44	75/10245 (0.7%)	1.35	71/13988 (0.5%)

All (75) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	150	GLY	N-CA	9.38	1.52	1.44
1	C	112	PRO	CA-C	-8.83	1.44	1.52
1	C	152	HIS	CA-C	-8.14	1.41	1.52
1	C	152	HIS	C-O	-7.94	1.13	1.24
1	C	109	GLY	C-O	-7.63	1.14	1.23
1	C	46	LEU	C-O	-7.39	1.15	1.24
1	B	112	PRO	CA-C	7.03	1.58	1.52
1	C	45	ASP	CA-C	6.96	1.61	1.53
1	B	295	HIS	N-CA	6.94	1.55	1.46
1	B	381	GLU	C-O	-6.94	1.15	1.24
1	B	408[A]	ASN	C-O	6.88	1.32	1.24
1	B	408[B]	ASN	C-O	6.88	1.32	1.24
1	B	193	TYR	N-CA	6.83	1.54	1.46
1	C	411	PHE	C-O	-6.77	1.15	1.24
1	A	50	PRO	C-O	-6.64	1.14	1.24
1	C	199	THR	CA-C	6.61	1.61	1.52
1	B	79	VAL	C-O	-6.49	1.15	1.24
1	B	212	LEU	C-O	-6.30	1.16	1.24
1	C	43	VAL	CA-C	6.27	1.60	1.52
1	C	321	PRO	N-CA	-6.18	1.42	1.47
1	C	104	PHE	C-O	6.16	1.30	1.24
1	C	138	SER	C-O	-6.13	1.17	1.24
1	C	49	ASP	CA-C	6.11	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	252	HIS	C-O	-6.11	1.18	1.23
1	B	317	PRO	CA-C	6.10	1.59	1.52
1	B	339	GLN	CA-C	-6.09	1.45	1.52
1	B	217	ASN	CA-C	6.08	1.60	1.52
1	C	333	PRO	CA-C	5.99	1.60	1.52
1	B	347	LEU	N-CA	5.96	1.53	1.46
1	B	290	PHE	C-O	5.86	1.30	1.23
1	C	150	GLY	N-CA	-5.83	1.39	1.44
1	C	165	SER	C-O	-5.77	1.17	1.23
1	C	369	LYS	C-O	5.74	1.30	1.23
1	A	370	LEU	C-O	-5.73	1.17	1.24
1	C	197	VAL	CA-CB	5.71	1.60	1.54
1	B	293	HIS	CA-C	-5.52	1.45	1.52
1	B	294[A]	THR	CA-C	-5.50	1.45	1.52
1	B	294[B]	THR	CA-C	-5.50	1.45	1.52
1	B	406	TYR	N-CA	-5.49	1.39	1.46
1	B	409	TYR	N-CA	-5.48	1.39	1.46
1	B	247	VAL	C-O	-5.47	1.18	1.24
1	C	82	ASP	N-CA	-5.45	1.39	1.45
1	C	408	ASN	C-O	-5.42	1.17	1.24
1	C	171	VAL	CA-CB	5.42	1.61	1.54
1	A	229	GLN	C-O	-5.39	1.17	1.24
1	B	381	GLU	CA-C	-5.38	1.45	1.52
1	B	372	TYR	C-O	-5.38	1.17	1.23
1	C	334	GLY	CA-C	5.36	1.56	1.51
1	B	117	VAL	CA-CB	5.34	1.56	1.54
1	C	294	THR	N-CA	5.33	1.53	1.46
1	A	185	SER	CA-C	-5.32	1.46	1.52
1	C	254	PRO	N-CA	-5.29	1.41	1.46
1	C	276	ILE	CA-CB	5.29	1.60	1.54
1	B	371	GLU	N-CA	5.28	1.52	1.46
1	B	350	MET	CA-C	-5.26	1.46	1.52
1	B	388	LEU	C-O	5.26	1.30	1.24
1	B	349	ASP	C-O	5.22	1.29	1.23
1	C	322	VAL	CA-CB	5.20	1.59	1.54
1	C	138	SER	CA-C	-5.19	1.46	1.52
1	B	111	SER	C-N	5.16	1.39	1.33
1	C	120	LEU	N-CA	5.16	1.52	1.45
1	A	321	PRO	N-CA	-5.15	1.43	1.47
1	B	405	LYS	C-O	5.14	1.30	1.24
1	C	48	LEU	N-CA	-5.13	1.39	1.46
1	C	62	CYS	C-O	-5.13	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	327	GLU	C-O	-5.13	1.17	1.23
1	C	354	TYR	CA-C	-5.13	1.46	1.52
1	C	64	SER	CA-C	5.11	1.59	1.52
1	A	112	PRO	C-O	-5.10	1.18	1.24
1	B	344	ASP	CA-C	5.10	1.59	1.52
1	C	205	ILE	CA-C	-5.07	1.46	1.52
1	A	352	GLN	CA-C	-5.05	1.46	1.52
1	B	292	GLY	N-CA	5.04	1.49	1.45
1	A	317	PRO	CA-C	5.02	1.58	1.52
1	C	108	THR	C-O	-5.01	1.17	1.24

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	112	PRO	CA-C-N	17.45	138.64	120.14
1	C	112	PRO	C-N-CA	17.45	138.64	120.14
1	C	108	THR	N-CA-C	11.01	124.64	112.97
1	C	258	LEU	CA-C-N	-9.28	109.95	120.25
1	C	258	LEU	C-N-CA	-9.28	109.95	120.25
1	B	34	PRO	CA-C-N	8.89	129.06	119.28
1	B	34	PRO	C-N-CA	8.89	129.06	119.28
1	C	110	ASP	N-CA-C	8.38	123.54	111.56
1	C	112	PRO	N-CA-C	-8.20	100.70	110.70
1	C	153	ASP	N-CA-C	8.15	122.89	113.19
1	C	112	PRO	O-C-N	8.00	130.90	121.46
1	C	437	ASN	N-CA-C	7.72	119.70	111.28
1	C	83	SER	N-CA-C	7.39	120.36	109.50
1	C	109	GLY	N-CA-C	7.36	125.35	112.83
1	A	285	VAL	CB-CA-C	-7.21	102.27	112.22
1	A	52	TYR	N-CA-C	7.03	120.85	110.30
1	B	71	SER	N-CA-C	6.91	118.70	111.03
1	B	110	ASP	N-CA-C	6.82	121.32	111.56
1	C	211	ASN	N-CA-C	-6.64	104.07	111.71
1	A	250	ILE	CA-CB-CG2	6.59	121.70	110.50
1	B	437	ASN	N-CA-C	6.59	119.30	111.33
1	C	75	PRO	N-CA-C	-6.58	105.29	113.84
1	B	417	SER	N-CA-C	-6.55	106.03	112.97
1	A	366	SER	CB-CA-C	-6.50	101.54	112.00
1	C	135	THR	N-CA-C	6.41	117.93	111.07
1	B	325	VAL	N-CA-CB	6.41	118.48	110.47
1	C	51	THR	N-CA-C	-6.39	105.24	114.12
1	C	113	PRO	N-CA-C	6.35	122.29	111.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	252	HIS	N-CA-C	6.28	120.78	111.04
1	B	372	TYR	N-CA-C	6.25	117.72	108.60
1	B	271	TYR	N-CA-C	6.23	117.87	111.14
1	C	336	ARG	N-CA-C	6.20	119.29	109.50
1	B	295	HIS	N-CA-C	6.18	125.19	112.02
1	A	138	SER	CB-CA-C	-6.01	100.82	110.79
1	B	146	PHE	CA-C-N	-5.96	112.39	119.84
1	B	146	PHE	C-N-CA	-5.96	112.39	119.84
1	C	199	THR	N-CA-C	5.96	120.16	113.01
1	B	349	ASP	N-CA-C	5.95	116.41	108.38
1	A	437	ASN	N-CA-C	5.93	118.51	111.33
1	A	422	LYS	N-CA-C	5.82	117.62	111.28
1	B	376	GLN	N-CA-C	5.73	117.33	111.14
1	C	83	SER	CA-C-N	-5.68	114.90	120.52
1	C	83	SER	C-N-CA	-5.68	114.90	120.52
1	B	325	VAL	CB-CA-C	-5.68	104.60	112.04
1	C	34	PRO	CA-C-N	5.67	125.34	119.05
1	C	34	PRO	C-N-CA	5.67	125.34	119.05
1	C	205	ILE	N-CA-C	-5.55	100.59	108.58
1	C	102	ALA	N-CA-C	5.49	117.75	109.23
1	B	386	GLU	N-CA-C	-5.49	105.38	111.36
1	B	297	ASP	N-CA-C	5.47	117.14	108.67
1	B	111	SER	N-CA-C	5.46	119.67	112.35
1	A	413	SER	N-CA-C	5.32	119.05	112.24
1	C	337	LEU	N-CA-C	5.32	117.08	108.41
1	C	278	ILE	CB-CA-C	-5.26	105.23	111.97
1	C	119	GLU	N-CA-C	-5.26	106.86	113.28
1	C	431	ALA	N-CA-C	5.24	116.99	111.28
1	C	285	VAL	CB-CA-C	-5.19	105.05	112.22
1	C	325	VAL	CB-CA-C	-5.16	105.17	112.14
1	C	113	PRO	CB-CA-C	-5.15	103.27	110.63
1	C	418	VAL	N-CA-CB	5.14	116.14	110.53
1	B	356	ASN	N-CA-C	-5.14	99.39	108.23
1	C	210	THR	N-CA-C	-5.13	106.28	112.54
1	B	278	ILE	N-CA-C	5.11	115.83	110.62
1	C	333	PRO	CA-C-N	5.11	125.12	121.65
1	C	333	PRO	C-N-CA	5.11	125.12	121.65
1	B	419	THR	N-CA-C	-5.10	102.47	110.17
1	A	138	SER	N-CA-C	5.09	116.83	111.28
1	B	217	ASN	N-CA-C	5.05	116.91	108.23
1	C	294	THR	N-CA-C	5.04	118.68	112.54
1	B	158	ASP	CB-CA-C	-5.00	102.85	110.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	419	THR	N-CA-C	-5.00	102.79	110.14

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	3302	0	3209	48	0
1	B	3327	0	3235	147	0
1	C	3319	0	3231	116	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
3	A	42	0	39	0	0
3	B	42	0	38	0	0
3	C	42	0	39	3	0
4	A	7	0	2	0	0
4	B	7	0	2	2	0
4	C	7	0	2	0	0
5	B	6	0	8	0	0
5	C	6	0	8	1	0
6	A	56	0	0	2	0
6	B	126	0	0	44	0
6	C	119	0	0	9	0
All	All	10414	0	9813	311	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

All (311) 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)
3:C:704:NAG:C2	3:C:704:NAG:C1	1.77	1.60
1:C:151:ASN:HD21	1:C:152:HIS:CD2	1.39	1.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:254:PRO:HB2	6:B:876:HOH:O	1.30	1.26
1:B:69:ASN:O	6:B:801:HOH:O	1.54	1.21
1:C:151:ASN:ND2	1:C:152:HIS:CD2	2.11	1.19
1:B:192:PHE:CG	6:B:853:HOH:O	2.15	0.99
1:A:51:THR:HG21	1:A:63:ALA:H	1.27	0.98
1:B:415:ASP:O	1:B:418:VAL:HG13	1.62	0.97
1:B:209:ASN:H	1:B:229:GLN:HE22	0.99	0.97
1:C:108:THR:CG2	1:C:250[B]:ILE:HG13	1.95	0.96
1:B:299[B]:ILE:HD11	1:B:388:LEU:HD13	1.43	0.96
1:B:252:HIS:C	6:B:809:HOH:O	2.09	0.96
1:B:299[B]:ILE:CD1	1:B:388:LEU:HD13	1.96	0.95
1:B:272:ASN:HB2	6:B:819:HOH:O	1.66	0.95
1:B:192:PHE:CD2	6:B:853:HOH:O	2.22	0.92
1:B:292:GLY:O	6:B:802:HOH:O	1.85	0.92
1:B:412:VAL:HG21	6:B:804:HOH:O	1.70	0.91
1:C:151:ASN:HD21	1:C:152:HIS:HD2	1.19	0.89
1:B:275:LEU:CD1	6:B:911:HOH:O	2.21	0.87
1:B:275:LEU:HD13	6:B:911:HOH:O	1.73	0.87
1:B:415:ASP:HB3	1:B:418:VAL:CG1	2.06	0.86
1:A:51:THR:CG2	1:A:63:ALA:H	1.88	0.86
1:C:108:THR:CG2	1:C:250[B]:ILE:CG1	2.53	0.86
1:B:315:VAL:HG23	6:B:840:HOH:O	1.77	0.85
1:C:154:TYR:HB2	6:C:841:HOH:O	1.77	0.85
1:B:338:PHE:CE2	6:B:855:HOH:O	2.30	0.83
1:B:106[B]:ILE:HD13	1:B:250:ILE:HD11	1.61	0.83
1:C:108:THR:HG21	1:C:250[B]:ILE:HG13	1.61	0.81
1:A:209:ASN:H	1:A:229:GLN:HE22	1.27	0.81
1:B:300:MET:HE1	6:B:876:HOH:O	1.80	0.80
1:C:35:PRO:HG2	6:C:896:HOH:O	1.80	0.80
1:C:151:ASN:ND2	1:C:152:HIS:HD2	1.74	0.79
1:C:51:THR:HG21	1:C:63:ALA:H	1.48	0.79
1:B:254:PRO:HD3	6:B:802:HOH:O	1.82	0.78
1:C:108:THR:HG21	1:C:250[B]:ILE:CG1	2.13	0.78
3:C:704:NAG:C1	3:C:704:NAG:H2	2.09	0.78
1:A:169:ASN:HD22	1:A:188:ARG:HH11	1.33	0.77
1:C:106[A]:ILE:HD12	1:C:250[A]:ILE:HG21	1.67	0.77
1:C:431:ALA:HB2	6:C:867:HOH:O	1.84	0.76
1:B:332:ASN:O	6:B:804:HOH:O	2.02	0.76
1:C:51:THR:CG2	1:C:63:ALA:H	2.00	0.75
1:C:169:ASN:HD22	1:C:188:ARG:HH11	1.34	0.74
1:C:217:ASN:O	1:C:268:ARG:NH2	2.19	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:169:ASN:HD22	1:C:188:ARG:NH1	1.85	0.74
1:B:272:ASN:ND2	6:B:807:HOH:O	2.20	0.73
1:B:415:ASP:CB	1:B:418:VAL:CG1	2.66	0.73
1:A:49:ASP:OD1	1:A:51:THR:HB	1.87	0.73
1:B:35:PRO:HG2	6:B:899:HOH:O	1.89	0.73
1:B:249:ILE:HB	1:B:289:GLN:HG2	1.71	0.72
1:C:319:VAL:HG11	6:C:892:HOH:O	1.88	0.72
1:B:300:MET:CE	6:B:876:HOH:O	2.36	0.72
1:B:129:ILE:HD11	1:B:153:ASP:HB3	1.71	0.72
1:C:267:MET:HE1	1:C:275:LEU:HD12	1.70	0.72
1:C:213:TYR:HB2	1:C:267:MET:HG2	1.72	0.72
1:B:412:VAL:CG2	6:B:804:HOH:O	2.36	0.70
1:B:415:ASP:HB3	1:B:418:VAL:HG13	1.74	0.69
1:B:169:ASN:HD22	1:B:188:ARG:HH11	1.40	0.69
1:C:207:SER:HA	1:C:250[B]:ILE:HG22	1.74	0.69
1:B:112:PRO:HG2	1:B:152:HIS:O	1.94	0.68
1:C:106[A]:ILE:CD1	1:C:250[A]:ILE:HG21	2.23	0.68
1:C:108:THR:HG21	1:C:250[B]:ILE:CD1	2.23	0.68
1:A:323:LYS:HD3	1:A:330:THR:HB	1.75	0.68
1:B:252:HIS:N	6:B:809:HOH:O	2.27	0.67
1:C:377:THR:HG21	1:C:409:TYR:OH	1.95	0.67
1:A:43:VAL:HG12	1:A:335:ILE:HD12	1.77	0.67
1:C:55:THR:OG1	1:C:56:ASP:N	2.27	0.66
1:B:293:HIS:ND1	4:B:706:MLI:O9	2.29	0.66
1:B:371:GLU:OE1	6:B:805:HOH:O	2.14	0.65
1:B:415:ASP:HB3	1:B:418:VAL:HG12	1.77	0.65
1:A:179:LEU:O	6:A:801:HOH:O	2.15	0.65
1:A:106[A]:ILE:HG23	1:A:250:ILE:HG12	1.77	0.65
1:A:377:THR:HG21	1:A:409:TYR:OH	1.97	0.65
1:B:254:PRO:CB	6:B:876:HOH:O	2.06	0.64
3:C:704:NAG:H83	5:C:707:GOL:H32	1.80	0.64
1:B:254:PRO:HG3	6:B:802:HOH:O	1.97	0.64
1:B:294[B]:THR:HG22	1:B:294[B]:THR:O	1.97	0.64
1:C:132:MET:HA	1:C:132:MET:HE2	1.81	0.62
1:B:185:SER:O	1:B:189:LYS:HD2	1.99	0.62
1:B:301:VAL:CG1	6:B:813:HOH:O	2.46	0.62
1:C:145:VAL:O	1:C:147:PRO:HD3	2.00	0.62
1:C:108:THR:HG22	1:C:250[B]:ILE:HG13	1.77	0.62
1:B:106[A]:ILE:HD12	1:B:250:ILE:HD13	1.82	0.61
1:B:331:ASN:HB2	6:B:804:HOH:O	2.00	0.61
1:C:43:VAL:HG21	6:C:908:HOH:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:323:LYS:HD3	1:B:330:THR:HB	1.82	0.60
1:A:363:LYS:HE2	6:B:843:HOH:O	2.01	0.60
1:B:394:GLN:NE2	1:B:402:GLN:HE21	2.00	0.60
1:C:49:ASP:OD1	1:C:51:THR:HB	2.02	0.60
1:C:106[B]:ILE:HD12	1:C:250[B]:ILE:HD13	1.84	0.59
1:C:108:THR:HG21	1:C:250[B]:ILE:HD11	1.82	0.59
1:C:90:SER:HB2	1:C:366:SER:OG	2.01	0.59
1:B:301:VAL:HG13	6:B:813:HOH:O	2.01	0.59
1:A:51:THR:HG21	1:A:63:ALA:N	2.09	0.59
1:A:96:LYS:NZ	1:A:139:LEU:O	2.35	0.59
1:B:415:ASP:O	1:B:418:VAL:CG1	2.46	0.59
1:B:415:ASP:C	1:B:418:VAL:HG13	2.28	0.59
1:C:250[B]:ILE:CD1	1:C:290:PHE:HB2	2.33	0.59
1:B:312:SER:HB3	1:B:388:LEU:HD12	1.85	0.58
1:C:188:ARG:HH11	1:C:188:ARG:HG2	1.69	0.58
1:B:339:GLN:OE1	6:B:806:HOH:O	2.17	0.57
1:C:106[A]:ILE:HD13	1:C:146:PHE:HB2	1.86	0.57
1:A:39:GLN:NE2	1:A:339:GLN:HE21	2.02	0.57
1:C:46:LEU:HB3	1:C:88:ILE:HD12	1.85	0.57
1:C:317:PRO:HD2	6:C:860:HOH:O	2.04	0.57
1:B:297:ASP:OD1	1:B:297:ASP:C	2.48	0.57
1:B:412:VAL:HG12	1:B:412:VAL:O	2.04	0.57
1:C:250[B]:ILE:HD13	1:C:290:PHE:HB2	1.85	0.57
1:C:132:MET:HE2	1:C:132:MET:CA	2.35	0.56
1:A:35:PRO:HG2	6:A:853:HOH:O	2.04	0.56
1:B:47:HIS:O	1:B:82:ASP:HB3	2.06	0.56
1:B:349:ASP:HA	1:B:383:LEU:HD13	1.87	0.56
1:A:249:ILE:HB	1:A:289:GLN:HG2	1.86	0.56
1:B:376:GLN:CG	1:C:35:PRO:HB3	2.35	0.56
1:B:106[B]:ILE:CD1	1:B:250:ILE:HD11	2.33	0.56
1:C:43:VAL:O	1:C:107:TRP:HA	2.06	0.56
1:A:437:ASN:HD22	1:A:438:ILE:H	1.54	0.55
1:B:251:ALA:C	6:B:809:HOH:O	2.49	0.55
1:C:79:VAL:O	1:C:323:LYS:N	2.39	0.55
1:B:299[B]:ILE:HG12	1:B:300:MET:N	2.21	0.55
1:C:145:VAL:HB	1:C:178:TRP:CE2	2.42	0.55
1:C:265:THR:OG1	1:C:267:MET:O	2.16	0.55
1:A:217:ASN:O	1:A:268:ARG:NH2	2.39	0.54
1:B:299[B]:ILE:HD11	1:B:388:LEU:CD1	2.27	0.54
1:B:112:PRO:HD3	1:B:153:ASP:OD1	2.07	0.54
1:B:58:HIS:HB2	1:B:69:ASN:OD1	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:289:GLN:N	6:B:814:HOH:O	2.40	0.54
1:B:346:LYS:HD2	1:B:384:GLN:NE2	2.23	0.54
1:B:377:THR:OG1	6:B:803:HOH:O	1.96	0.53
1:B:42:HIS:HB3	1:B:336:ARG:HG3	1.89	0.53
1:B:39:GLN:NE2	1:B:339:GLN:HE21	2.07	0.53
1:B:192:PHE:CB	1:B:229:GLN:HE21	2.22	0.53
1:C:334:GLY:O	1:C:335:ILE:HD13	2.07	0.53
1:B:178:TRP:O	1:B:179:LEU:HD23	2.09	0.53
1:B:435:LEU:N	1:B:435:LEU:HD12	2.24	0.53
1:B:254:PRO:CG	6:B:802:HOH:O	2.55	0.52
1:C:149:LEU:HD21	1:C:171:VAL:HG11	1.91	0.52
1:B:376:GLN:HG3	1:C:35:PRO:HB3	1.91	0.52
1:C:393:LYS:HG2	1:C:433:MET:HE1	1.91	0.52
1:B:51:THR:O	1:B:51:THR:HG22	2.10	0.52
1:C:169:ASN:ND2	1:C:188:ARG:HH11	2.05	0.52
1:B:38:GLY:HA3	1:B:340:TYR:CZ	2.45	0.51
1:B:318:ALA:HB1	1:B:320:THR:HG22	1.91	0.51
1:C:162:VAL:HG12	1:C:163:VAL:HG13	1.92	0.51
1:C:313:LEU:N	1:C:313:LEU:HD12	2.24	0.51
1:B:157:GLN:O	1:B:158:ASP:HB2	2.09	0.51
1:C:112:PRO:CB	1:C:113:PRO:HD2	2.37	0.51
1:A:39:GLN:HE21	1:A:339:GLN:HE21	1.57	0.51
1:B:62:CYS:SG	1:B:65:SER:HB3	2.51	0.51
1:B:106[B]:ILE:HG21	1:B:250:ILE:CD1	2.41	0.51
1:B:91:ALA:HB2	1:B:368:TRP:CZ2	2.45	0.51
1:A:112:PRO:HG2	1:A:152:HIS:O	2.10	0.50
1:B:156:PRO:O	1:B:157:GLN:C	2.55	0.50
1:B:162:VAL:HG13	1:B:227:ALA:HA	1.93	0.50
1:A:132:MET:HA	1:A:132:MET:HE2	1.93	0.50
1:B:246:LYS:HG3	1:B:344:ASP:O	2.12	0.50
1:C:250[B]:ILE:HD12	1:C:290:PHE:O	2.12	0.50
1:C:213:TYR:CB	1:C:267:MET:HG2	2.40	0.50
1:C:393:LYS:NZ	1:C:433:MET:HE1	2.26	0.50
1:A:441:ALA:O	1:A:442:ASP:C	2.54	0.50
1:B:192:PHE:CD1	6:B:853:HOH:O	2.53	0.50
1:B:175:TRP:HE3	1:B:187:LEU:HD21	1.76	0.50
1:B:45:ASP:OD2	1:B:252:HIS:HE1	1.94	0.50
1:B:252:HIS:CA	6:B:809:HOH:O	2.48	0.50
1:B:375:THR:O	1:B:379[A]:ASP:HA	2.12	0.50
1:C:134:THR:HG21	6:C:909:HOH:O	2.11	0.50
1:B:272:ASN:CG	6:B:807:HOH:O	2.53	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:415:ASP:CB	1:B:418:VAL:HG13	2.40	0.49
1:C:206:ILE:HG13	1:C:247:VAL:HG13	1.94	0.49
1:A:43:VAL:HG12	1:A:335:ILE:CD1	2.42	0.49
1:C:252:HIS:CD2	1:C:293:HIS:HB2	2.48	0.49
1:A:208:LEU:HD21	1:A:233:LEU:HD13	1.95	0.48
1:C:132:MET:HE2	1:C:132:MET:N	2.28	0.48
1:C:386:GLU:H	1:C:386:GLU:CD	2.22	0.48
1:C:106[B]:ILE:HD12	1:C:250[B]:ILE:CD1	2.43	0.48
1:A:374:LEU:C	1:A:374:LEU:HD23	2.37	0.48
1:B:293:HIS:CE1	4:B:706:MLI:O9	2.67	0.48
1:B:375:THR:HB	1:B:380:ILE:O	2.14	0.48
1:C:94:PHE:CZ	1:C:353:TYR:CD1	3.02	0.48
1:C:356:ASN:OD1	1:C:356:ASN:C	2.56	0.48
1:A:156:PRO:O	1:A:157:GLN:C	2.53	0.48
1:B:206:ILE:HD12	1:B:247:VAL:HG11	1.95	0.48
1:C:319:VAL:HG21	6:C:892:HOH:O	2.12	0.48
1:B:255:VAL:O	1:B:300:MET:HE1	2.14	0.48
1:C:181:GLU:O	1:C:185:SER:HB2	2.14	0.48
1:C:403:PHE:O	1:C:406:TYR:HB3	2.14	0.47
1:B:349:ASP:HA	1:B:383:LEU:CD1	2.43	0.47
1:A:437:ASN:HD22	1:A:438:ILE:N	2.12	0.47
1:B:254:PRO:CD	6:B:802:HOH:O	2.48	0.47
1:B:209:ASN:N	1:B:229:GLN:HE22	1.85	0.47
1:C:94:PHE:HZ	1:C:353:TYR:CD1	2.32	0.47
1:C:319:VAL:O	1:C:333:PRO:HB3	2.14	0.47
1:A:106[B]:ILE:HD13	1:A:250:ILE:HD11	1.97	0.47
1:B:175:TRP:CE3	1:B:187:LEU:HD21	2.50	0.47
1:B:375:THR:O	1:B:379[B]:ASP:HA	2.14	0.47
1:B:197:VAL:HG21	1:B:203:LEU:HD23	1.96	0.47
1:B:106[B]:ILE:HG21	1:B:250:ILE:HD11	1.95	0.47
1:B:267:MET:HB2	6:B:819:HOH:O	2.14	0.47
1:B:294[B]:THR:O	1:B:294[B]:THR:CG2	2.62	0.47
1:B:298:SER:C	1:B:299[A]:ILE:CG2	2.85	0.47
1:C:58:HIS:HA	1:C:61:VAL:HG23	1.97	0.47
1:C:249:ILE:HB	1:C:289:GLN:HG2	1.97	0.47
1:C:323:LYS:HB3	1:C:330:THR:HB	1.96	0.47
1:A:51:THR:HG22	1:A:62:CYS:HA	1.97	0.46
1:C:160:LEU:HD23	1:C:209:ASN:HD21	1.80	0.46
1:A:252:HIS:CD2	1:A:293:HIS:HB2	2.51	0.46
1:B:115:VAL:CG2	1:B:120:LEU:HG	2.45	0.46
1:B:137:GLN:HG3	1:B:178:TRP:CZ2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145:VAL:HB	1:B:178:TRP:CE2	2.50	0.46
1:C:151:ASN:CG	1:C:152:HIS:HD2	2.21	0.46
1:B:109:GLY:HA2	6:B:829:HOH:O	2.15	0.46
1:B:151:ASN:N	1:B:211:ASN:ND2	2.63	0.46
1:C:91:ALA:HB1	1:C:335:ILE:HD11	1.97	0.46
1:C:42:HIS:HB3	1:C:336:ARG:HG3	1.98	0.46
1:B:254:PRO:HA	1:B:291:TYR:CD1	2.51	0.46
1:B:346:LYS:HD2	1:B:384:GLN:HE22	1.79	0.45
1:C:175:TRP:CE3	1:C:187:LEU:HD21	2.51	0.45
1:A:267:MET:HE1	1:A:275:LEU:HD12	1.99	0.45
1:C:276:ILE:O	1:C:280:GLN:HG3	2.16	0.45
1:A:312:SER:C	1:A:313:LEU:HD12	2.41	0.45
1:B:133:THR:HG21	1:B:174:LEU:HB3	1.99	0.45
1:A:94:PHE:O	1:A:95:ILE:C	2.57	0.44
1:B:151:ASN:HB2	1:B:158:ASP:OD1	2.17	0.44
1:A:294:THR:O	1:A:295:HIS:HB2	2.18	0.44
1:B:303:SER:HA	1:B:308:SER:O	2.18	0.44
1:B:408[B]:ASN:OD1	1:B:409:TYR:CD1	2.69	0.44
1:C:276:ILE:HG23	1:C:302:LEU:HD11	1.99	0.44
1:B:106[B]:ILE:HD11	6:B:855:HOH:O	2.16	0.44
1:B:192:PHE:HB3	1:B:229:GLN:NE2	2.32	0.44
1:B:115:VAL:HB	1:B:116:PRO:HD2	2.00	0.44
1:B:220:THR:O	1:B:221:LEU:C	2.60	0.44
1:B:376:GLN:CD	1:C:35:PRO:HB3	2.42	0.44
1:A:115:VAL:CG2	1:A:120:LEU:HG	2.48	0.44
1:A:185:SER:O	1:A:189:LYS:HD2	2.18	0.44
1:C:170:ALA:O	1:C:174:LEU:HG	2.17	0.44
1:C:42:HIS:CE1	1:C:290:PHE:HB3	2.54	0.43
1:C:166[B]:LYS:O	1:C:166[B]:LYS:HD3	2.18	0.43
1:C:437:ASN:HD22	1:C:438:ILE:N	2.16	0.43
1:C:295:HIS:CD2	1:C:318:ALA:HB2	2.52	0.43
1:B:42:HIS:HB3	1:B:336:ARG:CG	2.48	0.43
1:B:325:VAL:HG23	6:B:872:HOH:O	2.18	0.43
1:C:48:LEU:HD22	1:C:132:MET:HE3	2.00	0.43
1:C:162:VAL:HG13	6:C:891:HOH:O	2.18	0.43
1:C:49:ASP:C	1:C:51:THR:H	2.26	0.43
1:C:151:ASN:CG	1:C:152:HIS:N	2.76	0.43
1:C:188:ARG:NH1	1:C:188:ARG:HG2	2.34	0.43
1:B:41:TRP:HB2	1:B:105:MET:HG3	2.00	0.43
1:B:43:VAL:HG12	1:B:335:ILE:HD12	2.01	0.43
1:C:156:PRO:O	1:C:157:GLN:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:171:VAL:HB	1:C:175:TRP:CZ3	2.52	0.43
1:A:55:THR:OG1	1:A:56:ASP:N	2.52	0.43
1:A:204:ARG:O	1:A:247:VAL:HA	2.18	0.43
1:A:386:GLU:H	1:A:386:GLU:CD	2.27	0.43
1:B:301:VAL:CG2	6:B:813:HOH:O	2.67	0.43
1:C:112:PRO:HG2	1:C:152:HIS:O	2.18	0.42
1:C:171:VAL:HB	1:C:175:TRP:CH2	2.53	0.42
1:C:210:THR:O	1:C:211:ASN:C	2.59	0.42
1:A:239:ASN:OD1	1:A:239:ASN:C	2.61	0.42
1:A:289:GLN:HB2	1:A:313:LEU:HG	2.00	0.42
1:A:416:SER:C	1:A:418:VAL:H	2.26	0.42
1:B:151:ASN:O	1:B:158:ASP:N	2.41	0.42
1:B:147:PRO:HG2	1:B:175:TRP:CD2	2.54	0.42
1:B:106[A]:ILE:CG2	1:B:250:ILE:HG12	2.49	0.42
1:B:298:SER:C	1:B:299[A]:ILE:HG22	2.45	0.42
1:B:115:VAL:HG23	1:B:120:LEU:HG	2.01	0.42
1:B:385:PRO:HA	6:B:813:HOH:O	2.19	0.42
1:A:150:GLY:HA2	1:A:252:HIS:CG	2.55	0.42
1:B:289:GLN:NE2	1:B:311:ASN:OD1	2.47	0.42
1:B:268:ARG:NH1	1:B:271:TYR:HE2	2.18	0.42
1:B:388:LEU:HD23	1:B:388:LEU:HA	1.80	0.42
1:B:85:TYR:CE2	1:B:89:LEU:HD22	2.55	0.42
1:C:62:CYS:O	1:C:62:CYS:SG	2.77	0.42
1:A:374:LEU:HD23	1:A:374:LEU:O	2.20	0.41
1:B:106[A]:ILE:HG21	1:B:250:ILE:HD11	2.00	0.41
1:C:175:TRP:HE3	1:C:187:LEU:HD21	1.84	0.41
1:C:206:ILE:HD12	1:C:247:VAL:HG11	2.01	0.41
1:C:210:THR:C	1:C:212:LEU:N	2.74	0.41
1:C:441:ALA:O	1:C:442:ASP:C	2.63	0.41
1:B:295:HIS:HA	6:B:833:HOH:O	2.19	0.41
1:C:298:SER:HA	1:C:406:TYR:OH	2.20	0.41
1:A:51:THR:HG21	1:A:63:ALA:CB	2.49	0.41
1:C:257:TYR:CE2	1:C:265:THR:HG23	2.56	0.41
1:C:296:ARG:HB3	1:C:410:PHE:CE1	2.55	0.41
1:A:362:LEU:HD23	1:A:362:LEU:HA	1.89	0.41
1:C:39:GLN:NE2	1:C:339:GLN:HE21	2.18	0.41
1:C:94:PHE:CD1	1:C:368:TRP:HB2	2.54	0.41
1:B:253:VAL:HG22	1:B:293:HIS:CD2	2.56	0.41
1:C:267:MET:CE	1:C:275:LEU:HD12	2.44	0.41
1:C:49:ASP:OD1	1:C:51:THR:CB	2.67	0.41
1:C:226:PRO:C	1:C:228:ASN:H	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:336:ARG:HD3	1:B:338:PHE:CE2	2.56	0.41
1:B:338:PHE:HE2	6:B:855:HOH:O	1.87	0.41
1:B:371:GLU:OE2	1:B:412:VAL:HA	2.21	0.41
1:B:401:LYS:N	1:B:401:LYS:HD2	2.34	0.41
1:B:434:ASN:OD1	1:B:439:SER:HB3	2.21	0.41
1:C:94:PHE:HZ	1:C:353:TYR:CE1	2.39	0.41
1:A:62:CYS:SG	1:A:65:SER:HB3	2.61	0.41
1:A:207:SER:HA	1:A:250:ILE:HG22	2.02	0.41
1:B:94:PHE:O	1:B:95:ILE:C	2.63	0.41
1:B:271:TYR:O	1:B:272:ASN:C	2.65	0.41
1:C:112:PRO:HB3	1:C:113:PRO:HD2	2.03	0.41
1:C:122:THR:HG22	1:C:126:ILE:HD12	2.02	0.41
1:C:437:ASN:HD22	1:C:438:ILE:H	1.69	0.41
1:B:325:VAL:O	1:B:325:VAL:HG12	2.21	0.40
1:B:218:ILE:HD13	1:B:218:ILE:N	2.37	0.40
1:C:117:VAL:HB	1:C:118:PRO:HD3	2.03	0.40
1:C:250[B]:ILE:HD12	1:C:250[B]:ILE:HA	1.51	0.40
1:B:204:ARG:O	1:B:247:VAL:HA	2.21	0.40
1:B:257:TYR:CE2	1:B:265:THR:HG23	2.57	0.40
1:C:39:GLN:HA	1:C:338:PHE:O	2.21	0.40
1:C:378:TYR:OH	1:C:406:TYR:HA	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	411/410 (100%)	387 (94%)	23 (6%)	1 (0%)	43 66
1	B	415/410 (101%)	385 (93%)	26 (6%)	4 (1%)	12 28
1	C	413/410 (101%)	380 (92%)	33 (8%)	0	100 100
All	All	1239/1230 (101%)	1152 (93%)	82 (7%)	5 (0%)	36 51

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	295	HIS
1	B	379[A]	ASP
1	B	379[B]	ASP
1	A	190	GLY
1	B	321	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	375/372 (101%)	359 (96%)	16 (4%)	26	51
1	B	379/372 (102%)	353 (93%)	26 (7%)	14	32
1	C	377/372 (101%)	348 (92%)	29 (8%)	12	27
All	All	1131/1116 (101%)	1060 (94%)	71 (6%)	17	36

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	THR
1	A	66	LYS
1	A	80	LEU
1	A	162	VAL
1	A	176	LYS
1	A	239	ASN
1	A	250	ILE
1	A	285	VAL
1	A	306	LYS
1	A	308	SER
1	A	311	ASN
1	A	346	LYS
1	A	377	THR
1	A	412	VAL
1	A	416	SER
1	A	437	ASN

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Mol	Chain	Res	Type
1	B	46	LEU
1	B	69	ASN
1	B	80	LEU
1	B	176	LYS
1	B	185	SER
1	B	218	ILE
1	B	239	ASN
1	B	250	ILE
1	B	261	SER
1	B	262	GLN
1	B	276	ILE
1	B	298	SER
1	B	299[A]	ILE
1	B	299[B]	ILE
1	B	306	LYS
1	B	308	SER
1	B	311	ASN
1	B	313	LEU
1	B	346	LYS
1	B	379[A]	ASP
1	B	379[B]	ASP
1	B	384	GLN
1	B	386	GLU
1	B	404	ILE
1	B	415	ASP
1	B	437	ASN
1	C	51	THR
1	C	55	THR
1	C	80	LEU
1	C	86	GLN
1	C	125	VAL
1	C	139	LEU
1	C	162	VAL
1	C	176	LYS
1	C	184	ILE
1	C	185	SER
1	C	228	ASN
1	C	238	ASN
1	C	250[A]	ILE
1	C	250[B]	ILE
1	C	262	GLN
1	C	281	LYS

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Mol	Chain	Res	Type
1	C	285	VAL
1	C	299	ILE
1	C	305	LYS
1	C	306	LYS
1	C	311	ASN
1	C	346	LYS
1	C	367	ILE
1	C	377	THR
1	C	398	LEU
1	C	412	VAL
1	C	416	SER
1	C	418	VAL
1	C	437	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	GLN
1	A	58	HIS
1	A	169	ASN
1	A	200	ASN
1	A	211	ASN
1	A	229	GLN
1	A	262	GLN
1	A	263	ASN
1	A	332	ASN
1	A	384	GLN
1	A	437	ASN
1	B	39	GLN
1	B	169	ASN
1	B	200	ASN
1	B	211	ASN
1	B	229	GLN
1	B	263	ASN
1	B	339	GLN
1	B	376	GLN
1	B	394	GLN
1	B	402	GLN
1	C	39	GLN
1	C	53	HIS
1	C	58	HIS
1	C	86	GLN

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Mol	Chain	Res	Type
1	C	127	ASN
1	C	169	ASN
1	C	200	ASN
1	C	239	ASN
1	C	241	GLN
1	C	263	ASN
1	C	332	ASN
1	C	437	ASN

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 20 ligands modelled in this entry, 6 are monoatomic - leaving 14 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
3	NAG	A	703	1	14,14,15	1.94	5 (35%)	17,19,21	1.66	5 (29%)
3	NAG	B	705	1	14,14,15	2.32	4 (28%)	17,19,21	2.36	8 (47%)
3	NAG	C	705	1	14,14,15	2.38	4 (28%)	17,19,21	2.16	6 (35%)
5	GOL	B	707	-	5,5,5	0.66	0	5,5,5	0.44	0
5	GOL	C	707	-	5,5,5	0.46	0	5,5,5	1.08	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	MLI	B	706	2	6,6,6	2.06	1 (16%)	7,7,7	1.61	2 (28%)
4	MLI	A	706	2	6,6,6	2.07	2 (33%)	7,7,7	2.27	2 (28%)
4	MLI	C	706	2	6,6,6	2.05	2 (33%)	7,7,7	1.51	2 (28%)
3	NAG	A	704	1	14,14,15	1.72	3 (21%)	17,19,21	1.30	2 (11%)
3	NAG	A	705	1	14,14,15	2.18	2 (14%)	17,19,21	3.57	11 (64%)
3	NAG	B	703	1	14,14,15	2.49	5 (35%)	17,19,21	1.42	2 (11%)
3	NAG	C	703	1	14,14,15	2.04	4 (28%)	17,19,21	1.87	6 (35%)
3	NAG	B	704	1	14,14,15	1.71	4 (28%)	17,19,21	1.85	3 (17%)
3	NAG	C	704	1	14,14,15	5.96	6 (42%)	17,19,21	3.52	10 (58%)

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
3	NAG	A	703	1	-	2/6/23/26	0/1/1/1
3	NAG	B	705	1	-	4/6/23/26	0/1/1/1
3	NAG	C	705	1	-	0/6/23/26	0/1/1/1
5	GOL	B	707	-	-	2/4/4/4	-
5	GOL	C	707	-	-	4/4/4/4	-
4	MLI	B	706	2	-	0/4/4/4	-
4	MLI	A	706	2	-	0/4/4/4	-
4	MLI	C	706	2	-	0/4/4/4	-
3	NAG	A	704	1	-	2/6/23/26	0/1/1/1
3	NAG	A	705	1	-	2/6/23/26	0/1/1/1
3	NAG	B	703	1	-	2/6/23/26	0/1/1/1
3	NAG	C	703	1	-	2/6/23/26	0/1/1/1
3	NAG	B	704	1	-	2/6/23/26	0/1/1/1
3	NAG	C	704	1	1/1/5/7	4/6/23/26	0/1/1/1

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	704	NAG	C1-C2	18.24	1.77	1.52
3	C	704	NAG	O5-C1	8.28	1.57	1.43
3	A	705	NAG	O4-C4	6.69	1.59	1.43
3	C	705	NAG	O4-C4	6.31	1.58	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	703	NAG	C1-C2	6.02	1.60	1.52
3	C	704	NAG	O5-C5	5.89	1.54	1.43
3	B	705	NAG	O4-C4	5.41	1.56	1.43
3	C	703	NAG	C1-C2	4.94	1.59	1.52
3	C	704	NAG	C3-C2	4.75	1.62	1.52
3	A	704	NAG	O5-C1	4.56	1.51	1.43
3	C	704	NAG	C2-N2	4.54	1.53	1.46
3	B	705	NAG	O3-C3	-4.41	1.32	1.43
3	B	704	NAG	O5-C1	4.34	1.51	1.43
4	B	706	MLI	C1-C3	4.06	1.57	1.51
4	A	706	MLI	C1-C2	3.96	1.57	1.51
4	C	706	MLI	C1-C3	3.82	1.57	1.51
3	A	703	NAG	C1-C2	3.57	1.57	1.52
3	B	703	NAG	O5-C1	3.55	1.49	1.43
3	A	703	NAG	O4-C4	3.53	1.51	1.43
3	B	703	NAG	O4-C4	3.52	1.51	1.43
3	C	703	NAG	C8-C7	3.27	1.57	1.50
3	C	705	NAG	O5-C5	3.16	1.49	1.43
3	B	703	NAG	C8-C7	3.15	1.57	1.50
3	C	705	NAG	C4-C5	3.12	1.59	1.53
3	A	704	NAG	C8-C7	3.05	1.56	1.50
3	B	705	NAG	C2-N2	3.05	1.51	1.46
3	A	703	NAG	O5-C5	2.93	1.49	1.43
3	B	705	NAG	C1-C2	2.83	1.56	1.52
3	B	704	NAG	O5-C5	2.82	1.48	1.43
3	C	705	NAG	C1-C2	2.82	1.56	1.52
3	A	703	NAG	C8-C7	2.78	1.56	1.50
3	A	704	NAG	O5-C5	2.57	1.48	1.43
4	A	706	MLI	C1-C3	2.54	1.55	1.51
3	B	704	NAG	C8-C7	2.43	1.55	1.50
3	B	703	NAG	C4-C5	2.29	1.57	1.53
4	C	706	MLI	C1-C2	2.27	1.54	1.51
3	A	705	NAG	O5-C5	2.21	1.47	1.43
3	A	703	NAG	O5-C1	2.17	1.47	1.43
3	C	703	NAG	O3-C3	2.17	1.48	1.43
3	C	704	NAG	O3-C3	2.13	1.48	1.43
3	C	703	NAG	O4-C4	2.07	1.48	1.43
3	B	704	NAG	C2-N2	2.04	1.49	1.46

All (60) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	705	NAG	C1-O5-C5	10.57	126.35	112.19
3	C	704	NAG	O5-C5-C6	8.12	123.46	107.66
3	C	704	NAG	C2-N2-C7	7.22	132.57	122.90
3	C	704	NAG	C1-C2-N2	5.33	118.83	110.43
3	A	705	NAG	O5-C5-C6	-4.94	98.04	107.66
3	B	704	NAG	C1-O5-C5	4.44	118.14	112.19
3	A	705	NAG	O3-C3-C2	-4.39	100.28	109.40
3	B	704	NAG	O5-C5-C6	4.20	115.84	107.66
3	B	705	NAG	C2-N2-C7	4.15	128.46	122.90
4	A	706	MLI	O6-C2-C1	-4.04	110.59	122.11
3	C	703	NAG	O5-C5-C6	4.04	115.52	107.66
3	C	705	NAG	O4-C4-C5	4.00	119.18	109.32
3	C	704	NAG	C4-C3-C2	3.93	116.78	111.02
3	C	705	NAG	O5-C1-C2	-3.93	105.22	111.29
3	B	705	NAG	C3-C4-C5	-3.86	103.22	110.23
3	C	703	NAG	C1-O5-C5	-3.78	107.12	112.19
4	A	706	MLI	O7-C2-C1	3.61	125.69	114.51
3	C	705	NAG	C1-O5-C5	3.58	116.99	112.19
3	A	703	NAG	O5-C5-C6	3.52	114.51	107.66
3	B	705	NAG	C1-C2-N2	-3.44	105.01	110.43
3	A	704	NAG	C1-O5-C5	3.41	116.75	112.19
3	A	705	NAG	O4-C4-C3	3.35	118.27	110.38
3	A	705	NAG	O6-C6-C5	-3.32	100.02	111.33
3	C	704	NAG	C1-O5-C5	3.27	116.57	112.19
3	C	704	NAG	O7-C7-N2	3.21	127.66	121.98
3	C	705	NAG	C3-C4-C5	-3.15	104.53	110.23
3	B	703	NAG	O4-C4-C5	3.12	117.01	109.32
4	B	706	MLI	C3-C1-C2	-3.08	102.07	112.95
3	A	703	NAG	O4-C4-C5	3.03	116.78	109.32
3	B	705	NAG	O4-C4-C3	2.89	117.19	110.38
3	B	705	NAG	O4-C4-C5	2.86	116.37	109.32
3	A	705	NAG	C1-C2-N2	-2.86	105.93	110.43
3	A	705	NAG	O5-C5-C4	2.76	117.55	110.83
3	C	705	NAG	O3-C3-C2	-2.75	103.69	109.40
3	C	704	NAG	O5-C5-C4	-2.72	104.22	110.83
4	C	706	MLI	O8-C3-C1	-2.70	114.41	122.11
3	A	703	NAG	C3-C4-C5	-2.69	105.36	110.23
3	B	705	NAG	C1-O5-C5	2.65	115.73	112.19
3	B	703	NAG	C3-C4-C5	-2.59	105.53	110.23
3	B	705	NAG	O5-C5-C6	2.50	112.54	107.66
3	A	703	NAG	O5-C5-C4	-2.41	104.96	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	703	NAG	C3-C4-C5	-2.40	105.88	110.23
3	A	704	NAG	O5-C5-C6	2.40	112.33	107.66
4	C	706	MLI	O9-C3-C1	2.39	121.93	114.51
3	C	705	NAG	C1-C2-N2	-2.35	106.72	110.43
3	C	703	NAG	C2-N2-C7	-2.33	119.78	122.90
4	B	706	MLI	O6-C2-C1	-2.31	115.54	122.11
3	B	705	NAG	O5-C5-C4	-2.31	105.22	110.83
3	B	704	NAG	C4-C3-C2	2.27	114.34	111.02
3	A	705	NAG	O4-C4-C5	2.27	114.91	109.32
3	A	705	NAG	O3-C3-C4	-2.23	105.11	110.38
3	A	705	NAG	C6-C5-C4	-2.23	107.55	113.02
3	C	704	NAG	O3-C3-C2	2.20	113.97	109.40
3	C	704	NAG	O7-C7-C8	-2.11	118.30	122.05
3	C	703	NAG	C1-C2-N2	-2.08	107.16	110.43
3	C	704	NAG	O4-C4-C5	2.05	114.37	109.32
3	A	705	NAG	O5-C1-C2	-2.02	108.16	111.29
3	C	703	NAG	O4-C4-C5	2.02	114.30	109.32
3	A	703	NAG	O3-C3-C2	-2.02	105.21	109.40
5	C	707	GOL	O3-C3-C2	-2.00	101.36	110.38

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	C	704	NAG	C1

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	707	GOL	O2-C2-C3-O3
5	C	707	GOL	C1-C2-C3-O3
5	C	707	GOL	O2-C2-C3-O3
3	B	704	NAG	O5-C5-C6-O6
3	A	704	NAG	O5-C5-C6-O6
3	A	703	NAG	O5-C5-C6-O6
3	B	704	NAG	C4-C5-C6-O6
3	A	704	NAG	C4-C5-C6-O6
3	A	703	NAG	C4-C5-C6-O6
3	C	703	NAG	O5-C5-C6-O6
3	C	704	NAG	C4-C5-C6-O6
3	C	703	NAG	C4-C5-C6-O6
3	B	705	NAG	C8-C7-N2-C2
3	B	705	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
3	A	705	NAG	C4-C5-C6-O6
3	B	703	NAG	O5-C5-C6-O6
3	B	703	NAG	C4-C5-C6-O6
3	B	705	NAG	O5-C5-C6-O6
3	B	705	NAG	C4-C5-C6-O6
3	C	704	NAG	O5-C5-C6-O6
3	A	705	NAG	O5-C5-C6-O6
5	B	707	GOL	C1-C2-C3-O3
5	C	707	GOL	O1-C1-C2-C3
3	C	704	NAG	C3-C2-N2-C7
3	C	704	NAG	C1-C2-N2-C7
5	C	707	GOL	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	707	GOL	1	0
4	B	706	MLI	2	0
3	C	704	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

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	410/410 (100%)	-0.36	6 (1%) 72 68	3, 13, 32, 56	3 (0%)
1	B	410/410 (100%)	0.87	37 (9%) 15 11	4, 23, 41, 60	7 (1%)
1	C	410/410 (100%)	0.89	34 (8%) 17 13	7, 23, 43, 65	5 (1%)
All	All	1230/1230 (100%)	0.47	77 (6%) 26 20	3, 20, 40, 65	15 (1%)

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	305	LYS	7.1
1	C	151	ASN	6.0
1	C	166[A]	LYS	5.3
1	B	294[A]	THR	5.2
1	B	390	GLY	4.6
1	B	34	PRO	4.4
1	B	408[A]	ASN	4.3
1	C	306	LYS	4.1
1	B	260[A]	SER	4.0
1	B	306	LYS	3.9
1	B	416	SER	3.8
1	B	284	ASP	3.6
1	B	305	LYS	3.5
1	C	437	ASN	3.5
1	C	277	ASP	3.5
1	C	260[A]	SER	3.4
1	B	379[A]	ASP	3.3
1	B	269	GLU	3.2
1	B	277	ASP	3.1
1	B	347	LEU	3.1
1	B	299[A]	ILE	3.1
1	B	258	LEU	3.0
1	C	259	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	389	TYR	2.9
1	C	50	PRO	2.8
1	B	266	ALA	2.8
1	B	70	ALA	2.8
1	A	306	LYS	2.8
1	C	250[A]	ILE	2.7
1	C	217	ASN	2.7
1	C	417	SER	2.6
1	C	172	ALA	2.6
1	C	266	ALA	2.6
1	B	241	GLN	2.6
1	C	201	PRO	2.6
1	C	261	SER	2.5
1	C	192	PHE	2.5
1	B	259	PRO	2.5
1	A	239	ASN	2.5
1	B	346	LYS	2.5
1	C	415	ASP	2.4
1	B	189	LYS	2.4
1	C	176	LYS	2.4
1	C	53	HIS	2.4
1	C	171	VAL	2.4
1	C	418	VAL	2.4
1	B	261	SER	2.4
1	C	234	GLU	2.4
1	B	399	ASP	2.4
1	C	167	VAL	2.4
1	C	89	LEU	2.3
1	C	224	THR	2.3
1	B	393	LYS	2.3
1	B	418	VAL	2.3
1	B	265	THR	2.3
1	C	242	GLN	2.2
1	B	381	GLU	2.2
1	B	394	GLN	2.2
1	C	112	PRO	2.2
1	C	120	LEU	2.2
1	A	86	GLN	2.1
1	C	86	GLN	2.1
1	B	396	THR	2.1
1	A	242	GLN	2.1
1	C	228	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	359	GLU	2.1
1	B	320	THR	2.1
1	B	388	LEU	2.1
1	A	417	SER	2.1
1	B	392	ALA	2.1
1	C	416	SER	2.1
1	B	398	LEU	2.1
1	B	239	ASN	2.1
1	B	361	ASN	2.1
1	C	87	LEU	2.0
1	C	152	HIS	2.0
1	A	437	ASN	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
5	GOL	C	707	6/6	0.62	0.24	43,49,51,52	0
3	NAG	C	704	14/15	0.73	0.24	40,47,55,56	0
3	NAG	B	703	14/15	0.75	0.18	35,43,53,56	0
3	NAG	C	703	14/15	0.76	0.16	29,41,51,58	0
3	NAG	B	705	14/15	0.80	0.18	31,33,35,36	0
3	NAG	B	704	14/15	0.82	0.15	34,44,49,54	0
3	NAG	A	703	14/15	0.86	0.13	25,30,38,43	0
5	GOL	B	707	6/6	0.88	0.13	32,36,37,41	0
3	NAG	A	704	14/15	0.88	0.13	26,31,39,44	0
3	NAG	A	705	14/15	0.89	0.11	16,18,20,21	0
3	NAG	C	705	14/15	0.91	0.09	22,24,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	MLI	B	706	7/7	0.91	0.17	21,28,35,35	0
4	MLI	C	706	7/7	0.94	0.17	38,49,50,54	0
4	MLI	A	706	7/7	0.97	0.10	22,35,41,41	0
2	ZN	C	702	1/1	0.98	0.09	23,23,23,23	0
2	ZN	C	701	1/1	0.99	0.02	13,13,13,13	0
2	ZN	B	702	1/1	0.99	0.04	23,23,23,23	0
2	ZN	B	701	1/1	1.00	0.04	19,19,19,19	0
2	ZN	A	701	1/1	1.00	0.02	14,14,14,14	0
2	ZN	A	702	1/1	1.00	0.02	7,7,7,7	0

6.5 Other polymers [i](#)

There are no such residues in this entry.