



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:03 PM GMT

PDB ID : 3SQM  
Title : Crystal Structure of Glycoside Hydrolase from Synechococcus Complexed with N-acetyl-D-glucosamine  
Authors : Kim, Y.; Chhor, G.; Bearden, J.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)  
Deposited on : 2011-07-05  
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

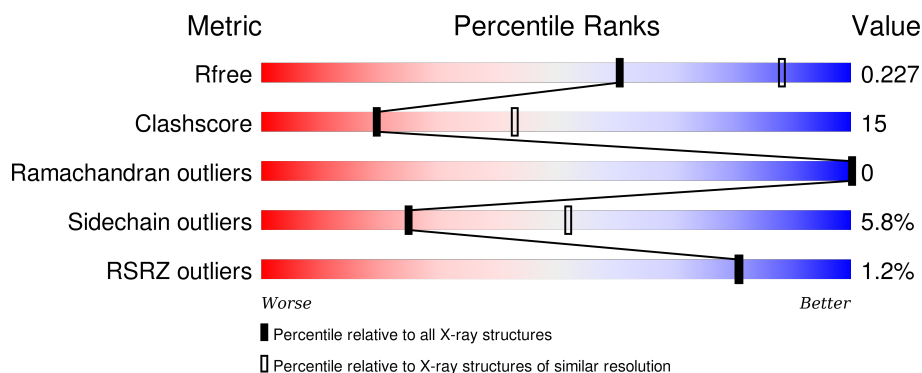
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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))
$R_{free}$	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	535	<div> <div> <div>2%</div> <div>66%</div> <div>28%</div> <div>• •</div> </div> </div>
1	B	535	<div> <div> <div>2%</div> <div>67%</div> <div>28%</div> <div>• •</div> </div> </div>
1	C	535	<div> <div> <div>69%</div> <div>26%</div> <div>• •</div> </div> </div>
1	D	535	<div> <div> <div>2%</div> <div>60%</div> <div>35%</div> <div>• •</div> </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	ACY	D	541	-	-	-	X
4	GOL	B	541	-	-	-	X
4	GOL	B	544	-	-	X	X
4	GOL	C	541	-	-	-	X
4	GOL	C	542	-	-	-	X
4	GOL	C	546	-	-	-	X
5	PEG	B	542	-	-	-	X
6	SO4	C	545	-	-	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 16306 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.

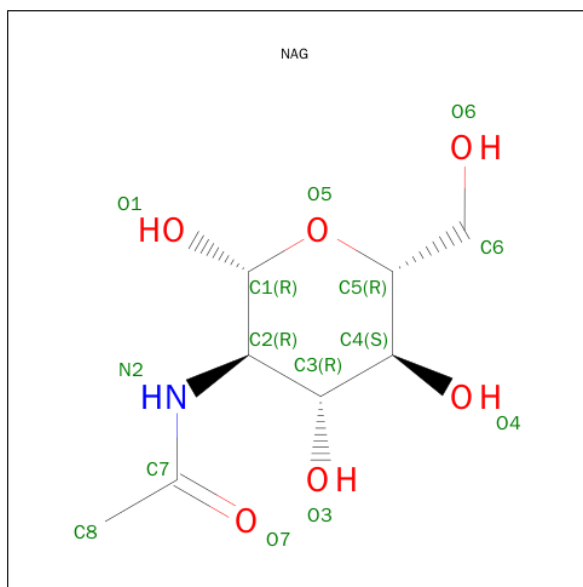
- Molecule 1 is a protein called Glycosyl hydrolase family 3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	514	Total	C	N	O	S	Se	0	1	0
			3957	2548	670	727	3	9			
1	B	516	Total	C	N	O	S	Se	0	2	0
			3984	2562	675	735	3	9			
1	C	519	Total	C	N	O	S	Se	0	2	0
			4008	2579	680	735	3	11			
1	D	519	Total	C	N	O	S	Se	0	2	0
			4006	2576	682	736	3	9			

There are 12 discrepancies between the modelled and reference sequences:

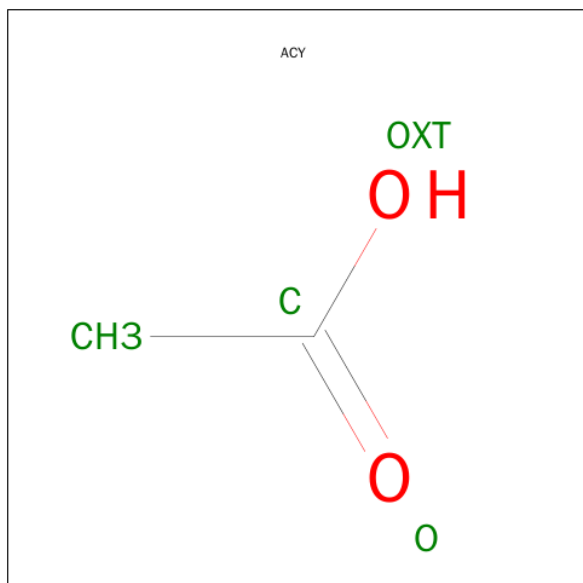
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	EXPRESSION TAG	UNP B1XLD2
A	-1	ASN	-	EXPRESSION TAG	UNP B1XLD2
A	0	ALA	-	EXPRESSION TAG	UNP B1XLD2
B	-2	SER	-	EXPRESSION TAG	UNP B1XLD2
B	-1	ASN	-	EXPRESSION TAG	UNP B1XLD2
B	0	ALA	-	EXPRESSION TAG	UNP B1XLD2
C	-2	SER	-	EXPRESSION TAG	UNP B1XLD2
C	-1	ASN	-	EXPRESSION TAG	UNP B1XLD2
C	0	ALA	-	EXPRESSION TAG	UNP B1XLD2
D	-2	SER	-	EXPRESSION TAG	UNP B1XLD2
D	-1	ASN	-	EXPRESSION TAG	UNP B1XLD2
D	0	ALA	-	EXPRESSION TAG	UNP B1XLD2

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



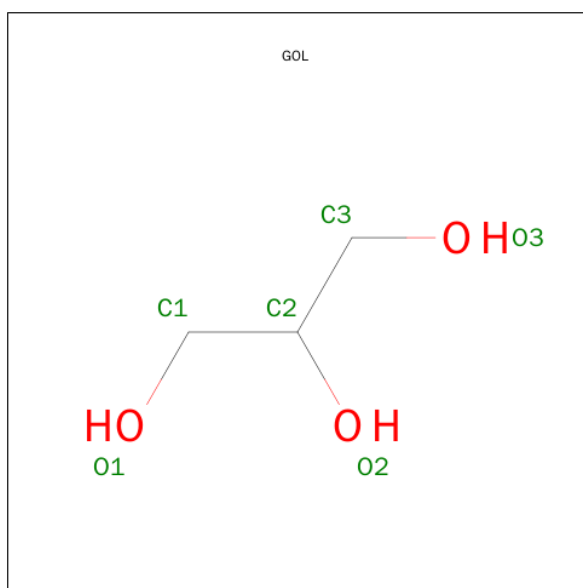
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			15	8	1	6		
2	B	1	Total	C	N	O	0	0
			15	8	1	6		
2	C	1	Total	C	N	O	0	0
			15	8	1	6		
2	D	1	Total	C	N	O	0	0
			15	8	1	6		

- Molecule 3 is ACETIC ACID (three-letter code: ACY) (formula: C<sub>2</sub>H<sub>4</sub>O<sub>2</sub>).



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

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



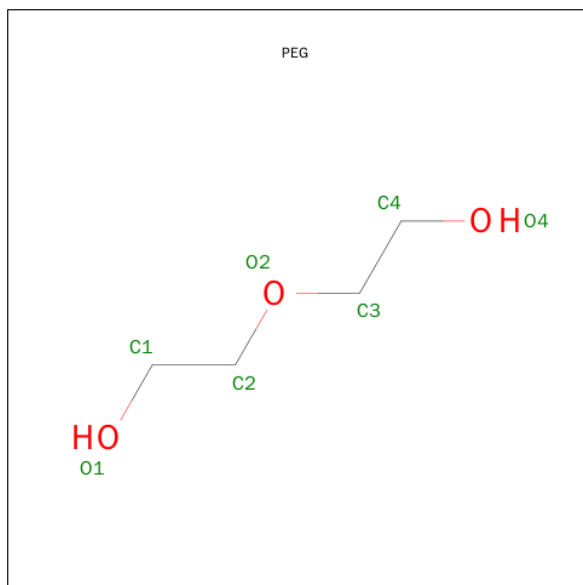
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	C	1	Total C O 6 3 3	0	0
4	C	1	Total C O 6 3 3	0	0

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

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



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

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is water.

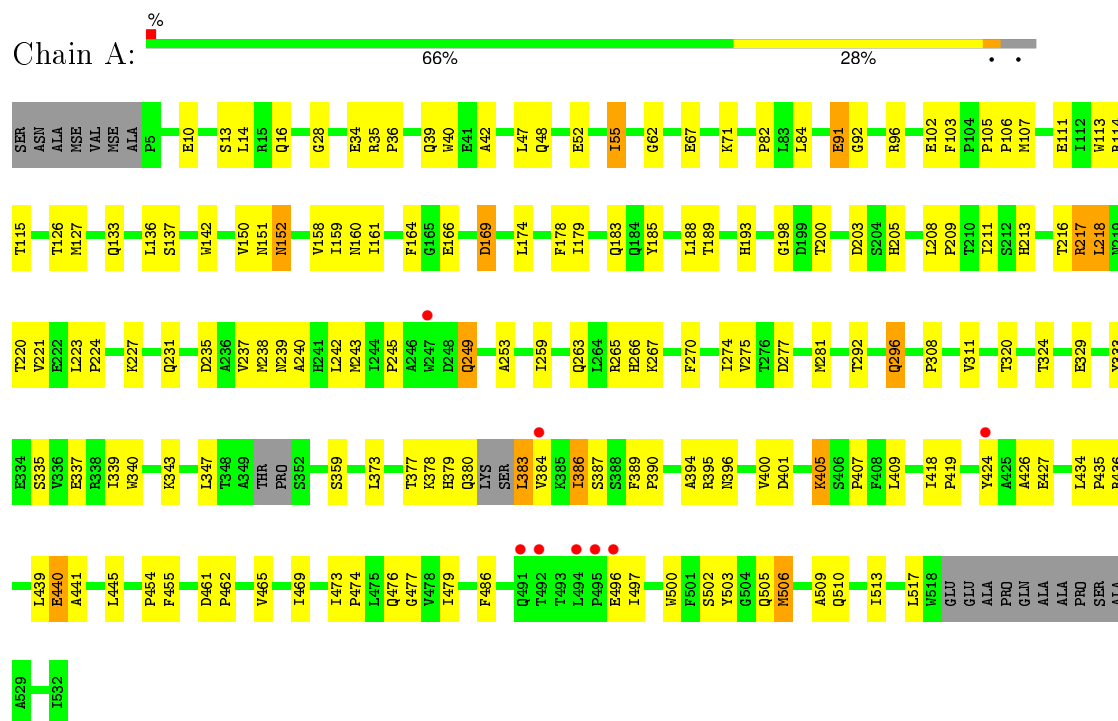
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	36	Total	O	0	0
			36	36		
7	B	73	Total	O	0	0
			73	73		
7	C	61	Total	O	0	0
			61	61		
7	D	41	Total	O	0	0
			41	41		



### 3 Residue-property plots

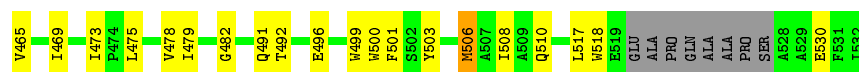
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: Glycosyl hydrolase family 3



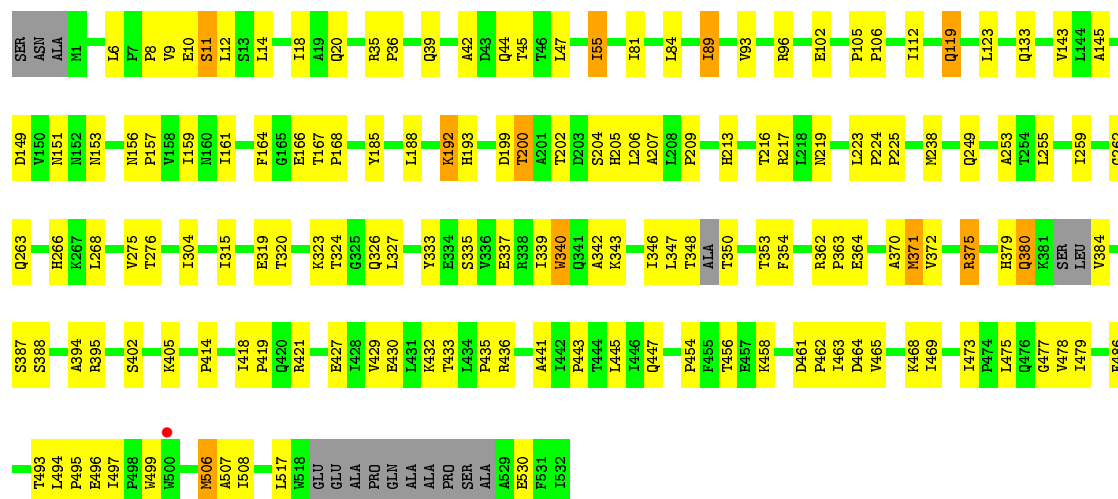
#### • Molecule 1: Glycosyl hydrolase family 3





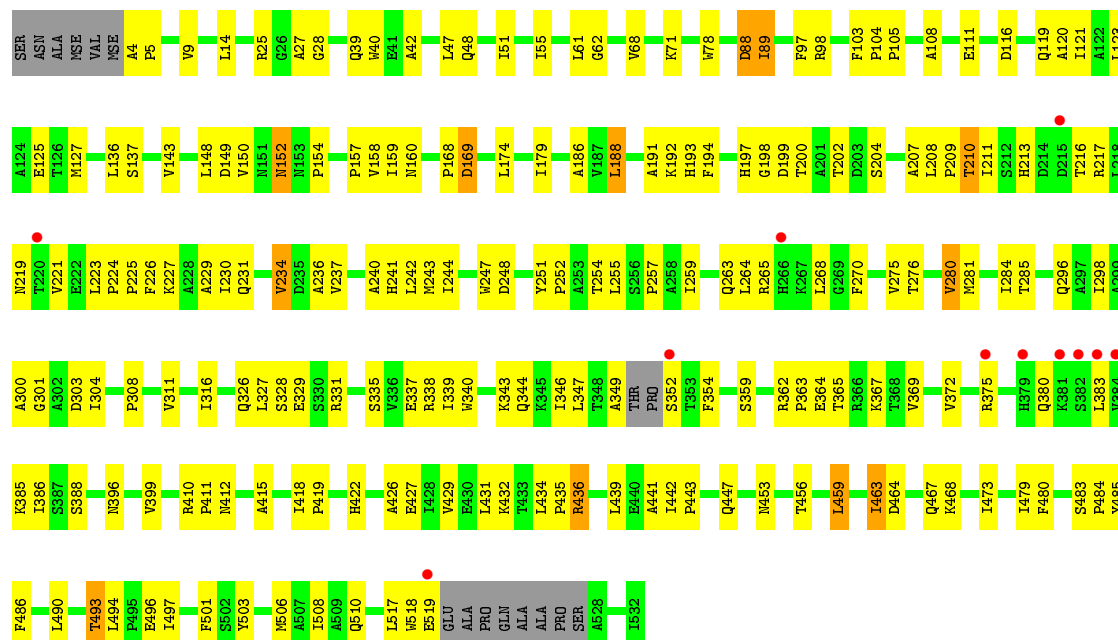
• Molecule 1: Glycosyl hydrolase family 3

Chain C: 69% 26%



• Molecule 1: Glycosyl hydrolase family 3

Chain D: 2% 60% 35%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	125.14Å 125.14Å 233.75Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.96 – 2.70 49.16 – 2.70	Depositor EDS
% Data completeness (in resolution range)	85.9 (40.96-2.70) 85.9 (49.16-2.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.44 (at 2.69Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_761)	Depositor
R, $R_{free}$	0.159 , 0.231 0.159 , 0.227	Depositor DCC
$R_{free}$ test set	2548 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	40.5	Xtriage
Anisotropy	0.384	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 44.6	EDS
Estimated twinning fraction	0.025 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	2 of 50457 reflections (0.004%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	16306	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.46% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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, ACY, PEG, NAG, SO4

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	0.41	0/4046	0.62	0/5511
1	B	0.42	0/4071	0.65	0/5545
1	C	0.46	0/4095	0.68	1/5576 (0.0%)
1	D	0.43	0/4094	0.63	0/5577
All	All	0.43	0/16306	0.65	1/22209 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	206	LEU	CA-CB-CG	-5.60	102.41	115.30

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	3957	0	3989	133	0
1	B	3984	0	4007	116	0
1	C	4008	0	4039	104	0
1	D	4006	0	4033	142	0
2	A	15	0	15	4	0
2	B	15	0	15	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	15	0	15	1	0
2	D	15	0	15	0	0
3	A	12	0	9	0	0
3	B	4	0	3	0	0
3	C	4	0	3	0	0
3	D	12	0	9	0	0
4	B	12	0	16	13	0
4	C	24	0	32	2	0
5	B	7	0	10	1	0
6	C	5	0	0	0	0
7	A	36	0	0	8	0
7	B	73	0	0	3	0
7	C	61	0	0	3	0
7	D	41	0	0	3	0
All	All	16306	0	16210	485	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 (485) 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:D:209:PRO:HG2	1:D:242:LEU:HD23	1.47	0.97
1:D:441:ALA:HA	1:D:473:ILE:HG21	1.43	0.96
1:B:119:GLN:HE22	1:B:371:MSE:SE	2.07	0.86
1:A:220:THR:HG22	1:A:221:VAL:HG23	1.56	0.86
1:A:461:ASP:HA	1:A:486:PHE:HE1	1.40	0.86
1:C:375:ARG:HH21	1:C:375:ARG:CG	1.92	0.82
1:B:35:ARG:HH12	4:B:541:GOL:H11	1.44	0.82
1:A:461:ASP:HA	1:A:486:PHE:CE1	2.13	0.82
1:B:479:ILE:HD11	1:B:517:LEU:HD11	1.65	0.79
1:C:119:GLN:HA	1:C:119:GLN:HE21	1.47	0.78
1:D:385:LYS:HG3	1:D:519:GLU:HG2	1.63	0.78
1:A:277:ASP:OD2	1:A:281:MSE:SE	2.52	0.78
1:A:213:HIS:HB3	1:A:217:ARG:HG2	1.67	0.76
1:D:152:ASN:HD21	1:D:199:ASP:HB2	1.51	0.76
1:A:462:PRO:HD2	1:A:486:PHE:CD1	2.21	0.76
1:B:290:PRO:HD3	4:B:544:GOL:H12	1.66	0.76
1:D:441:ALA:HA	1:D:473:ILE:CG2	2.17	0.74
1:C:432:LYS:HE2	1:D:427:GLU:HG3	1.70	0.74
1:A:227:LYS:O	1:A:231:GLN:HG2	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:123:LEU:HD13	1:D:372:VAL:HG22	1.70	0.74
1:B:290:PRO:HA	4:B:544:GOL:H32	1.68	0.74
1:D:359:SER:OG	1:D:365:THR:HG21	1.88	0.73
1:C:200:THR:HG21	1:C:209:PRO:HB3	1.71	0.72
1:A:380:GLN:OE1	1:A:380:GLN:N	2.18	0.72
1:C:188:LEU:HD21	1:C:342:ALA:HB1	1.72	0.72
1:A:102:GLU:HG2	1:A:506:MSE:HE3	1.70	0.72
1:D:152:ASN:ND2	1:D:199:ASP:HB2	2.05	0.72
1:C:375:ARG:HG2	1:C:375:ARG:NH2	2.04	0.71
1:B:380:GLN:HG3	1:B:491:GLN:HE22	1.56	0.71
1:D:158:VAL:HG13	1:D:159:ILE:HG12	1.73	0.70
1:C:375:ARG:HH21	1:C:375:ARG:HG2	1.56	0.70
1:B:285:THR:CB	4:B:544:GOL:H2	2.22	0.70
1:D:213:HIS:HB3	1:D:217:ARG:HG2	1.73	0.70
1:B:397:LEU:HD23	1:B:446:ILE:HD13	1.74	0.70
1:D:369:VAL:CG1	1:D:508:ILE:HD11	2.24	0.68
1:A:249[A]:GLN:NE2	7:A:571:HOH:O	2.26	0.68
1:C:479:ILE:HD11	1:C:517:LEU:HD11	1.76	0.67
1:D:441:ALA:O	1:D:442:ILE:HG23	1.94	0.67
1:C:414:PRO:HG2	1:C:507:ALA:O	1.95	0.67
1:A:462:PRO:HD2	1:A:486:PHE:HD1	1.55	0.67
1:D:493:THR:HG22	1:D:494:LEU:HG	1.77	0.67
1:D:157:PRO:HA	1:D:459:LEU:CD1	2.25	0.67
1:D:255:LEU:HD11	1:D:284:ILE:HD11	1.76	0.66
1:C:371:MSE:HA	1:C:371:MSE:HE2	1.77	0.66
1:D:303:ASP:OD1	1:D:338:ARG:NH2	2.29	0.66
1:C:427:GLU:OE2	1:D:436:ARG:NH2	2.29	0.66
1:A:395:ARG:NH2	1:A:440:GLU:OE2	2.29	0.66
1:A:205:HIS:HE1	2:A:540:NAG:O1	1.80	0.65
1:C:370:ALA:HB2	1:C:508:ILE:HD11	1.77	0.65
1:A:265:ARG:NH2	1:A:274:ILE:HG13	2.10	0.65
1:D:179:ILE:HD13	1:D:234:VAL:HG13	1.79	0.65
1:B:107:MSE:HG2	1:B:503:TYR:CE1	2.32	0.65
1:A:111:GLU:OE1	1:A:114:ARG:NH2	2.29	0.64
1:C:395:ARG:NH1	1:C:427:GLU:OE1	2.30	0.64
1:D:169:ASP:N	1:D:169:ASP:OD1	2.29	0.64
1:D:188:LEU:HD13	1:D:346:ILE:HD11	1.80	0.64
1:B:285:THR:HG22	4:B:544:GOL:H2	1.79	0.63
1:B:491:GLN:NE2	1:B:499:TRP:HE1	1.95	0.63
1:A:441:ALA:HA	1:A:473:ILE:HD12	1.80	0.63
1:A:386:ILE:CG1	1:A:476:GLN:HB3	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:GLN:O	1:A:52:GLU:HG3	1.98	0.63
1:C:275:VAL:HG22	1:C:304:ILE:HB	1.81	0.63
1:A:441:ALA:HA	1:A:473:ILE:CD1	2.29	0.63
1:B:226:PHE:O	1:B:230:ILE:HG13	1.98	0.63
1:D:157:PRO:HA	1:D:459:LEU:HD13	1.81	0.62
1:D:188:LEU:CD1	1:D:346:ILE:HD11	2.30	0.62
1:A:151:ASN:O	1:A:166:GLU:HG3	1.99	0.62
1:B:353:THR:O	1:B:356:GLN:HB2	1.98	0.62
1:A:427:GLU:CD	1:B:436:ARG:HH12	2.03	0.62
1:C:123:LEU:HD13	1:C:372:VAL:HG22	1.79	0.62
1:D:210:THR:HG23	1:D:243:MSE:HB2	1.80	0.62
1:C:436:ARG:NH1	1:D:427:GLU:OE1	2.32	0.62
1:D:369:VAL:HG11	1:D:508:ILE:HD11	1.82	0.62
1:B:68:VAL:HG21	1:B:97:PHE:CD1	2.34	0.62
1:B:179:ILE:O	1:B:183:GLN:HG3	2.00	0.61
1:A:107:MSE:HG2	1:A:503:TYR:CE1	2.36	0.61
1:A:265:ARG:HH22	1:A:274:ILE:HG13	1.65	0.61
1:A:335:SER:O	1:A:339:ILE:HG13	2.01	0.61
1:C:346:ILE:HD12	1:C:347:LEU:HD23	1.83	0.61
1:B:123:LEU:HD13	1:B:372:VAL:HG22	1.83	0.60
1:B:285:THR:HB	4:B:544:GOL:H2	1.83	0.60
1:B:399:VAL:HB	1:B:448:CYS:HB3	1.84	0.60
1:A:434:LEU:HB3	1:A:435:PRO:HD3	1.84	0.60
1:B:290:PRO:CA	4:B:544:GOL:H32	2.31	0.60
1:D:68:VAL:HG21	1:D:97:PHE:CD1	2.37	0.59
1:D:149:ASP:OD2	1:D:159:ILE:HD12	2.00	0.59
1:B:14:LEU:HD13	1:B:329:GLU:HG3	1.84	0.59
1:D:467:GLN:OE1	1:D:493:THR:HG23	2.02	0.59
1:A:439:LEU:HD12	1:A:439:LEU:N	2.16	0.59
1:D:418:ILE:HB	1:D:419:PRO:HD3	1.84	0.59
1:C:262:GLY:O	1:C:266[B]:HIS:HB3	2.03	0.59
1:D:230:ILE:HD13	1:D:270:PHE:HB2	1.84	0.59
1:B:207:ALA:O	1:B:209:PRO:HD3	2.03	0.59
1:D:257:PRO:HD2	7:D:561:HOH:O	2.02	0.59
1:D:150:VAL:O	1:D:198:GLY:HA3	2.03	0.59
1:C:346:ILE:C	1:C:346:ILE:HD12	2.23	0.58
1:B:389:PHE:HB3	1:B:390:PRO:HD2	1.85	0.58
1:D:467:GLN:HA	1:D:494:LEU:HD11	1.86	0.58
1:D:179:ILE:HD13	1:D:234:VAL:CG1	2.33	0.58
1:B:356:GLN:HA	1:B:356:GLN:HE21	1.68	0.58
1:A:150:VAL:O	1:A:198:GLY:HA3	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:221:VAL:HG12	1:B:222:GLU:N	2.19	0.58
1:B:285:THR:CG2	4:B:544:GOL:H2	2.33	0.58
1:C:143:VAL:HG12	1:C:145:ALA:HB3	1.85	0.57
1:A:209:PRO:HG2	1:A:242:LEU:HD23	1.86	0.57
1:C:447:GLN:HG2	1:C:479:ILE:HD12	1.85	0.57
1:B:103:PHE:HB3	1:B:127:MSE:HE3	1.87	0.57
1:A:373:LEU:HD13	1:A:509:ALA:HA	1.85	0.57
1:C:496:GLU:HG2	1:C:497:ILE:HG13	1.86	0.57
1:D:186:ALA:HB3	1:D:349:ALA:HB2	1.86	0.57
1:D:111:GLU:HG3	1:D:503:TYR:HE2	1.69	0.57
1:D:9:VAL:HG21	1:D:337:GLU:OE1	2.05	0.57
1:D:442:ILE:HB	1:D:443:PRO:CD	2.35	0.57
1:A:217:ARG:HG3	1:A:218:LEU:N	2.19	0.56
1:A:386:ILE:HG12	1:A:476:GLN:HB3	1.86	0.56
1:B:39:GLN:HG2	1:B:40:TRP:CD1	2.40	0.56
1:D:237:VAL:HG23	1:D:270:PHE:CZ	2.40	0.56
1:A:42:ALA:HB3	1:A:47:LEU:HD13	1.86	0.56
1:A:405:LYS:C	1:A:407:PRO:HD3	2.26	0.56
1:A:203:ASP:OD2	1:A:205:HIS:HD2	1.89	0.56
1:B:290:PRO:HG3	4:B:544:GOL:O2	2.06	0.56
1:C:335:SER:O	1:C:339:ILE:HG13	2.06	0.56
1:D:42:ALA:HB3	1:D:47:LEU:HG	1.88	0.56
1:C:320:THR:O	1:C:324:THR:HG23	2.06	0.55
1:C:494:LEU:HD13	1:C:497:ILE:HD12	1.88	0.55
1:B:113:TRP:CE3	1:B:170:GLN:HG3	2.41	0.55
1:D:328:SER:OG	1:D:331:ARG:N	2.37	0.55
1:C:402:SER:HB3	1:C:405:LYS:HB2	1.88	0.55
1:B:410:ARG:HB3	1:B:411:PRO:HD2	1.87	0.55
1:C:275:VAL:HG12	1:C:276:THR:O	2.07	0.55
1:D:207:ALA:O	1:D:209:PRO:HD3	2.07	0.55
1:D:14:LEU:HD13	1:D:329:GLU:HG3	1.89	0.55
1:A:505:GLN:HG3	7:A:564:HOH:O	2.06	0.55
1:B:330:SER:O	1:B:334:GLU:HG3	2.07	0.55
1:A:418:ILE:HB	1:A:419:PRO:HD3	1.89	0.54
1:A:84:LEU:HG	1:A:343:LYS:HE2	1.89	0.54
1:A:237:VAL:HG23	1:A:270:PHE:CZ	2.42	0.54
1:C:371:MSE:SE	1:C:375:ARG:HE	2.40	0.54
1:D:4:ALA:HB1	1:D:5:PRO:HD2	1.89	0.54
1:C:418:ILE:HB	1:C:419:PRO:HD3	1.88	0.54
1:A:439:LEU:N	1:A:439:LEU:CD1	2.69	0.54
1:A:436:ARG:HH12	1:B:427:GLU:CD	2.11	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:255:LEU:O	1:D:300:ALA:HB2	2.08	0.54
1:B:237:VAL:HG23	1:B:270:PHE:CZ	2.43	0.54
1:C:441:ALA:HA	1:C:473:ILE:CD1	2.37	0.53
1:A:383:LEU:HD12	1:A:383:LEU:C	2.29	0.53
1:A:28:GLY:HA3	1:A:62:GLY:O	2.08	0.53
1:A:239:ASN:O	1:A:277:ASP:HB2	2.08	0.53
1:A:401:ASP:N	7:A:572:HOH:O	2.41	0.53
1:B:221:VAL:O	1:B:224:PRO:HD2	2.09	0.53
1:A:396:ASN:HB3	1:A:426:ALA:HA	1.91	0.53
1:C:375:ARG:HH21	1:C:375:ARG:HG3	1.70	0.53
1:D:219:ASN:HA	1:D:223:LEU:HB2	1.91	0.53
1:B:446:ILE:HG13	1:B:475:LEU:HD11	1.90	0.53
1:A:142:TRP:CD1	1:A:188:LEU:HB2	2.43	0.53
1:D:27:ALA:O	1:D:71:LYS:HE2	2.07	0.53
1:C:188:LEU:HD13	1:C:346:ILE:CG2	2.39	0.53
1:B:337:GLU:HA	1:B:337:GLU:OE2	2.09	0.53
1:A:221:VAL:O	1:A:224:PRO:HD2	2.09	0.52
1:D:441:ALA:O	1:D:442:ILE:CG2	2.56	0.52
1:D:229:ALA:O	1:D:234:VAL:HG22	2.08	0.52
1:D:154:PRO:HB3	1:D:485:TYR:CD1	2.44	0.52
1:B:263:GLN:O	1:B:268:LEU:HG	2.08	0.52
1:B:204:SER:HA	1:B:207:ALA:O	2.09	0.52
1:D:247:TRP:CE3	1:D:263:GLN:HG3	2.44	0.52
1:A:189:THR:HG22	1:A:235:ASP:OD1	2.09	0.52
1:B:441:ALA:HA	1:B:473:ILE:CD1	2.39	0.52
1:D:335:SER:O	1:D:339:ILE:HG13	2.09	0.52
1:B:386:ILE:HG22	1:B:518:TRP:NE1	2.25	0.52
1:D:447:GLN:HG2	1:D:479:ILE:HB	1.92	0.52
1:C:151:ASN:O	1:C:166:GLU:HG2	2.09	0.52
1:D:281:MSE:O	1:D:285:THR:HG23	2.10	0.52
1:C:207:ALA:O	1:C:209:PRO:HD3	2.10	0.51
1:A:380:GLN:NE2	1:A:384:VAL:HB	2.25	0.51
1:D:221:VAL:O	1:D:224:PRO:HD2	2.11	0.51
1:B:241:HIS:NE2	1:B:277:ASP:HB3	2.24	0.51
1:D:248:ASP:OD1	1:D:251:TYR:N	2.40	0.51
1:C:343:LYS:O	1:C:347:LEU:HG	2.10	0.51
1:B:107:MSE:HE2	1:B:165:GLY:HA2	1.93	0.51
1:D:224:PRO:HB2	1:D:225:PRO:HD3	1.93	0.51
1:B:373:LEU:CD1	1:B:508:ILE:HG23	2.41	0.51
1:A:497:ILE:HG13	1:A:497:ILE:O	2.10	0.51
1:C:8:PRO:O	1:C:11:SER:HB3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:192:LYS:HB3	1:D:193:HIS:CD2	2.46	0.51
1:C:380:GLN:HG3	1:C:499:TRP:NE1	2.26	0.51
1:D:137:SER:HA	1:D:352:SER:HB2	1.92	0.51
1:A:502:SER:HB2	1:A:513:ILE:HD11	1.92	0.51
1:B:401:ASP:HB2	7:B:603:HOH:O	2.09	0.51
1:A:265:ARG:HH22	1:A:274:ILE:CG1	2.23	0.51
1:D:197:HIS:NE2	1:D:204:SER:OG	2.32	0.51
1:C:263:GLN:O	1:C:268:LEU:HD13	2.10	0.51
1:B:119:GLN:NE2	1:B:371:MSE:SE	2.86	0.51
1:A:386:ILE:HD12	1:A:387:SER:N	2.26	0.51
1:A:208:LEU:HD23	1:A:209:PRO:HD2	1.93	0.51
1:D:298:ILE:O	1:D:331:ARG:NH2	2.44	0.51
1:A:343:LYS:NZ	7:A:547:HOH:O	2.42	0.51
1:A:436:ARG:NH1	1:B:427:GLU:OE1	2.44	0.51
1:A:238:MSE:SE	1:A:277:ASP:OD1	2.79	0.50
1:B:208:LEU:HD13	1:B:283:GLY:O	2.12	0.50
1:C:105:PRO:HG3	1:C:161:ILE:HD12	1.92	0.50
1:B:144:LEU:HA	1:B:190:THR:OG1	2.12	0.50
1:C:463:ILE:HD13	1:C:463:ILE:N	2.26	0.50
1:D:380:GLN:O	1:D:380:GLN:HG3	2.12	0.50
1:D:463:ILE:HD11	1:D:486:PHE:HB2	1.93	0.50
1:A:218:LEU:O	1:A:223:LEU:HG	2.12	0.50
1:D:28:GLY:HA3	1:D:62:GLY:O	2.11	0.50
1:C:200:THR:HG22	1:C:202:THR:H	1.77	0.50
1:A:386:ILE:CG1	1:A:387:SER:H	2.25	0.50
2:A:540:NAG:H62	2:A:540:NAG:O1	2.12	0.50
1:C:418:ILE:HG12	1:C:421:ARG:HH11	1.76	0.50
1:A:263:GLN:OE1	1:A:267:LYS:HD3	2.11	0.50
1:D:121:ILE:O	1:D:125:GLU:HB2	2.11	0.50
1:D:343:LYS:O	1:D:347:LEU:HG	2.11	0.50
1:B:39:GLN:N	1:B:39:GLN:OE1	2.32	0.49
1:A:105:PRO:HG3	1:A:161:ILE:HD12	1.93	0.49
1:A:178:PHE:CD2	1:A:178:PHE:C	2.86	0.49
1:D:480:PHE:CD1	1:D:486:PHE:HZ	2.30	0.49
1:A:126:THR:HG21	7:A:552:HOH:O	2.11	0.49
1:B:415:ALA:HB2	1:B:510:GLN:HB3	1.94	0.49
1:C:465:VAL:O	1:C:469:ILE:HG13	2.11	0.49
1:C:14:LEU:O	1:C:18:ILE:HG13	2.12	0.49
1:B:161:ILE:HD11	1:B:451:ARG:CZ	2.42	0.49
1:C:119:GLN:HA	1:C:119:GLN:NE2	2.22	0.49
1:A:106:PRO:HB3	1:A:164:PHE:CE1	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:482:GLY:O	1:B:501:PHE:HE1	1.96	0.49
1:D:199:ASP:O	1:D:200:THR:HG23	2.11	0.49
1:C:167:THR:HB	1:C:168:PRO:HD2	1.95	0.49
1:A:169:ASP:OD1	1:A:169:ASP:N	2.39	0.49
1:A:179:ILE:O	1:A:183:GLN:HG3	2.13	0.48
1:B:288:ALA:O	4:B:544:GOL:H11	2.13	0.48
1:A:308:PRO:HG2	1:A:311:VAL:HG22	1.96	0.48
1:D:148:LEU:HD12	1:D:191:ALA:HB1	1.96	0.48
1:B:251:TYR:O	7:B:576:HOH:O	2.20	0.48
1:A:389:PHE:HB3	1:A:390:PRO:CD	2.43	0.48
1:A:150:VAL:HG12	1:A:152:ASN:OD1	2.13	0.48
1:A:213:HIS:CD2	1:A:217:ARG:NH1	2.81	0.48
1:A:263:GLN:O	1:A:267:LYS:HB3	2.14	0.48
1:D:227:LYS:HG3	1:D:268:LEU:HD22	1.95	0.48
1:D:496:GLU:HG2	1:D:497:ILE:N	2.29	0.48
1:D:493:THR:CG2	1:D:494:LEU:HG	2.42	0.48
1:C:224:PRO:HB2	1:C:225:PRO:HD3	1.96	0.48
1:D:48:GLN:HG3	1:D:78:TRP:CD2	2.49	0.48
1:C:156:ASN:HD21	1:C:159:ILE:HG12	1.79	0.48
1:C:55:ILE:HA	1:C:55:ILE:HD12	1.63	0.48
1:B:144:LEU:HA	1:B:190:THR:HG1	1.79	0.48
1:B:206:LEU:HD13	1:B:457:GLU:HG2	1.96	0.48
1:C:20:GLN:NE2	7:C:555:HOH:O	2.44	0.48
1:A:320:THR:O	1:A:324:THR:HG23	2.14	0.48
1:D:308:PRO:HG2	1:D:311:VAL:HG22	1.94	0.48
1:B:23:VAL:HA	1:B:57:GLY:O	2.13	0.48
1:A:39:GLN:HG2	1:A:40:TRP:CD1	2.49	0.48
1:D:88:ASP:OD1	1:D:88:ASP:N	2.44	0.48
1:D:439:LEU:HA	1:D:439:LEU:HD23	1.69	0.48
1:A:386:ILE:HD12	1:A:387:SER:H	1.79	0.47
1:B:270:PHE:CZ	1:B:272:GLY:HA3	2.49	0.47
1:B:400:VAL:HG11	1:B:409:LEU:HD11	1.96	0.47
1:B:250:GLN:CG	1:B:250:GLN:O	2.61	0.47
1:A:92:GLY:HA2	7:A:537:HOH:O	2.13	0.47
1:A:394:ALA:HB3	1:A:424:TYR:HA	1.96	0.47
1:D:275:VAL:HG12	1:D:276:THR:O	2.15	0.47
1:C:204:SER:HA	1:C:207:ALA:O	2.15	0.47
1:A:405:LYS:O	1:A:407:PRO:HD3	2.13	0.47
1:C:192:LYS:HB3	1:C:238:MSE:HB3	1.97	0.47
1:C:337:GLU:OE2	4:C:543:GOL:H32	2.14	0.47
1:C:253:ALA:HA	1:C:259:ILE:HD12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:400:VAL:HG11	1:A:409:LEU:HD11	1.97	0.47
1:D:159:ILE:O	1:D:160:ASN:C	2.52	0.47
1:D:105:PRO:HG2	1:D:503:TYR:HB3	1.97	0.47
1:C:319:GLU:O	1:C:323:LYS:HG3	2.15	0.47
1:A:220:THR:HG22	1:A:221:VAL:CG2	2.38	0.47
1:C:315:ILE:O	1:C:319:GLU:HG3	2.15	0.47
1:A:266:HIS:HD2	7:A:567:HOH:O	1.98	0.47
1:A:34:GLU:OE2	1:B:99:GLY:HA2	2.14	0.47
1:A:427:GLU:OE2	1:B:436:ARG:NH1	2.46	0.47
1:C:96:ARG:HA	1:C:96:ARG:HD3	1.79	0.47
1:B:86:ALA:HB2	1:B:142:TRP:HB3	1.97	0.47
1:B:206:LEU:CD1	1:B:457:GLU:HG2	2.44	0.46
1:C:157:PRO:HB2	1:C:456:THR:O	2.15	0.46
1:D:422:HIS:CD2	1:D:518:TRP:CD2	3.03	0.46
1:D:441:ALA:C	1:D:442:ILE:HG23	2.35	0.46
1:B:343:LYS:O	1:B:347:LEU:HG	2.15	0.46
1:D:431:LEU:O	1:D:435:PRO:HD3	2.16	0.46
1:C:362:ARG:HA	1:C:363:PRO:HD3	1.80	0.46
1:D:236:ALA:HA	1:D:270:PHE:HZ	1.80	0.46
1:C:81:ILE:HD13	1:C:340:TRP:CH2	2.51	0.46
1:B:241:HIS:ND1	1:B:284:ILE:HB	2.31	0.46
1:B:418:ILE:HB	1:B:419:PRO:HD3	1.98	0.46
2:C:540:NAG:O1	2:C:540:NAG:C6	2.64	0.46
1:D:160:ASN:OD1	1:D:483:SER:HB2	2.16	0.46
1:C:493:THR:C	1:C:495:PRO:HD3	2.36	0.46
1:D:149:ASP:OD2	1:D:159:ILE:CD1	2.64	0.46
1:B:111:GLU:OE2	1:B:114:ARG:NH1	2.49	0.46
1:A:395:ARG:NH1	1:A:440:GLU:O	2.41	0.46
1:B:398:ILE:HG23	1:B:449:PHE:HE2	1.80	0.46
1:D:194:PHE:CE1	1:D:264:LEU:HD13	2.51	0.46
1:D:396:ASN:HB3	1:D:426:ALA:HA	1.98	0.46
1:D:240:ALA:HB3	1:D:242:LEU:HD12	1.97	0.45
1:C:89:ILE:HG21	1:C:93:VAL:HA	1.97	0.45
1:A:13:SER:OG	1:A:16:GLN:HG3	2.16	0.45
1:C:205:HIS:CE1	1:C:454:PRO:HB3	2.51	0.45
1:D:259:ILE:O	1:D:263:GLN:HB2	2.15	0.45
1:B:260:LEU:O	1:B:264:LEU:HB3	2.17	0.45
1:B:264:LEU:HD23	1:B:274:ILE:HD13	1.97	0.45
1:A:218:LEU:HD12	1:A:218:LEU:HA	1.78	0.45
1:B:35:ARG:HH12	4:B:541:GOL:C1	2.21	0.45
1:A:205:HIS:CE1	2:A:540:NAG:O1	2.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:ARG:NH2	1:A:274:ILE:CG1	2.77	0.45
1:A:217:ARG:O	1:A:220:THR:N	2.50	0.45
1:C:495:PRO:HD2	1:C:496:GLU:OE1	2.17	0.45
1:A:396:ASN:O	1:A:426:ALA:HA	2.15	0.45
1:B:111:GLU:OE1	5:B:542:PEG:H31	2.17	0.45
1:A:103:PHE:HB3	1:A:127:MSE:HE3	1.98	0.45
1:B:48:GLN:HG3	1:B:78:TRP:CD2	2.52	0.45
1:C:445:LEU:HD12	1:C:477:GLY:O	2.16	0.45
1:D:385:LYS:HA	1:D:517:LEU:O	2.17	0.45
1:B:478:VAL:O	1:B:499:TRP:HA	2.17	0.45
1:B:224:PRO:HB2	1:B:225:PRO:HD3	1.98	0.45
1:D:385:LYS:HG3	1:D:519:GLU:CG	2.42	0.45
1:B:105:PRO:HG3	1:B:161:ILE:HD12	1.98	0.45
1:B:377:THR:HG23	1:B:501:PHE:O	2.16	0.45
1:C:102:GLU:HG2	1:C:506:MSE:CE	2.47	0.45
1:C:475:LEU:HD12	1:C:497:ILE:HD13	1.97	0.45
1:D:501:PHE:C	1:D:501:PHE:CD2	2.90	0.45
1:C:395:ARG:HH11	1:C:427:GLU:HB2	1.82	0.45
1:A:160:ASN:OD1	1:A:161:ILE:N	2.47	0.45
1:C:429:VAL:HG22	1:C:430:GLU:N	2.32	0.45
1:A:445:LEU:HD12	1:A:477:GLY:O	2.16	0.44
1:C:394:ALA:HB1	1:C:443:PRO:O	2.17	0.44
1:D:25:ARG:NH1	1:D:61:LEU:HD23	2.32	0.44
1:D:411:PRO:O	1:D:412:ASN:HB2	2.16	0.44
1:B:399:VAL:O	1:B:448:CYS:HA	2.17	0.44
1:C:441:ALA:HA	1:C:473:ILE:HD12	1.98	0.44
1:B:106:PRO:HB3	1:B:164:PHE:CD1	2.52	0.44
1:D:209:PRO:CG	1:D:242:LEU:HD23	2.32	0.44
1:C:202:THR:HG22	1:C:209:PRO:HG3	2.00	0.44
1:B:241:HIS:CE1	1:B:284:ILE:HB	2.53	0.44
1:D:410:ARG:NH1	7:D:544:HOH:O	2.42	0.44
1:D:486:PHE:CD1	1:D:486:PHE:C	2.91	0.44
1:A:479:ILE:HD11	1:A:517:LEU:HD11	2.00	0.44
1:B:116:ASP:OD2	1:B:119:GLN:HB2	2.17	0.44
1:A:208:LEU:HD23	1:A:209:PRO:CD	2.47	0.44
1:B:239[A]:ASN:OD1	1:B:276:THR:HA	2.18	0.44
1:C:192:LYS:HB2	1:C:193:HIS:CG	2.52	0.44
1:A:113:TRP:HB2	1:A:174:LEU:HD11	1.99	0.44
1:D:354:PHE:CD2	1:D:354:PHE:C	2.91	0.44
1:C:219:ASN:HA	1:C:223:LEU:HB2	1.99	0.43
1:A:35:ARG:HA	1:A:36:PRO:HD2	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:377:THR:HG22	1:A:378:LYS:N	2.33	0.43
1:B:380:GLN:HB2	1:B:499:TRP:NE1	2.33	0.43
1:B:103:PHE:CB	1:B:127:MSE:HE3	2.48	0.43
1:A:253:ALA:HA	1:A:259:ILE:HD12	2.00	0.43
1:D:364:GLU:N	1:D:364:GLU:OE1	2.45	0.43
1:D:40:TRP:CZ3	1:D:280:VAL:HG22	2.52	0.43
1:D:116:ASP:OD2	1:D:119:GLN:HB2	2.18	0.43
1:B:153:ASN:HB2	1:B:199:ASP:OD1	2.18	0.43
1:D:244:ILE:HG22	1:D:247:TRP:H	1.82	0.43
1:D:265:ARG:NH2	1:D:303:ASP:OD2	2.46	0.43
1:C:223:LEU:N	1:C:224:PRO:CD	2.82	0.43
1:D:209:PRO:HG2	1:D:242:LEU:CD2	2.34	0.43
1:B:386:ILE:HD13	1:B:500:TRP:CH2	2.54	0.43
1:A:55:ILE:HA	1:A:55:ILE:HD12	1.70	0.43
1:D:359:SER:OG	1:D:365:THR:CG2	2.64	0.43
1:D:363:PRO:O	1:D:367:LYS:HG2	2.18	0.43
1:C:213:HIS:HB3	1:C:217:ARG:HG2	2.00	0.43
1:A:461:ASP:CA	1:A:486:PHE:HE1	2.23	0.43
1:B:506:MSE:O	1:B:510:GLN:HG3	2.18	0.43
1:D:119:GLN:HG2	1:D:375:ARG:HH22	1.83	0.43
1:D:383:LEU:HD12	1:D:383:LEU:HA	1.80	0.43
1:A:14:LEU:HD13	1:A:329:GLU:HG3	2.00	0.43
1:A:67:GLU:OE1	1:B:98:ARG:NH1	2.51	0.43
1:C:112:ILE:HG12	1:C:375:ARG:HB3	2.01	0.43
1:A:205:HIS:CE1	1:A:454:PRO:HB3	2.53	0.43
1:A:39:GLN:HG2	1:A:40:TRP:N	2.34	0.43
1:B:96:ARG:HD3	1:B:96:ARG:HA	1.56	0.43
1:B:290:PRO:CD	4:B:544:GOL:H12	2.43	0.42
1:D:396:ASN:O	1:D:426:ALA:HA	2.19	0.42
1:D:136:LEU:HD23	1:D:136:LEU:HA	1.80	0.42
1:C:9:VAL:HG12	1:C:333:TYR:HD1	1.82	0.42
1:C:464:ASP:HB3	7:C:582:HOH:O	2.18	0.42
1:B:134:GLU:O	1:B:137:SER:HB3	2.19	0.42
1:C:10:GLU:OE2	4:C:543:GOL:O3	2.37	0.42
1:B:332:ILE:O	1:B:336:VAL:HG23	2.19	0.42
1:B:394:ALA:HB1	1:B:443:PRO:O	2.19	0.42
1:B:192:LYS:HB3	1:B:193:HIS:CG	2.54	0.42
1:B:328:SER:O	1:B:331:ARG:HB3	2.19	0.42
1:C:427:GLU:HG3	1:D:432:LYS:NZ	2.34	0.42
1:B:104:PRO:HG2	1:B:372:VAL:CG1	2.50	0.42
1:C:475:LEU:HA	1:C:475:LEU:HD23	1.89	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:192:LYS:HA	1:B:193:HIS:HA	1.80	0.42
1:A:455:PHE:CZ	1:B:530:GLU:HA	2.55	0.42
1:D:179:ILE:CD1	1:D:234:VAL:CG1	2.97	0.42
1:C:192:LYS:HA	1:C:193:HIS:HA	1.79	0.42
1:C:461:ASP:HA	1:C:462:PRO:HD2	1.86	0.42
1:A:102:GLU:HG2	1:A:506:MSE:CE	2.46	0.42
1:D:226:PHE:O	1:D:230:ILE:HG13	2.19	0.42
1:C:106:PRO:HB3	1:C:164:PHE:CD1	2.54	0.42
1:B:133:GLN:HB2	1:B:185:TYR:CZ	2.55	0.42
1:A:213:HIS:HB3	1:A:217:ARG:CG	2.41	0.42
1:A:386:ILE:CD1	1:A:387:SER:H	2.31	0.42
1:D:111:GLU:CG	1:D:503:TYR:HE2	2.32	0.42
1:D:223:LEU:HD11	1:D:247:TRP:HH2	1.85	0.42
1:C:192:LYS:HB2	1:C:193:HIS:CD2	2.54	0.42
1:C:364:GLU:CD	1:C:364:GLU:H	2.22	0.42
1:D:241:HIS:CE1	1:D:254:THR:HG21	2.55	0.42
1:D:301:GLY:HA2	1:D:331:ARG:NH2	2.34	0.42
1:C:47:LEU:HA	1:C:47:LEU:HD12	1.61	0.42
1:A:238:MSE:HA	1:A:275:VAL:O	2.19	0.42
1:D:108:ALA:HA	1:D:503:TYR:CD2	2.54	0.42
1:A:91:GLU:HG3	1:A:105:PRO:HA	2.02	0.42
1:A:500:TRP:CE2	1:A:517:LEU:HD23	2.55	0.42
1:A:506:MSE:O	1:A:510:GLN:HG3	2.20	0.42
1:D:188:LEU:CD2	1:D:346:ILE:HD11	2.50	0.42
1:C:433:THR:C	1:C:435:PRO:HD2	2.41	0.41
1:D:399:VAL:HA	1:D:429:VAL:O	2.20	0.41
1:A:133:GLN:HB2	1:A:185:TYR:CZ	2.55	0.41
1:B:496:GLU:HB2	7:B:585:HOH:O	2.19	0.41
1:A:193:HIS:HB3	1:A:240:ALA:HB2	2.01	0.41
1:A:473:ILE:HA	1:A:474:PRO:HD3	1.90	0.41
1:B:123:LEU:HD13	1:B:372:VAL:CG2	2.48	0.41
1:C:42:ALA:HB3	1:C:47:LEU:HD13	2.02	0.41
1:B:465:VAL:O	1:B:469:ILE:HG13	2.19	0.41
1:A:209:PRO:HG2	1:A:242:LEU:CD2	2.49	0.41
1:A:373:LEU:HD13	1:A:509:ALA:CA	2.50	0.41
1:D:484:PRO:HB3	1:D:501:PHE:CZ	2.55	0.41
1:C:464:ASP:OD1	1:C:464:ASP:C	2.58	0.41
1:B:506:MSE:HG2	1:B:508:ILE:HG22	2.02	0.41
1:D:410:ARG:HB3	1:D:411:PRO:HD2	2.02	0.41
1:D:415:ALA:HB2	1:D:510:GLN:HG2	2.02	0.41
1:A:136:LEU:HA	1:A:136:LEU:HD23	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:468:LYS:HB3	1:D:468:LYS:HE2	1.71	0.41
1:D:255:LEU:HB3	1:D:296:GLN:HG3	2.02	0.41
1:C:427:GLU:CD	1:D:436:ARG:NH2	2.74	0.41
1:B:508:ILE:HD12	1:B:508:ILE:HA	1.87	0.41
1:D:453:ASN:O	1:D:456:THR:HG23	2.20	0.41
1:A:333:TYR:O	1:A:337:GLU:HG2	2.20	0.41
1:B:479:ILE:CD1	1:B:517:LEU:HD11	2.43	0.41
1:D:168:PRO:HD3	1:D:221:VAL:HG13	2.02	0.41
1:B:284:ILE:HA	1:B:284:ILE:HD12	1.97	0.41
1:C:133:GLN:HB2	1:C:185:TYR:CZ	2.55	0.41
1:B:290:PRO:N	4:B:544:GOL:H32	2.35	0.41
1:C:427:GLU:HA	7:D:552:HOH:O	2.20	0.41
1:A:203:ASP:OD2	1:A:205:HIS:CD2	2.72	0.41
1:A:394:ALA:HB1	1:A:424:TYR:CD1	2.56	0.41
1:C:149:ASP:HA	7:C:591:HOH:O	2.20	0.41
1:D:89:ILE:HG12	1:D:89:ILE:H	1.52	0.41
1:D:120:ALA:HB1	1:D:174:LEU:HD21	2.02	0.41
1:B:89:ILE:HD11	1:B:143:VAL:HG22	2.02	0.41
1:A:213:HIS:HB2	1:A:218:LEU:CD1	2.50	0.41
1:C:84:LEU:HG	1:C:343:LYS:HE2	2.02	0.41
1:B:461:ASP:HA	1:B:462:PRO:HD2	1.96	0.41
1:B:136:LEU:HA	1:B:136:LEU:HD23	1.81	0.41
1:D:51:ILE:HA	1:D:55:ILE:HG22	2.03	0.41
1:A:386:ILE:HG13	1:A:387:SER:H	1.85	0.41
1:C:478:VAL:O	1:C:499:TRP:HA	2.21	0.41
1:D:275:VAL:HG22	1:D:304:ILE:HB	2.02	0.41
1:C:506:MSE:H	1:C:506:MSE:SE	2.53	0.41
1:C:153:ASN:HB2	1:C:199:ASP:OD1	2.20	0.41
1:D:326:GLN:O	1:D:327:LEU:HD23	2.21	0.41
1:A:158:VAL:HG13	1:A:159:ILE:HG12	2.03	0.41
1:B:431:LEU:CD2	1:B:460:ALA:HB1	2.51	0.41
1:D:251:TYR:HA	1:D:252:PRO:HD2	1.91	0.41
1:B:89:ILE:O	1:B:89:ILE:HG13	2.21	0.41
1:A:465:VAL:O	1:A:469:ILE:HG13	2.21	0.41
1:A:82:PRO:CG	1:A:347:LEU:HD11	2.51	0.41
1:D:208:LEU:HD12	1:D:209:PRO:HD2	2.02	0.40
1:D:434:LEU:N	1:D:435:PRO:CD	2.85	0.40
1:A:160:ASN:HA	7:A:550:HOH:O	2.20	0.40
1:D:422:HIS:CD2	1:D:518:TRP:CE3	3.09	0.40
1:D:39:GLN:HG2	1:D:40:TRP:CD1	2.56	0.40
1:A:243:MSE:C	1:A:245:PRO:HD3	2.42	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:HIS:CD2	2:A:540:NAG:HN2	2.40	0.40
1:C:326[B]:GLN:O	1:C:327:LEU:HD23	2.21	0.40
1:A:292:THR:O	1:A:296:GLN:HB2	2.22	0.40
1:A:71:LYS:HD2	1:A:71:LYS:HA	1.89	0.40
1:D:98[A]:ARG:HH11	1:D:98[A]:ARG:HG2	1.87	0.40
1:C:354:PHE:C	1:C:354:PHE:CD2	2.94	0.40
1:C:143:VAL:CG1	1:C:145:ALA:HB3	2.51	0.40
1:C:35:ARG:HA	1:C:36:PRO:HD2	1.99	0.40
1:D:104:PRO:HD3	1:D:369:VAL:HG13	2.03	0.40
1:A:386:ILE:HG13	1:A:476:GLN:HB3	2.01	0.40
1:C:441:ALA:HA	1:C:473:ILE:HD13	2.04	0.40
1:B:335:SER:O	1:B:339:ILE:HG13	2.21	0.40
1:B:150:VAL:O	1:B:198:GLY:HA3	2.21	0.40
1:A:96:ARG:HD3	1:A:96:ARG:HA	1.74	0.40
1:D:103:PHE:CB	1:D:127:MSE:HE3	2.51	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	507/535 (95%)	489 (96%)	18 (4%)	0	100	100
1	B	512/535 (96%)	499 (98%)	13 (2%)	0	100	100
1	C	513/535 (96%)	500 (98%)	13 (2%)	0	100	100
1	D	515/535 (96%)	502 (98%)	13 (2%)	0	100	100
All	All	2047/2140 (96%)	1990 (97%)	57 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	417/420 (99%)	393 (94%)	24 (6%)	25	52
1	B	420/420 (100%)	402 (96%)	18 (4%)	35	66
1	C	423/420 (101%)	393 (93%)	30 (7%)	18	41
1	D	421/420 (100%)	395 (94%)	26 (6%)	23	49
All	All	1681/1680 (100%)	1583 (94%)	98 (6%)	25	52

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	GLU
1	A	55	ILE
1	A	91	GLU
1	A	115	THR
1	A	137	SER
1	A	152	ASN
1	A	169	ASP
1	A	200	THR
1	A	211	ILE
1	A	216	THR
1	A	217	ARG
1	A	218	LEU
1	A	249[A]	GLN
1	A	249[B]	GLN
1	A	296	GLN
1	A	340	TRP
1	A	359	SER
1	A	379	HIS
1	A	383	LEU
1	A	386	ILE
1	A	405	LYS
1	A	440	GLU
1	A	496	GLU
1	A	506	MSE

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Mol	Chain	Res	Type
1	B	45	THR
1	B	67	GLU
1	B	189	THR
1	B	190	THR
1	B	211	ILE
1	B	249	GLN
1	B	291	ASP
1	B	294	VAL
1	B	340	TRP
1	B	364	GLU
1	B	379	HIS
1	B	386	ILE
1	B	401	ASP
1	B	442	ILE
1	B	448	CYS
1	B	458	LYS
1	B	492	THR
1	B	506	MSE
1	C	6	LEU
1	C	11	SER
1	C	12	LEU
1	C	39	GLN
1	C	44	GLN
1	C	45	THR
1	C	55	ILE
1	C	89	ILE
1	C	119	GLN
1	C	192	LYS
1	C	200	THR
1	C	216	THR
1	C	249	GLN
1	C	255	LEU
1	C	340	TRP
1	C	348	THR
1	C	350	THR
1	C	353	THR
1	C	371	MSE
1	C	375	ARG
1	C	379	HIS
1	C	380	GLN
1	C	384	VAL
1	C	387	SER

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Mol	Chain	Res	Type
1	C	388	SER
1	C	458	LYS
1	C	468	LYS
1	C	486	PHE
1	C	506	MSE
1	C	530	GLU
1	D	88	ASP
1	D	89	ILE
1	D	143	VAL
1	D	152	ASN
1	D	169	ASP
1	D	188	LEU
1	D	202	THR
1	D	210	THR
1	D	211	ILE
1	D	216	THR
1	D	231	GLN
1	D	234	VAL
1	D	280	VAL
1	D	316	ILE
1	D	340	TRP
1	D	344	GLN
1	D	362	ARG
1	D	386	ILE
1	D	388	SER
1	D	436	ARG
1	D	459	LEU
1	D	463	ILE
1	D	464	ASP
1	D	490	LEU
1	D	493	THR
1	D	506	MSE

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

Mol	Chain	Res	Type
1	A	74	GLN
1	A	151	ASN
1	A	205	HIS
1	A	266	HIS
1	A	420	GLN
1	A	422	HIS

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Mol	Chain	Res	Type
1	A	447	GLN
1	A	505	GLN
1	B	119	GLN
1	B	231	GLN
1	B	356	GLN
1	B	380	GLN
1	B	422	HIS
1	B	447	GLN
1	B	491	GLN
1	C	74	GLN
1	C	119	GLN
1	C	250	GLN
1	C	263	GLN
1	C	380	GLN
1	C	412	ASN
1	C	447	GLN
1	D	119	GLN
1	D	133	GLN
1	D	152	ASN
1	D	170	GLN
1	D	239	ASN
1	D	263	GLN
1	D	379	HIS
1	D	380	GLN
1	D	392	ASN
1	D	422	HIS
1	D	447	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

20 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
2	NAG	A	540	-	15,15,15	0.51	0	17,21,21	0.95	1 (5%)
3	ACY	A	541	-	1,3,3	1.88	0	0,3,3	0.00	-
3	ACY	A	542	-	1,3,3	1.75	0	0,3,3	0.00	-
3	ACY	A	543	-	1,3,3	1.90	0	0,3,3	0.00	-
2	NAG	B	540	-	15,15,15	1.38	1 (6%)	17,21,21	1.69	2 (11%)
4	GOL	B	541	-	5,5,5	0.34	0	5,5,5	0.49	0
5	PEG	B	542	-	6,6,6	0.50	0	5,5,5	0.19	0
3	ACY	B	543	-	1,3,3	1.44	0	0,3,3	0.00	-
4	GOL	B	544	-	5,5,5	0.40	0	5,5,5	0.67	0
2	NAG	C	540	-	15,15,15	0.51	0	17,21,21	0.85	0
4	GOL	C	541	-	5,5,5	0.31	0	5,5,5	0.19	0
4	GOL	C	542	-	5,5,5	0.40	0	5,5,5	0.54	0
4	GOL	C	543	-	5,5,5	0.30	0	5,5,5	0.43	0
3	ACY	C	544	-	1,3,3	1.18	0	0,3,3	0.00	-
6	SO4	C	545	-	4,4,4	0.21	0	6,6,6	0.12	0
4	GOL	C	546	-	5,5,5	0.32	0	5,5,5	0.47	0
2	NAG	D	540	-	15,15,15	0.43	0	17,21,21	0.86	0
3	ACY	D	541	-	1,3,3	1.43	0	0,3,3	0.00	-
3	ACY	D	542	-	1,3,3	1.07	0	0,3,3	0.00	-
3	ACY	D	543	-	1,3,3	1.72	0	0,3,3	0.00	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	540	-	-	0/6/26/26	0/1/1/1
3	ACY	A	541	-	-	0/0/0/0	0/0/0/0
3	ACY	A	542	-	-	0/0/0/0	0/0/0/0
3	ACY	A	543	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	540	-	-	0/6/26/26	0/1/1/1
4	GOL	B	541	-	-	0/4/4/4	0/0/0/0
5	PEG	B	542	-	-	0/4/4/4	0/0/0/0
3	ACY	B	543	-	-	0/0/0/0	0/0/0/0
4	GOL	B	544	-	-	0/4/4/4	0/0/0/0
2	NAG	C	540	-	-	0/6/26/26	0/1/1/1
4	GOL	C	541	-	-	0/4/4/4	0/0/0/0
4	GOL	C	542	-	-	0/4/4/4	0/0/0/0
4	GOL	C	543	-	-	0/4/4/4	0/0/0/0
3	ACY	C	544	-	-	0/0/0/0	0/0/0/0
6	SO4	C	545	-	-	0/0/0/0	0/0/0/0
4	GOL	C	546	-	-	0/4/4/4	0/0/0/0
2	NAG	D	540	-	-	0/6/26/26	0/1/1/1
3	ACY	D	541	-	-	0/0/0/0	0/0/0/0
3	ACY	D	542	-	-	0/0/0/0	0/0/0/0
3	ACY	D	543	-	-	0/0/0/0	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	540	NAG	O3-C3	-2.39	1.37	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	540	NAG	O3-C3-C2	-3.56	102.41	109.66
2	A	540	NAG	O5-C5-C6	2.42	112.48	106.36
2	B	540	NAG	C1-O5-C5	4.41	121.64	113.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	540	NAG	4	0
4	B	541	GOL	2	0
5	B	542	PEG	1	0
4	B	544	GOL	11	0
2	C	540	NAG	1	0
4	C	543	GOL	2	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	505/535 (94%)	-0.21	8 (1%) 74 75	20, 46, 83, 124	0
1	B	507/535 (94%)	-0.41	5 (0%) 84 85	17, 39, 74, 119	0
1	C	508/535 (94%)	-0.40	1 (0%) 95 96	14, 32, 66, 112	0
1	D	510/535 (95%)	-0.10	11 (2%) 65 66	17, 50, 85, 117	0
All	All	2030/2140 (94%)	-0.28	25 (1%) 81 81	14, 41, 81, 124	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	382	SER	4.5
1	D	383	LEU	4.1
1	D	381	LYS	3.9
1	D	382	SER	3.5
1	D	384	VAL	3.4
1	D	266	HIS	3.1
1	D	379	HIS	3.0
1	B	384	VAL	2.7
1	C	500	TRP	2.7
1	D	220	THR	2.7
1	A	384	VAL	2.6
1	B	10	GLU	2.5
1	A	491	GLN	2.5
1	A	496	GLU	2.5
1	D	215	ASP	2.5
1	B	383	LEU	2.4
1	D	519	GLU	2.4
1	A	247	TRP	2.4
1	A	494	LEU	2.4
1	A	424	TYR	2.4
1	A	495	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	352	SER	2.3
1	A	492	THR	2.2
1	B	12	LEU	2.2
1	D	375	ARG	2.1

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
6	SO4	C	545	5/5	0.82	0.44	11.31	169,169,170,174	0
4	GOL	B	544	6/6	0.82	0.31	6.69	61,77,88,98	0
4	GOL	C	542	6/6	0.92	0.32	6.64	48,53,59,62	0
5	PEG	B	542	7/7	0.92	0.21	3.62	67,69,73,74	0
4	GOL	C	546	6/6	0.90	0.31	3.35	74,78,102,108	0
3	ACY	D	541	4/4	0.96	0.16	3.12	45,59,59,63	0
4	GOL	B	541	6/6	0.86	0.19	2.59	62,69,76,78	0
4	GOL	C	541	6/6	0.83	0.18	2.53	75,82,84,88	0
3	ACY	A	543	4/4	0.89	0.17	1.54	65,68,71,72	0
4	GOL	C	543	6/6	0.89	0.23	1.34	58,63,68,69	0
2	NAG	C	540	15/15	0.98	0.18	1.22	13,31,44,53	0
3	ACY	D	543	4/4	0.95	0.16	1.14	41,55,56,64	0
2	NAG	D	540	15/15	0.97	0.18	0.81	42,52,65,70	0
3	ACY	D	542	4/4	0.86	0.24	0.57	66,71,74,79	0
2	NAG	B	540	15/15	0.97	0.13	0.22	19,35,52,53	0
2	NAG	A	540	15/15	0.97	0.14	-0.01	40,51,58,63	0
3	ACY	C	544	4/4	0.96	0.14	-0.68	63,64,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	ACY	B	543	4/4	0.96	0.16	-	46,46,47,49	4
3	ACY	A	542	4/4	0.85	0.20	-	76,86,86,87	0
3	ACY	A	541	4/4	0.92	0.15	-	58,60,68,75	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.