



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 08:58 pm GMT

PDB ID : 5EBB  
Title : Structure of human sphingomyelinase phosphodiesterase like 3A (SMPDL3A) with Zn<sup>2+</sup>  
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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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

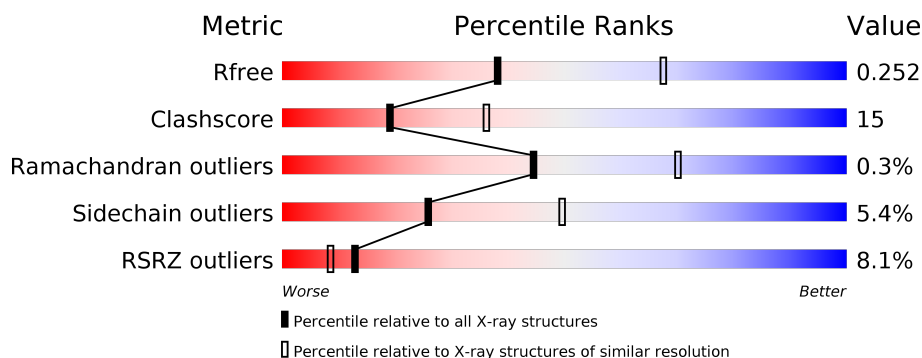
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	100719	2542 (2.60-2.60)
Clashscore	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)
RSRZ outliers	101464	2550 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	410	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> <span>%</span> <div style="width: 82%; height: 10px; background-color: green;"></div> <div style="width: 17%; height: 10px; background-color: yellow;"></div> <span>•</span> </div> <div style="display: flex; justify-content: space-between; align-items: center;"> <span>82%</span> <span>17%</span> </div> </div>
1	B	410	<div> <div style="width: 10%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> <span>10%</span> <div style="width: 66%; height: 10px; background-color: green;"></div> <div style="width: 30%; height: 10px; background-color: yellow;"></div> <span>•</span> </div> <div style="display: flex; justify-content: space-between; align-items: center;"> <span>66%</span> <span>30%</span> </div> </div>
1	C	410	<div> <div style="width: 13%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> <span>13%</span> <div style="width: 68%; height: 10px; background-color: green;"></div> <div style="width: 29%; height: 10px; background-color: yellow;"></div> <span>•</span> </div> <div style="display: flex; justify-content: space-between; align-items: center;"> <span>68%</span> <span>29%</span> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	A	703	-	-	-	X
3	NAG	A	704	-	-	-	X
3	NAG	C	704	X	-	-	-
4	MLI	A	706	-	-	-	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
1	A	410	Total	C	N	O	S	0	3	0
			3302	2127	529	633	13			
1	B	410	Total	C	N	O	S	0	7	0
			3327	2143	532	639	13			
1	C	410	Total	C	N	O	S	0	5	0
			3319	2139	532	635	13			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

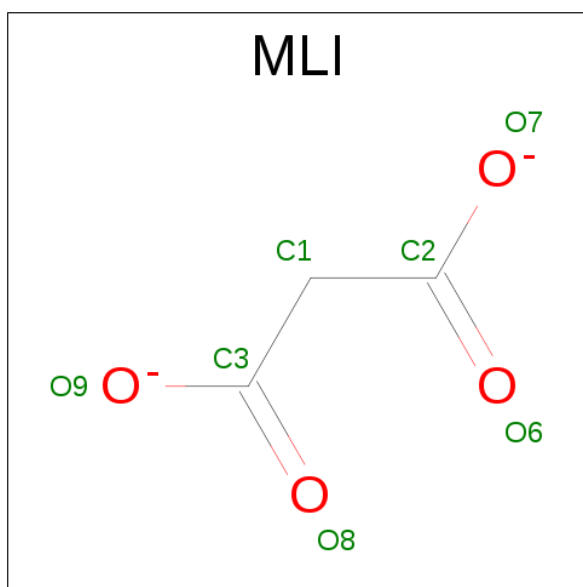
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Zn	0	0
			2	2		
2	A	2	Total	Zn	0	0
			2	2		
2	C	2	Total	Zn	0	0
			2	2		

- Molecule 3 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



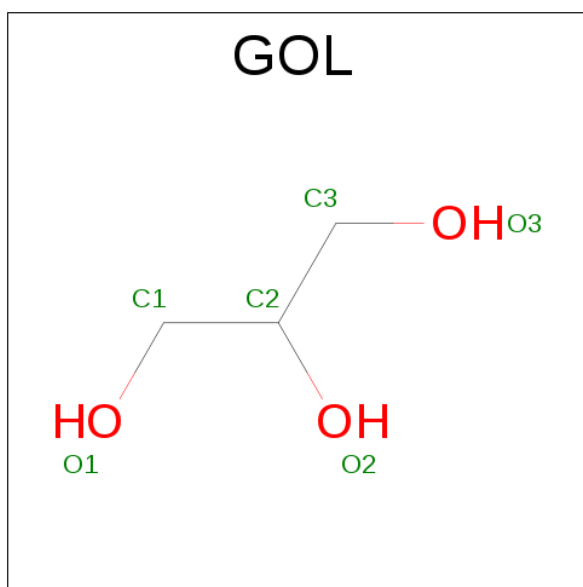
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1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

- Molecule 4 is MALONATE ION (three-letter code: 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 (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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		

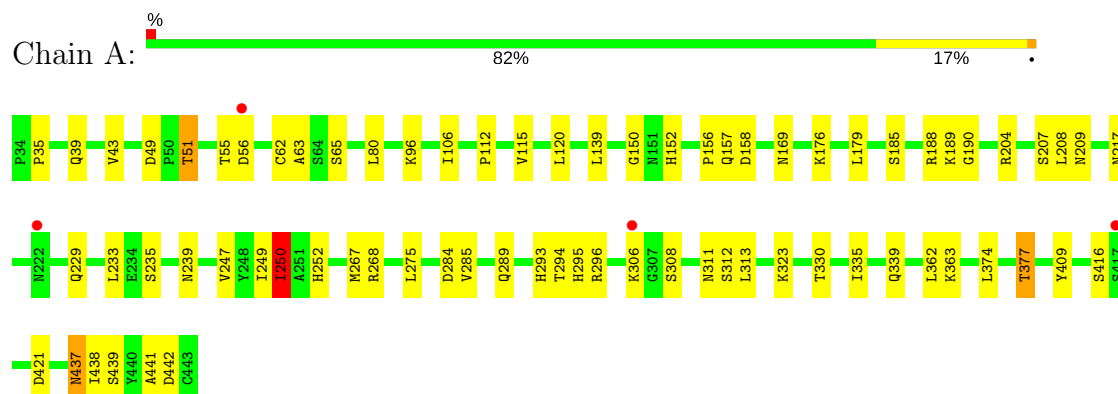
- Molecule 6 is water.

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

- Molecule 1: Acid sphingomyelinase-like phosphodiesterase 3a



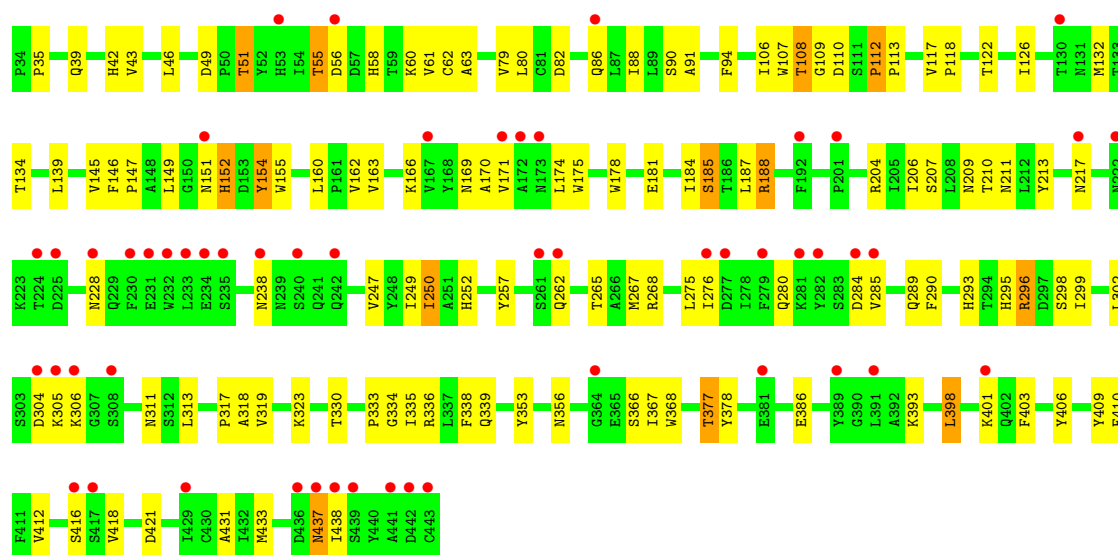
- Molecule 1: Acid sphingomyelinase-like phosphodiesterase 3a



- 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, $\alpha$ , $\beta$ , $\gamma$	147.79Å 147.79Å 139.90Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.38 – 2.60 47.22 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.3 (48.38-2.60) 99.4 (47.22-2.60)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.61 (at 2.61Å)	Xtriage
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 (5.15%)	DCC
Wilson B-factor (Å <sup>2</sup> )	22.8	Xtriage
Anisotropy	0.108	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.45 , 61.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	10414	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtriage'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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

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

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.96	0/3399	0.95	6/4641 (0.1%)
1	B	1.12	1/3430 (0.0%)	1.10	16/4684 (0.3%)
1	C	1.12	4/3416 (0.1%)	1.12	11/4663 (0.2%)
All	All	1.07	5/10245 (0.0%)	1.06	33/13988 (0.2%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	109	GLY	C-O	-6.04	1.14	1.23
1	B	284	ASP	CB-CG	5.90	1.64	1.51
1	C	155	TRP	CB-CG	-5.57	1.40	1.50
1	C	154	TYR	CB-CG	5.19	1.59	1.51
1	C	152	HIS	C-O	-5.04	1.13	1.23

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	296	ARG	NE-CZ-NH2	-8.53	116.04	120.30
1	C	296	ARG	NE-CZ-NH2	-8.02	116.29	120.30
1	C	421	ASP	CB-CG-OD1	7.07	124.67	118.30
1	A	296	ARG	NE-CZ-NH1	6.87	123.73	120.30
1	C	188	ARG	NE-CZ-NH1	6.62	123.61	120.30
1	B	158	ASP	CB-CG-OD1	6.51	124.16	118.30
1	C	296	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	C	284	ASP	CB-CG-OD2	6.19	123.87	118.30
1	A	421	ASP	CB-CG-OD1	6.15	123.83	118.30
1	C	204	ARG	NE-CZ-NH1	6.13	123.36	120.30
1	B	110	ASP	CB-CG-OD1	6.09	123.78	118.30
1	B	168	TYR	CB-CG-CD1	6.04	124.62	121.00
1	B	313	LEU	CA-CB-CG	5.96	129.02	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	336	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	C	110	ASP	CB-CG-OD2	-5.90	112.99	118.30
1	C	398	LEU	CA-CB-CG	5.83	128.71	115.30
1	B	268	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	B	267	MET	CG-SD-CE	-5.79	90.94	100.20
1	B	443	CYS	CA-CB-SG	5.77	124.39	114.00
1	C	304	ASP	CB-CG-OD1	5.74	123.47	118.30
1	B	284	ASP	CB-CG-OD1	5.67	123.40	118.30
1	B	296	ARG	NE-CZ-NH1	5.51	123.05	120.30
1	B	188	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	A	250	ILE	CA-CB-CG2	5.40	121.70	110.90
1	B	379[A]	ASP	CB-CA-C	5.36	121.11	110.40
1	B	379[B]	ASP	CB-CA-C	5.36	121.11	110.40
1	B	295	HIS	N-CA-C	5.25	125.19	111.00
1	B	371	GLU	OE1-CD-OE2	-5.24	117.02	123.30
1	A	284	ASP	CB-CG-OD1	5.18	122.96	118.30
1	B	275	LEU	CB-CG-CD2	5.17	119.78	111.00
1	A	158	ASP	CB-CG-OD1	5.16	122.94	118.30
1	C	112	PRO	O-C-N	5.16	130.90	121.10
1	C	108	THR	N-CA-C	5.05	124.64	111.00

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	3302	0	3209	43	0
1	B	3327	0	3235	142	0
1	C	3319	0	3231	106	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	45	0
6	C	119	0	0	9	0
All	All	10414	0	9813	292	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 15.

All (292) 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:C1	3:C:704:NAG:C2	1.77	1.60
1:C:151:ASN:HD21	1:C:152:HIS:CD2	1.39	1.40
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: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:252:HIS:C	6:B:809:HOH:O	2.09	0.91
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:H2	3:C:704:NAG:C1	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O	1:B:294[B]:THR:HG22	1.97	0.64
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
1:B:252:HIS:CA	6:B:809:HOH:O	2.48	0.60
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:108:THR:HG21	1:C:250[B]:ILE:HD11	1.82	0.59
1:C:106[B]:ILE:HD12	1:C:250[B]:ILE:HD13	1.84	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: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:300:MET:HE1	6:B:876:HOH:O	1.99	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:412:VAL:O	1:B:412:VAL:HG12	2.04	0.57
1:C:250[B]:ILE:HD13	1:C:290:PHE:HB2	1.85	0.57
1:A:35:PRO:HG2	6:A:853:HOH:O	2.04	0.56
1:B:349:ASP:HA	1:B:383:LEU:HD13	1.87	0.56
1:B:47:HIS:O	1:B:82:ASP:HB3	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:415:ASP:C	1:B:418:VAL:HG13	2.28	0.54
1:B:58:HIS:HB2	1:B:69:ASN:OD1	2.08	0.54
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:HD12	1:B:435:LEU:N	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:297:ASP:C	1:B:297:ASP:OD1	2.48	0.52
1:B:376:GLN:HG3	1:C:35:PRO:HB3	1.91	0.52
1:B:51:THR:HG22	1:B:51:THR:O	2.10	0.52
1:C:169:ASN:ND2	1:C:188:ARG:HH11	2.05	0.52
1:B:318:ALA:HB1	1:B:320:THR:HG22	1.91	0.51
1:B:38:GLY:HA3	1:B:340:TYR:CZ	2.45	0.51
1:C:162:VAL:HG12	1:C:163:VAL:HG13	1.92	0.51
1:C:313:LEU:HD12	1:C:313:LEU:N	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:106[B]:ILE:HG21	1:B:250:ILE:CD1	2.41	0.51
1:B:62:CYS:SG	1:B:65:SER:HB3	2.51	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:162:VAL:HG13	1:B:227:ALA:HA	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:C:393:LYS:HG2	1:C:433:MET:HE1	1.94	0.49
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:B:251:ALA:C	6:B:809:HOH:O	2.49	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:106[B]:ILE:HD12	1:C:250[B]:ILE:CD1	2.43	0.48
1:C:267:MET:CE	1:C:275:LEU:HD12	2.44	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:267:MET:HE1	1:C:275:LEU:HD12	1.95	0.48
1:C:94:PHE:CZ	1:C:353:TYR:CD1	3.02	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: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:319:VAL:O	1:C:333:PRO:HB3	2.14	0.47
1:C:94:PHE:HZ	1:C:353:TYR:CD1	2.32	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:C:249:ILE:HB	1:C:289:GLN:HG2	1.97	0.47
1:C:58:HIS:HA	1:C:61:VAL:HG23	1.97	0.47
1:B:294[B]:THR:O	1:B:294[B]:THR:CG2	2.62	0.47
1:C:323:LYS:HB3	1:C:330:THR:HB	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:145:VAL:HB	1:B:178:TRP:CE2	2.50	0.46
1:B:137:GLN:HG3	1:B:178:TRP:CZ2	2.51	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:156:PRO:O	1:B:157:GLN:C	2.55	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:A:441:ALA:O	1:A:442:ASP:C	2.54	0.45
1:C:175:TRP:CE3	1:C:187:LEU:HD21	2.51	0.45
1:C:276:ILE:O	1:C:280:GLN:HG3	2.16	0.45
1:B:133:THR:HG21	1:B:174:LEU:HB3	1.99	0.45
1:B:272:ASN:CG	6:B:807:HOH:O	2.53	0.45
1:A:267:MET:HE1	1:A:275:LEU:HD12	1.99	0.45
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:C:356:ASN:OD1	1:C:356:ASN:C	2.56	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:A:374:LEU:HD23	1:A:374:LEU:C	2.37	0.44
1:C:170:ALA:O	1:C:174:LEU:HG	2.17	0.44
1:C:386:GLU:H	1:C:386:GLU:CD	2.22	0.44
1:C:166[B]:LYS:O	1:C:166[B]:LYS:HD3	2.18	0.43
1:C:42:HIS:CE1	1:C:290:PHE:HB3	2.54	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:A:156:PRO:O	1:A:157:GLN:C	2.53	0.43
1:B:325:VAL:HG23	6:B:872:HOH:O	2.18	0.43
1:B:42:HIS:HB3	1:B:336:ARG:CG	2.48	0.43
1:C:162:VAL:HG13	6:C:891:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:A:289:GLN:HB2	1:A:313:LEU:HG	2.00	0.42
1:B:151:ASN:O	1:B:158:ASP:N	2.41	0.42
1:B:298:SER:C	1:B:299[A]:ILE:CG2	2.85	0.42
1:B:147:PRO:HG2	1:B:175:TRP:CD2	2.54	0.42
1:C:62:CYS:O	1:C:62:CYS:SG	2.77	0.42
1:B:106[A]:ILE:CG2	1:B:250:ILE:HG12	2.49	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:HA	1:B:388:LEU:HD23	1.80	0.42
1:B:85:TYR:CE2	1:B:89:LEU:HD22	2.55	0.42
1:C:132:MET:HA	1:C:132:MET:HE2	2.00	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: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:C:151:ASN:CG	1:C:152:HIS:HD2	2.21	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:HA	1:A:362:LEU:HD23	1.89	0.41
1:C:94:PHE:CD1	1:C:368:TRP:HB2	2.54	0.41
1:C:39:GLN:NE2	1:C:339:GLN:HE21	2.18	0.41
1:B:253:VAL:HG22	1:B:293:HIS:CD2	2.56	0.41
1:B:300:MET:HE3	6:B:876:HOH:O	2.08	0.41
1:C:49:ASP:OD1	1:C:51:THR:CB	2.67	0.41
1:B:371:GLU:OE2	1:B:412:VAL:HA	2.21	0.41
1:C:94:PHE:HZ	1:C:353:TYR:CE1	2.39	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:401:LYS:HD2	1:B:401:LYS:N	2.34	0.41
1:B:434:ASN:OD1	1:B:439:SER:HB3	2.21	0.41
1:C:210:THR:O	1:C:211:ASN:C	2.59	0.41
1:A:207:SER:HA	1:A:250:ILE:HG22	2.02	0.41
1:A:62:CYS:SG	1:A:65:SER:HB3	2.61	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:132:MET:HA	1:C:132:MET:CE	2.51	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:A:312:SER:C	1:A:313:LEU:HD12	2.41	0.40
1:B:218:ILE:N	1:B:218:ILE:HD13	2.37	0.40
1:C:117:VAL:HB	1:C:118:PRO:HD3	2.03	0.40
1:C:250[B]:ILE:HA	1:C:250[B]:ILE:HD12	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 ⓘ

### 5.3.1 Protein backbone ⓘ

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%)	51	76
1	B	415/410 (101%)	385 (93%)	26 (6%)	4 (1%)	18	37
1	C	413/410 (101%)	380 (92%)	33 (8%)	0	100	100
All	All	1239/1230 (101%)	1152 (93%)	82 (7%)	5 (0%)	44	63

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 ⓘ

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%)	361 (96%)	14 (4%)	39	66
1	B	379/372 (102%)	357 (94%)	22 (6%)	23	46
1	C	377/372 (101%)	350 (93%)	27 (7%)	17	33
All	All	1131/1116 (101%)	1068 (94%)	63 (6%)	26	48

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	THR
1	A	80	LEU
1	A	176	LYS
1	A	235	SER
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	377	THR
1	A	416	SER
1	A	437	ASN
1	A	439	SER
1	B	46	LEU
1	B	80	LEU

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Mol	Chain	Res	Type
1	B	176	LYS
1	B	185	SER
1	B	239	ASN
1	B	250	ILE
1	B	261	SER
1	B	262	GLN
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	349	ASP
1	B	379[A]	ASP
1	B	379[B]	ASP
1	B	401	LYS
1	B	404	ILE
1	B	415	ASP
1	B	437	ASN
1	C	51	THR
1	C	55	THR
1	C	60	LYS
1	C	80	LEU
1	C	82	ASP
1	C	86	GLN
1	C	139	LEU
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	285	VAL
1	C	299	ILE
1	C	305	LYS
1	C	306	LYS
1	C	311	ASN
1	C	367	ILE
1	C	377	THR
1	C	398	LEU

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Mol	Chain	Res	Type
1	C	401	LYS
1	C	412	VAL
1	C	416	SER
1	C	418	VAL
1	C	437	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	GLN
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	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	394	GLN
1	B	437	ASN
1	C	39	GLN
1	C	53	HIS
1	C	169	ASN
1	C	211	ASN
1	C	229	GLN
1	C	263	ASN
1	C	332	ASN
1	C	437	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 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	1.92	5 (35%)	15,19,21	1.39	2 (13%)
3	NAG	A	704	1	14,14,15	1.71	3 (21%)	15,19,21	1.23	1 (6%)
3	NAG	A	705	1	14,14,15	2.27	2 (14%)	15,19,21	3.48	9 (60%)
4	MLI	A	706	2	0,6,6	0.00	-	0,7,7	0.00	-
3	NAG	B	703	1	14,14,15	2.47	5 (35%)	15,19,21	1.34	2 (13%)
3	NAG	B	704	1	14,14,15	1.68	3 (21%)	15,19,21	1.61	3 (20%)
3	NAG	B	705	1	14,14,15	2.40	4 (28%)	15,19,21	2.32	6 (40%)
4	MLI	B	706	2	0,6,6	0.00	-	0,7,7	0.00	-
5	GOL	B	707	-	5,5,5	0.62	0	5,5,5	0.37	0
3	NAG	C	703	1	14,14,15	2.00	4 (28%)	15,19,21	1.58	3 (20%)
3	NAG	C	704	1	14,14,15	5.85	6 (42%)	15,19,21	2.86	8 (53%)
3	NAG	C	705	1	14,14,15	2.44	4 (28%)	15,19,21	2.34	7 (46%)
4	MLI	C	706	2	0,6,6	0.00	-	0,7,7	0.00	-
5	GOL	C	707	-	5,5,5	0.47	0	5,5,5	0.94	0

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

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	705	NAG	O3-C3	-4.74	1.32	1.43
3	A	705	NAG	O5-C5	2.04	1.47	1.43
3	A	703	NAG	O5-C1	2.22	1.47	1.43
3	C	703	NAG	O4-C4	2.22	1.48	1.43
3	B	703	NAG	C4-C5	2.29	1.57	1.53
3	C	704	NAG	O3-C3	2.30	1.48	1.43
3	C	703	NAG	O3-C3	2.33	1.48	1.43
3	B	704	NAG	C8-C7	2.33	1.55	1.50
3	A	704	NAG	O5-C5	2.37	1.48	1.43
3	B	704	NAG	O5-C5	2.61	1.48	1.43
3	A	703	NAG	C8-C7	2.67	1.56	1.50
3	A	703	NAG	O5-C5	2.70	1.49	1.43
3	C	705	NAG	C1-C2	2.72	1.56	1.52
3	B	705	NAG	C1-C2	2.72	1.56	1.52
3	B	705	NAG	C2-N2	2.83	1.51	1.46
3	C	705	NAG	O5-C5	2.92	1.49	1.43
3	A	704	NAG	C8-C7	2.93	1.56	1.50
3	B	703	NAG	C8-C7	3.03	1.57	1.50
3	C	705	NAG	C4-C5	3.12	1.59	1.53
3	C	703	NAG	C8-C7	3.14	1.57	1.50
3	A	703	NAG	C1-C2	3.45	1.57	1.52
3	B	703	NAG	O5-C1	3.63	1.49	1.43
3	B	703	NAG	O4-C4	3.79	1.51	1.43
3	A	703	NAG	O4-C4	3.80	1.51	1.43
3	C	704	NAG	C2-N2	4.23	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	704	NAG	O5-C1	4.44	1.51	1.43
3	C	704	NAG	C3-C2	4.56	1.62	1.52
3	A	704	NAG	O5-C1	4.67	1.51	1.43
3	C	703	NAG	C1-C2	4.80	1.59	1.52
3	C	704	NAG	O5-C5	5.44	1.54	1.43
3	B	705	NAG	O4-C4	5.82	1.56	1.43
3	B	703	NAG	C1-C2	5.86	1.60	1.52
3	C	705	NAG	O4-C4	6.78	1.58	1.43
3	A	705	NAG	O4-C4	7.20	1.59	1.43
3	C	704	NAG	O5-C1	8.48	1.57	1.43
3	C	704	NAG	C1-C2	17.90	1.77	1.52

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	705	NAG	O5-C1-C2	-4.50	105.22	111.47
3	A	705	NAG	O3-C3-C2	-4.25	100.28	109.39
3	B	705	NAG	C3-C4-C5	-3.97	103.22	110.22
3	C	703	NAG	C1-O5-C5	-3.66	107.12	112.17
3	A	705	NAG	O6-C6-C5	-3.36	100.02	111.34
3	C	705	NAG	C3-C4-C5	-3.23	104.53	110.22
3	B	705	NAG	C1-C2-N2	-3.21	105.01	110.49
3	A	703	NAG	C3-C4-C5	-2.76	105.36	110.22
3	A	705	NAG	C1-C2-N2	-2.67	105.93	110.49
3	B	703	NAG	C3-C4-C5	-2.66	105.53	110.22
3	C	705	NAG	O3-C3-C2	-2.66	103.69	109.39
3	C	703	NAG	C3-C4-C5	-2.46	105.88	110.22
3	A	705	NAG	O3-C3-C4	-2.41	105.11	110.36
3	A	705	NAG	O5-C1-C2	-2.38	108.16	111.47
3	A	705	NAG	C6-C5-C4	-2.33	107.55	113.00
3	C	705	NAG	C1-C2-N2	-2.20	106.72	110.49
3	C	703	NAG	C2-N2-C7	-2.17	119.78	122.94
3	C	704	NAG	O7-C7-C8	-2.07	118.30	122.06
3	B	704	NAG	O3-C3-C4	-2.01	105.99	110.36
3	C	704	NAG	O4-C4-C5	2.02	114.37	109.28
3	C	705	NAG	O4-C4-C3	2.03	114.77	110.36
3	C	704	NAG	O3-C3-C2	2.14	113.97	109.39
3	A	705	NAG	O4-C4-C5	2.23	114.91	109.28
3	B	704	NAG	C4-C3-C2	2.27	114.34	111.02
3	B	705	NAG	C1-O5-C5	2.59	115.73	112.17
3	B	705	NAG	O4-C4-C5	2.81	116.37	109.28
3	A	703	NAG	O4-C4-C5	2.97	116.78	109.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	704	NAG	O7-C7-N2	2.98	127.66	121.92
3	B	703	NAG	O4-C4-C5	3.07	117.01	109.28
3	B	705	NAG	O4-C4-C3	3.14	117.19	110.36
3	C	704	NAG	C1-O5-C5	3.20	116.57	112.17
3	A	704	NAG	C1-O5-C5	3.33	116.75	112.17
3	C	705	NAG	C1-O5-C5	3.50	116.99	112.17
3	A	705	NAG	O4-C4-C3	3.64	118.27	110.36
3	B	705	NAG	C2-N2-C7	3.78	128.46	122.94
3	C	705	NAG	O4-C4-C5	3.93	119.18	109.28
3	C	704	NAG	C4-C3-C2	3.93	116.78	111.02
3	B	704	NAG	C1-O5-C5	4.33	118.14	112.17
3	C	704	NAG	C1-C2-N2	4.88	118.83	110.49
3	C	704	NAG	C2-N2-C7	6.60	132.57	122.94
3	A	705	NAG	C1-O5-C5	10.29	126.35	112.17

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	C	704	NAG	C1

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	706	MLI	2	0
3	C	704	NAG	3	0
5	C	707	GOL	1	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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	410/410 (100%)	-0.26	4 (0%) 82 79	3, 13, 32, 56	0
1	B	410/410 (100%)	0.73	43 (10%) 7 4	7, 23, 42, 60	0
1	C	410/410 (100%)	0.82	53 (12%) 4 2	7, 23, 43, 65	0
All	All	1230/1230 (100%)	0.43	100 (8%) 13 8	3, 20, 41, 65	0

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	283	SER	5.0
1	B	396	THR	5.0
1	B	56	ASP	4.8
1	B	277	ASP	4.8
1	B	284	ASP	4.6
1	C	234	GLU	4.5
1	B	285	VAL	4.2
1	B	281	LYS	4.1
1	C	151	ASN	4.1
1	C	277	ASP	4.0
1	C	305	LYS	4.0
1	C	238	ASN	3.9
1	B	391	LEU	3.9
1	B	303	SER	3.8
1	B	389	TYR	3.8
1	B	308	SER	3.8
1	B	393	LYS	3.7
1	C	306	LYS	3.7
1	C	53	HIS	3.6
1	C	56	ASP	3.6
1	B	72	ASN	3.5
1	B	304	ASP	3.5
1	B	399	ASP	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	238	ASN	3.5
1	B	242	GLN	3.5
1	B	239	ASN	3.4
1	C	235	SER	3.4
1	C	304	ASP	3.3
1	B	390	GLY	3.3
1	B	276	ILE	3.3
1	C	172	ALA	3.2
1	B	420	CYS	3.2
1	C	284	ASP	3.2
1	C	276	ILE	3.2
1	C	438	ILE	3.1
1	A	306	LYS	3.0
1	B	294[A]	THR	3.0
1	B	224	THR	3.0
1	C	171	VAL	3.0
1	C	437	ASN	2.9
1	B	417	SER	2.9
1	C	173	ASN	2.9
1	B	260[A]	SER	2.9
1	C	436	ASP	2.9
1	C	240	SER	2.8
1	C	417	SER	2.8
1	B	360	ALA	2.8
1	C	262	GLN	2.7
1	B	394	GLN	2.7
1	B	347	LEU	2.7
1	C	242	GLN	2.7
1	C	232	TRP	2.7
1	C	442	ASP	2.7
1	B	222	ASN	2.6
1	C	308	SER	2.6
1	B	243	ASN	2.6
1	B	414	TYR	2.6
1	C	130	THR	2.5
1	B	418	VAL	2.5
1	C	230	PHE	2.5
1	C	228	ASN	2.5
1	C	225	ASP	2.5
1	C	282	TYR	2.5
1	C	86	GLN	2.4
1	C	217	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	224	THR	2.4
1	B	237	LEU	2.4
1	C	364	GLY	2.4
1	B	280	GLN	2.3
1	B	235	SER	2.3
1	C	429	ILE	2.3
1	B	258	LEU	2.3
1	C	201	PRO	2.3
1	C	381	GLU	2.3
1	C	233	LEU	2.3
1	C	192	PHE	2.3
1	C	389	TYR	2.3
1	A	222	ASN	2.3
1	A	56	ASP	2.3
1	C	281	LYS	2.3
1	B	53	HIS	2.2
1	C	222	ASN	2.2
1	C	441	ALA	2.2
1	C	279	PHE	2.2
1	B	386	GLU	2.2
1	A	417	SER	2.1
1	C	391	LEU	2.1
1	B	274	LYS	2.1
1	C	443	CYS	2.1
1	B	34	PRO	2.1
1	C	231	GLU	2.1
1	B	388	LEU	2.1
1	C	401	LYS	2.1
1	C	439	SER	2.1
1	C	416	SER	2.1
1	B	398	LEU	2.0
1	C	261	SER	2.0
1	C	167	VAL	2.0
1	C	285	VAL	2.0
1	B	265	THR	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	NAG	A	704	14/15	0.89	0.20	5.95	26,31,39,44	0
4	MLI	A	706	7/7	0.97	0.19	3.39	22,35,41,41	0
3	NAG	A	703	14/15	0.89	0.26	2.62	25,30,38,43	0
3	NAG	B	703	14/15	0.79	0.33	1.36	35,43,53,56	0
3	NAG	B	704	14/15	0.83	0.23	1.35	34,44,49,54	0
4	MLI	C	706	7/7	0.94	0.29	0.99	38,49,50,54	0
4	MLI	B	706	7/7	0.94	0.20	0.62	21,28,35,35	0
3	NAG	C	703	14/15	0.80	0.28	0.39	29,41,51,58	0
3	NAG	A	705	14/15	0.93	0.17	0.07	16,18,20,21	0
3	NAG	C	705	14/15	0.89	0.18	-0.46	22,24,27,27	0
2	ZN	A	702	1/1	0.99	0.13	-0.83	7,7,7,7	0
2	ZN	C	701	1/1	0.99	0.10	-1.19	13,13,13,13	0
2	ZN	C	702	1/1	0.94	0.08	-1.51	23,23,23,23	0
3	NAG	B	705	14/15	0.87	0.19	-2.48	31,33,35,36	0
2	ZN	B	702	1/1	0.99	0.05	-4.52	23,23,23,23	0
2	ZN	B	701	1/1	0.99	0.05	-4.81	19,19,19,19	0
2	ZN	A	701	1/1	1.00	0.11	-4.95	14,14,14,14	0
3	NAG	C	704	14/15	0.62	0.32	-	40,47,55,56	0
5	GOL	B	707	6/6	0.89	0.23	-	32,36,37,41	0
5	GOL	C	707	6/6	0.78	0.20	-	43,49,51,52	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.