Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:08 AM GMT

PDB ID	:	2PM8
Title	:	Crystal structure of recombinant full length human butyrylcholinesterase
Authors	:	Ngamelue, M.N.; Homma, K.; Lockridge, O.; Asojo, O.A.
Deposited on	:	2007-04-20
Resolution	:	2.80 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

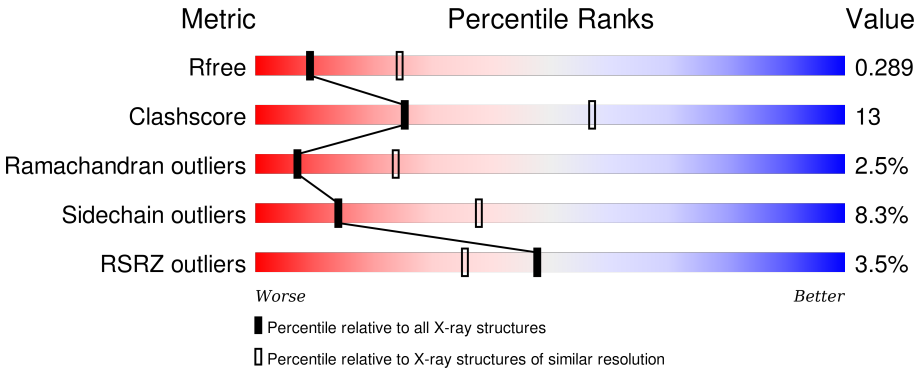
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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 >=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 <=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	574	4% 64% 24% • 8%
1	B	574	3% 61% 27% • 8%

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
4	NDG	A	678	X	-	-	-
5	SO4	A	603	-	-	X	-
5	SO4	A	606	-	-	X	-
6	GOL	A	774	-	-	-	X
6	GOL	A	777	-	-	-	X
6	GOL	A	999	-	-	-	X
6	GOL	B	774	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8699 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 Cholinesterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	530	Total	C	N	O	S	0	0	0
			4221	2725	708	772	16			
1	B	530	Total	C	N	O	S	0	0	0
			4221	2725	708	772	16			

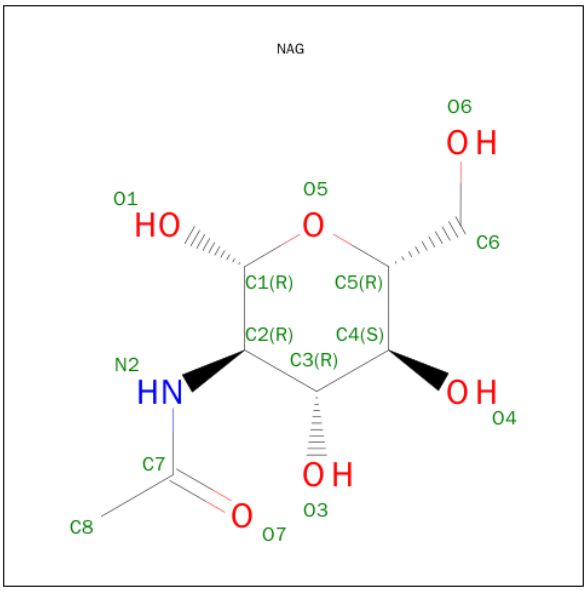
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	17	GLN	ASN	CONFLICT	UNP P06276
A	455	GLN	ASN	CONFLICT	UNP P06276
A	481	GLN	ASN	CONFLICT	UNP P06276
A	486	GLN	ASN	CONFLICT	UNP P06276
B	17	GLN	ASN	CONFLICT	UNP P06276
B	455	GLN	ASN	CONFLICT	UNP P06276
B	481	GLN	ASN	CONFLICT	UNP P06276
B	486	GLN	ASN	CONFLICT	UNP P06276

- Molecule 2 is a polymer of unknown type called SUGAR (2-MER).

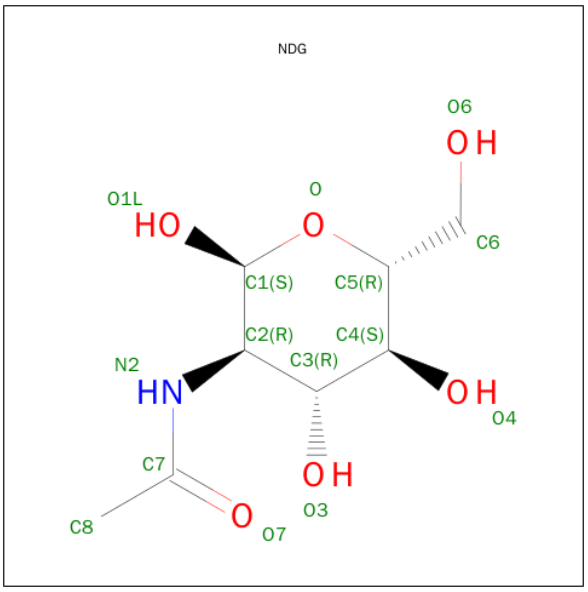
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



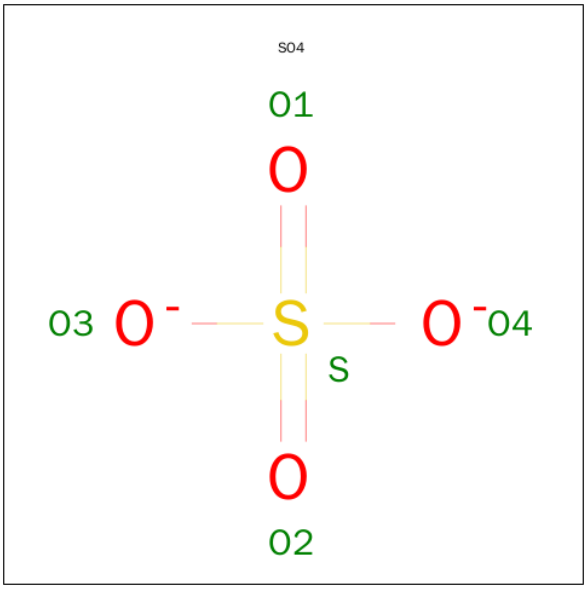
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 14 8 1 5	0	0
3	A	1	Total C N O 14 8 1 5	0	0
3	B	1	Total C N O 14 8 1 5	0	0
3	B	1	Total C N O 14 8 1 5	0	0

- Molecule 4 is SUGAR (2-(ACETYLAMINO)-2-DEOXY-A-D-GLUCOPYRANOSE) (three-letter code: NDG) (formula: $C_8H_{15}NO_6$).



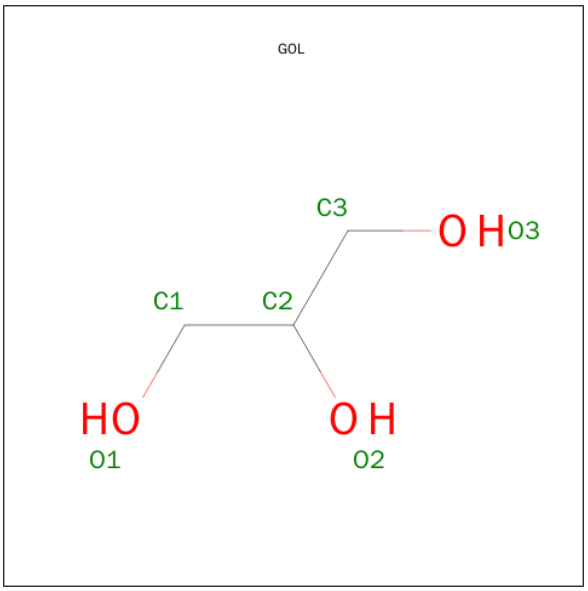
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 14 8 1 5	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O S 5 4 1	0	0
5	A	1	Total O S 5 4 1	0	0
5	A	1	Total O S 5 4 1	0	0
5	A	1	Total O S 5 4 1	0	0
5	A	1	Total O S 5 4 1	0	0
5	B	1	Total O S 5 4 1	0	0
5	B	1	Total O S 5 4 1	0	0

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 7 is water.

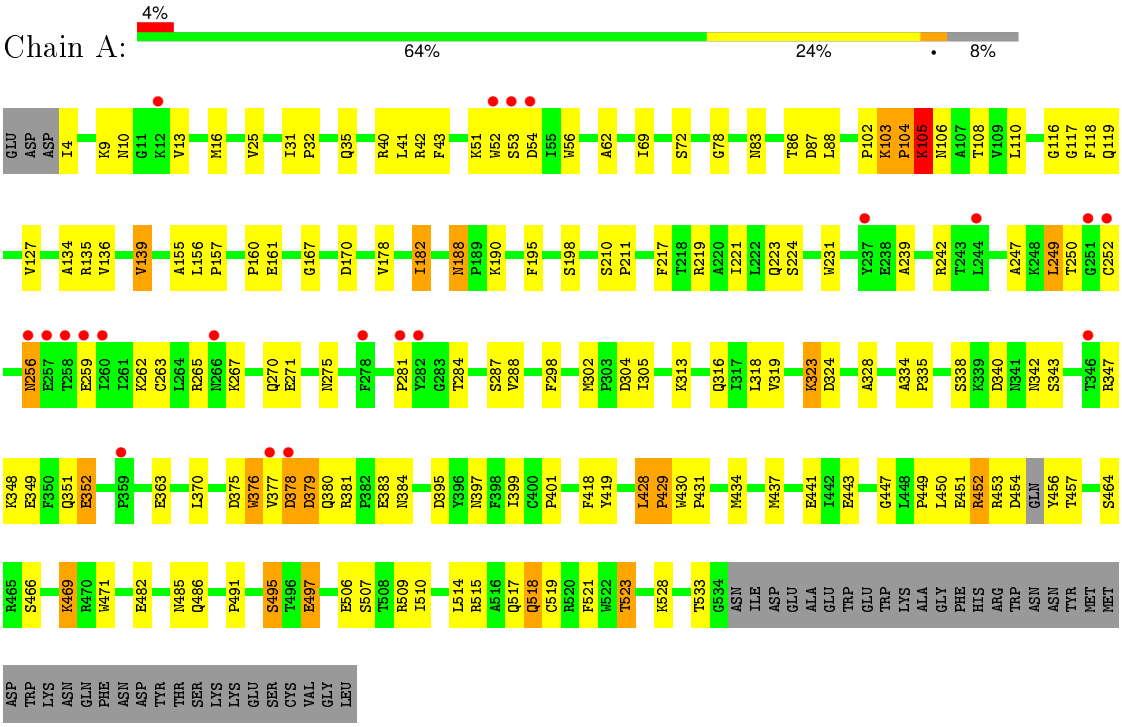
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	51	Total O 51 51	0	0
7	B	42	Total O 42 42	0	0
7	C	1	Total O 1 1	0	0

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 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.

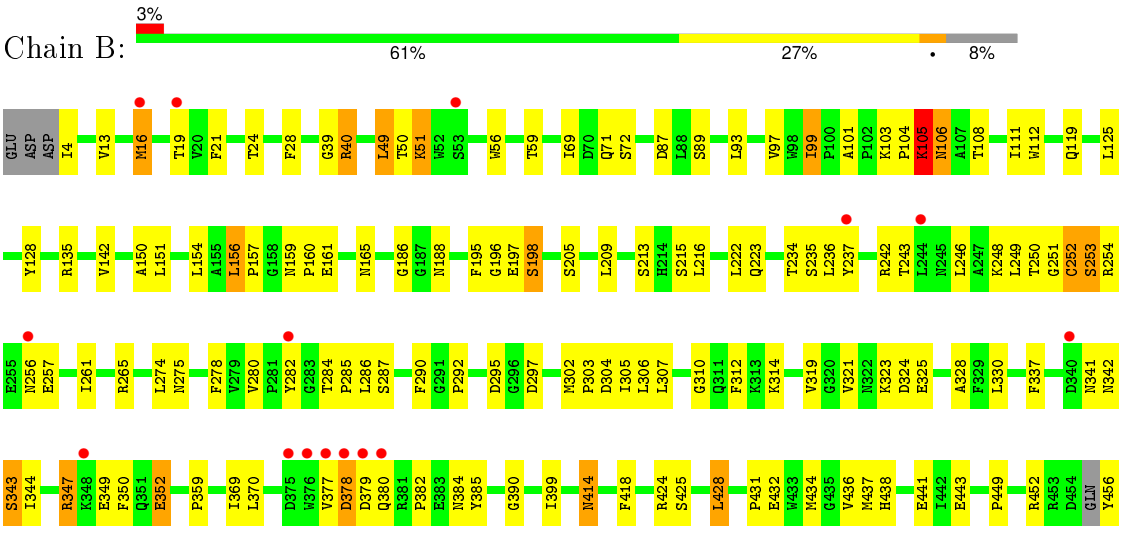
- Molecule 1: Cholinesterase

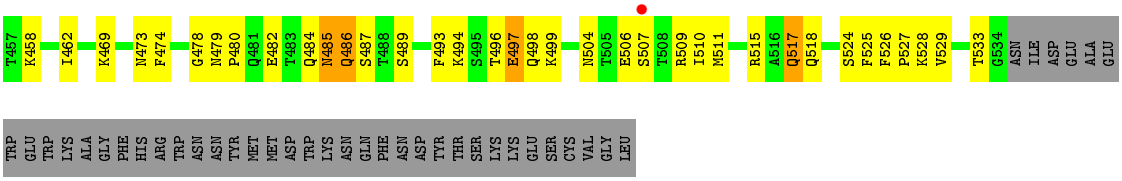
Chain A:



- Molecule 1: Cholinesterase

Chain B:




T457 K458 T462 K469 N473 F474 G478 N479 P480 Q481 E482 T483 Q484 N485 Q486 S487 T488 S489 F493 K494 S495 T496 E497 Q498 K499 N504 T505 E506 S507 T508 R509 I510 M511 R515 A516 Q517 Q518 S524 F525 F526 P527 K528 V529 T533 G534 ASN ILE ASP GLU ALA GLU
TRP GLU TRP LYS ALA GLY PHE HIS ARG TRP ASN ASN TYR MET MET ASP TRP LYS ASN GLN PHE ASN ASP TYR THR SER LYS LYS GLU SER CYS VAL GLY LEU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α, β, γ	150.80Å 150.80Å 142.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.80 50.27 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.8 (50.00-2.80) 98.8 (50.27-2.80)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	1.80 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.222 , 0.292 0.220 , 0.289	Depositor DCC
R_{free} test set	2026 reflections (5.27%)	DCC
Wilson B-factor (Å^2)	53.8	Xtriage
Anisotropy	0.073	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 65.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.26$	Xtriage
Outliers	0 of 40467 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	8699	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.29% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, NAG, NDG, 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	0.63	4/4339 (0.1%)	0.72	1/5889 (0.0%)
1	B	0.61	2/4339 (0.0%)	0.67	1/5889 (0.0%)
All	All	0.62	6/8678 (0.1%)	0.70	2/11778 (0.0%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	304	ASP	CB-CG	7.72	1.68	1.51
1	B	352	GLU	CD-OE2	7.49	1.33	1.25
1	A	352	GLU	CD-OE2	7.36	1.33	1.25
1	A	352	GLU	CG-CD	6.20	1.61	1.51
1	B	352	GLU	CG-CD	5.58	1.60	1.51
1	A	352	GLU	CB-CG	5.13	1.61	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	49	LEU	CA-CB-CG	6.33	129.86	115.30
1	A	104	PRO	C-N-CA	5.46	135.36	121.70

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	4221	0	4126	107	0
1	B	4221	0	4129	109	1
2	C	28	0	25	2	0
3	A	28	0	26	0	0
3	B	28	0	26	3	0
4	A	14	0	13	0	0
5	A	25	0	0	6	1
5	B	10	0	0	0	0
6	A	18	0	24	1	0
6	B	12	0	16	1	0
7	A	51	0	0	4	0
7	B	42	0	0	8	0
7	C	1	0	0	0	0
All	All	8699	0	8385	214	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (214) 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:B:341:ASN:HD21	3:B:781:NAG:C1	1.57	1.16
1:B:517:GLN:H	1:B:517:GLN:HE21	1.05	0.95
1:B:341:ASN:ND2	3:B:781:NAG:C1	2.30	0.95
1:B:425:SER:HB3	1:B:428:LEU:HD23	1.54	0.88
1:A:105:LYS:HG3	1:A:106:ASN:H	1.37	0.88
1:A:509:ARG:NH2	7:A:1038:HOH:O	2.09	0.83
1:B:103:LYS:NZ	7:B:827:HOH:O	1.70	0.83
1:A:105:LYS:CG	1:A:106:ASN:H	1.91	0.82
1:B:517:GLN:N	1:B:517:GLN:HE21	1.79	0.81
1:A:449:PRO:HG2	1:A:464:SER:HB2	1.61	0.81
1:A:518:GLN:H	1:A:518:GLN:HE21	1.28	0.80
1:B:104:PRO:CA	1:B:105:LYS:HB3	2.12	0.80
2:C:781:NAG:H61	2:C:782:NAG:HN2	1.45	0.79
1:B:157:PRO:HB3	1:B:236:LEU:HD22	1.66	0.77
1:B:103:LYS:CE	7:B:827:HOH:O	2.24	0.77
1:A:231:TRP:HD1	1:A:397:ASN:HD22	1.33	0.75
1:B:104:PRO:CB	1:B:105:LYS:HB3	2.18	0.74
1:B:246:LEU:O	1:B:250:THR:HG22	1.87	0.74
1:B:156:LEU:HD23	1:B:261:ILE:HD11	1.72	0.72
1:B:314:LYS:HB3	1:B:414:ASN:HD21	1.55	0.72
1:B:104:PRO:O	1:B:186:GLY:HA3	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:518:GLN:H	1:A:518:GLN:NE2	1.88	0.71
1:A:376:TRP:HD1	1:A:379:ASP:HB3	1.55	0.70
1:A:319:VAL:O	1:A:418:PHE:HA	1.92	0.70
1:A:104:PRO:HA	1:A:105:LYS:HB3	1.75	0.68
1:A:249:LEU:HD22	1:A:275:ASN:HD22	1.59	0.68
1:B:378:ASP:HB3	1:B:380:GLN:HG2	1.77	0.67
1:A:69:ILE:HG23	1:A:83:ASN:ND2	2.09	0.67
1:A:401:PRO:HA	5:A:604:SO4:O1	1.94	0.67
1:A:105:LYS:HG3	1:A:106:ASN:N	2.10	0.66
1:B:504:ASN:HB2	7:B:830:HOH:O	1.94	0.66
1:A:519:CYS:O	1:A:523:THR:HB	1.96	0.65
1:B:104:PRO:HA	1:B:105:LYS:HB3	1.79	0.64
1:B:105:LYS:O	1:B:106:ASN:HB2	1.98	0.64
1:A:376:TRP:CD1	1:A:379:ASP:HB3	2.32	0.64
1:A:42:ARG:O	1:A:43:PHE:HB2	1.97	0.63
1:B:165:ASN:OD1	1:B:292:PRO:HA	1.99	0.63
1:A:198:SER:HA	1:A:224:SER:O	1.97	0.63
1:B:21:PHE:O	1:B:135:ARG:NH1	2.18	0.63
1:A:252:CYS:SG	1:A:267:LYS:NZ	2.73	0.61
1:B:205:SER:HB3	1:B:222:LEU:HD21	1.83	0.61
1:A:528:LYS:HE3	5:A:603:SO4:O3	2.01	0.61
1:B:104:PRO:HA	1:B:105:LYS:CB	2.31	0.61
1:A:381:ARG:NH2	1:A:384:ASN:OD1	2.33	0.61
1:B:443:GLU:OE1	7:B:822:HOH:O	2.16	0.60
1:B:319:VAL:O	1:B:418:PHE:HA	2.02	0.60
1:A:370:LEU:HD12	5:A:606:SO4:O1	2.02	0.60
1:A:69:ILE:HD11	1:A:88:LEU:HD11	1.82	0.60
1:B:494:LYS:HB2	1:B:497:GLU:OE1	2.02	0.59
1:A:105:LYS:CG	1:A:106:ASN:N	2.64	0.59
1:A:347:ARG:O	1:A:351:GLN:HG3	2.03	0.59
1:B:13:VAL:HG12	1:B:56:TRP:HB3	1.84	0.59
1:A:378:ASP:O	1:A:380:GLN:N	2.34	0.59
1:B:16:MET:HG2	1:B:59:THR:HG22	1.84	0.58
1:A:399:ILE:HG21	1:A:515:ARG:HG3	1.83	0.58
1:A:62:ALA:O	1:A:86:THR:HG21	2.02	0.58
1:B:51:LYS:HD3	1:B:51:LYS:H	1.69	0.58
1:B:249:LEU:HB3	1:B:275:ASN:HD22	1.69	0.58
1:B:213:SER:HA	1:B:216:LEU:HD12	1.87	0.57
1:A:454:ASP:O	1:A:456:TYR:N	2.37	0.57
1:A:515:ARG:H	1:B:509:ARG:HH22	1.53	0.56
1:B:104:PRO:CA	1:B:105:LYS:CB	2.83	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:ASN:C	1:A:188:ASN:HD22	2.07	0.56
1:B:370:LEU:HD12	7:B:792:HOH:O	2.04	0.56
1:A:370:LEU:HD12	5:A:606:SO4:O2	2.06	0.56
1:B:302:MET:HB2	1:B:305:ILE:HD12	1.87	0.56
1:B:103:LYS:HE2	7:B:827:HOH:O	1.96	0.56
1:A:514:LEU:HG	1:A:515:ARG:HG2	1.87	0.55
1:A:250:THR:O	1:A:267:LYS:NZ	2.39	0.55
1:B:458:LYS:O	1:B:462:ILE:HD12	2.07	0.55
1:B:40:ARG:HA	1:B:265:ARG:HD2	1.87	0.55
1:B:209:LEU:HD23	1:B:312:PHE:HB3	1.89	0.55
1:B:342:ASN:HB2	1:B:344:ILE:HG12	1.88	0.55
1:B:159:ASN:HD21	1:B:161:GLU:HG2	1.72	0.55
1:A:449:PRO:HA	1:A:456:TYR:CD1	2.41	0.55
1:B:474:PHE:HB2	1:B:480:PRO:HB3	1.89	0.55
1:B:369:ILE:HD11	1:B:526:PHE:CE1	2.42	0.54
1:A:370:LEU:HD12	5:A:606:SO4:S	2.48	0.54
1:A:104:PRO:CA	1:A:105:LYS:HB3	2.37	0.53
1:B:515:ARG:HD2	1:B:518:GLN:HE21	1.73	0.53
1:A:217:PHE:O	1:A:313:LYS:HE2	2.08	0.53
1:A:302:MET:HB2	1:A:305:ILE:HD12	1.90	0.53
1:A:105:LYS:CD	1:A:106:ASN:H	2.21	0.53
1:A:323:LYS:HD2	1:A:324:ASP:OD2	2.08	0.53
1:B:242:ARG:HH12	6:B:774:GOL:H2	1.74	0.53
1:A:249:LEU:HD22	1:A:275:ASN:ND2	2.24	0.52
1:B:151:LEU:HB2	7:B:809:HOH:O	2.08	0.52
1:A:381:ARG:HB3	1:A:383:GLU:CD	2.30	0.52
1:A:349:GLU:HA	1:A:352:GLU:HB2	1.91	0.52
1:B:349:GLU:HA	1:B:352:GLU:HB2	1.92	0.52
1:B:106:ASN:OD1	1:B:188:ASN:HB2	2.09	0.52
1:A:134:ALA:HA	1:A:139:VAL:O	2.09	0.52
1:B:449:PRO:HA	1:B:456:TYR:CD1	2.45	0.52
1:A:363:GLU:H	1:A:363:GLU:CD	2.14	0.51
1:B:347:ARG:HD2	1:B:385:TYR:OH	2.09	0.51
1:A:395:ASP:OD2	1:A:399:ILE:HD12	2.10	0.51
1:A:469:LYS:HG2	1:A:482:GLU:HG2	1.91	0.51
1:B:197:GLU:HA	1:B:223:GLN:O	2.10	0.51
1:B:125:LEU:HD12	1:B:128:TYR:CE2	2.46	0.50
1:B:97:VAL:HG22	1:B:142:VAL:HG22	1.92	0.50
1:B:484:GLN:O	1:B:486:GLN:N	2.45	0.50
1:B:303:PRO:HA	1:B:306:LEU:HD12	1.93	0.50
1:A:517:GLN:HB2	7:A:1045:HOH:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:324:ASP:O	1:B:325:GLU:C	2.49	0.50
1:A:188:ASN:ND2	1:A:190:LYS:H	2.10	0.50
1:A:221:ILE:HG23	1:A:318:LEU:HB3	1.92	0.50
1:A:223:GLN:NE2	1:A:441:GLU:OE2	2.45	0.49
1:A:25:VAL:CG2	1:A:135:ARG:HB2	2.42	0.49
1:B:215:SER:O	1:B:216:LEU:HD23	2.13	0.49
1:B:284:THR:HB	1:B:285:PRO:HD2	1.94	0.49
1:B:493:PHE:CZ	1:B:498:GLN:HG2	2.48	0.49
1:A:338:SER:C	1:A:340:ASP:H	2.17	0.48
1:A:102:PRO:O	1:A:103:LYS:C	2.51	0.48
1:B:341:ASN:ND2	3:B:781:NAG:O7	2.47	0.48
1:A:119:GLN:HE21	1:A:288:VAL:HG13	1.77	0.48
1:B:525:PHE:O	1:B:529:VAL:HG23	2.13	0.48
1:A:155:ALA:HB3	1:A:239:ALA:HB1	1.95	0.48
1:A:160:PRO:HG2	1:A:161:GLU:OE1	2.14	0.48
1:A:219:ARG:HD3	1:A:316:GLN:OE1	2.13	0.48
1:A:491:PRO:HG2	1:A:510:ILE:CG2	2.44	0.48
1:A:78:GLY:HA2	1:A:429:PRO:HG2	1.96	0.47
1:A:347:ARG:HG2	1:A:351:GLN:HE21	1.79	0.47
1:B:344:ILE:HG23	1:B:382:PRO:O	2.13	0.47
1:A:31:ILE:HG22	1:A:32:PRO:O	2.15	0.47
1:A:69:ILE:N	1:A:69:ILE:HD12	2.29	0.47
1:B:198:SER:HB2	1:B:438:HIS:CE1	2.49	0.47
1:B:284:THR:HB	1:B:285:PRO:CD	2.45	0.47
1:A:430:TRP:HB3	1:A:431:PRO:HD2	1.96	0.47
1:A:116:GLY:O	1:A:118:PHE:N	2.47	0.47
1:B:198:SER:HB2	1:B:438:HIS:NE2	2.29	0.47
1:A:188:ASN:C	1:A:188:ASN:ND2	2.68	0.46
1:B:150:ALA:O	1:B:154:LEU:HB2	2.15	0.46
1:A:40:ARG:HA	1:A:265:ARG:HD2	1.96	0.46
1:A:428:LEU:HD13	1:A:430:TRP:H	1.80	0.46
1:A:495:SER:HB2	7:A:1039:HOH:O	2.15	0.46
1:B:323:LYS:HB3	1:B:436:VAL:HB	1.98	0.46
1:B:251:GLY:O	1:B:253:SER:N	2.49	0.45
1:B:99:ILE:HD12	1:B:104:PRO:HD2	1.98	0.45
1:A:521:PHE:HA	5:A:602:SO4:O1	2.16	0.45
1:B:40:ARG:HG2	1:B:40:ARG:H	1.47	0.45
1:B:489:SER:O	1:B:510:ILE:HD11	2.16	0.45
1:A:447:GLY:HA2	1:A:464:SER:OG	2.16	0.45
1:B:112:TRP:CZ3	1:B:196:GLY:HA2	2.52	0.45
1:B:330:LEU:HD11	1:B:390:GLY:HA2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:491:PRO:HD3	1:A:510:ILE:HD12	1.99	0.44
1:B:321:VAL:HG11	1:B:399:ILE:HA	1.98	0.44
1:B:328:ALA:HB2	1:B:437:MET:HE3	2.00	0.44
1:B:197:GLU:O	1:B:198:SER:C	2.56	0.44
1:B:359:PRO:HD2	7:B:795:HOH:O	2.17	0.44
1:B:159:ASN:ND2	1:B:161:GLU:HG2	2.31	0.44
1:A:256:ASN:O	1:A:259:GLU:HB2	2.18	0.44
1:A:167:GLY:O	1:A:170:ASP:HB2	2.18	0.44
1:B:252:CYS:HA	1:B:254:ARG:NH2	2.33	0.44
1:A:104:PRO:HB2	1:A:105:LYS:CG	2.47	0.44
1:A:136:VAL:HG21	1:A:450:LEU:HD13	2.00	0.44
1:B:119:GLN:HE22	1:B:290:PHE:H	1.66	0.43
1:A:395:ASP:HA	1:A:399:ILE:HB	2.00	0.43
1:A:328:ALA:HB2	1:A:437:MET:HE3	2.01	0.43
1:B:111:ILE:HG12	1:B:142:VAL:HB	2.00	0.43
1:A:104:PRO:HB2	1:A:105:LYS:HG3	2.00	0.43
1:B:104:PRO:HB2	1:B:105:LYS:HB3	1.98	0.43
1:A:428:LEU:HA	1:A:429:PRO:HD3	1.80	0.43
1:A:334:ALA:HA	1:A:335:PRO:HD2	1.80	0.43
1:A:338:SER:HB2	2:C:781:NAG:H62	2.00	0.43
1:A:250:THR:HB	1:A:267:LYS:HD3	2.00	0.43
1:B:474:PHE:O	1:B:478:GLY:N	2.51	0.43
1:B:24:THR:HB	1:B:101:ALA:HB3	2.00	0.43
1:B:524:SER:C	1:B:527:PRO:HD2	2.38	0.43
1:B:280:VAL:HG12	1:B:282:TYR:H	1.82	0.43
1:A:517:GLN:HG3	1:A:517:GLN:H	1.42	0.43
1:B:310:GLY:O	1:B:314:LYS:NZ	2.49	0.43
1:A:457:THR:HB	1:B:378:ASP:OD2	2.19	0.43
1:A:41:LEU:O	1:A:42:ARG:C	2.58	0.43
1:A:452:ARG:HG3	1:A:453:ARG:N	2.34	0.43
1:A:223:GLN:HG2	1:A:419:TYR:OH	2.19	0.42
1:A:491:PRO:HG2	1:A:510:ILE:HG23	2.01	0.42
1:B:223:GLN:NE2	1:B:441:GLU:OE2	2.52	0.42
1:B:248:LYS:HA	1:B:253:SER:OG	2.19	0.42
1:A:210:SER:HA	1:A:211:PRO:HD2	1.87	0.42
1:B:431:PRO:HG2	1:B:434:MET:HG3	2.02	0.42
1:A:13:VAL:HG12	1:A:56:TRP:HB3	2.02	0.42
1:B:469:LYS:HG3	1:B:473:ASN:ND2	2.35	0.42
1:A:178:VAL:O	1:A:182:ILE:HB	2.19	0.41
1:B:424:ARG:NH2	1:B:432:GLU:HA	2.35	0.41
1:A:247:ALA:HA	1:A:252:CYS:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:479:ASN:HA	1:B:480:PRO:HD3	1.92	0.41
1:A:156:LEU:HA	1:A:157:PRO:HD2	1.85	0.41
1:A:284:THR:H	1:A:287:SER:HB2	1.85	0.41
1:B:275:ASN:HA	1:B:278:PHE:HD1	1.85	0.41
1:B:493:PHE:HD2	1:B:499:LYS:O	2.02	0.41
1:A:434:MET:HE2	1:A:434:MET:HB3	1.94	0.41
1:B:105:LYS:HD3	1:B:106:ASN:C	2.41	0.41
1:B:261:ILE:O	1:B:265:ARG:HB2	2.20	0.41
1:B:28:PHE:N	1:B:28:PHE:CD1	2.89	0.41
1:A:259:GLU:O	1:A:263:CYS:N	2.44	0.41
1:A:182:ILE:HA	1:A:182:ILE:HD12	1.74	0.41
1:B:156:LEU:HD22	1:B:243:THR:HG21	2.03	0.41
1:B:249:LEU:HB3	1:B:275:ASN:ND2	2.33	0.41
7:A:1047:HOH:O	1:B:511:MET:HE3	2.21	0.41
1:B:337:PHE:HA	1:B:343:SER:OG	2.21	0.41
1:B:485:ASN:O	1:B:487:SER:N	2.54	0.41
1:B:497:GLU:HG3	1:B:497:GLU:H	1.60	0.41
1:B:159:ASN:HA	1:B:160:PRO:HD2	1.88	0.41
1:A:497:GLU:HG3	1:A:497:GLU:H	1.67	0.41
1:B:307:LEU:HD12	1:B:312:PHE:CE2	2.55	0.40
1:B:295:ASP:OD2	1:B:297:ASP:HB3	2.21	0.40
1:A:242:ARG:HH12	6:A:774:GOL:H2	1.86	0.40
1:A:449:PRO:HG2	1:A:464:SER:CB	2.42	0.40
1:A:514:LEU:HA	1:B:509:ARG:HH12	1.87	0.40
1:A:86:THR:HG22	1:A:87:ASP:N	2.36	0.40
1:B:347:ARG:O	1:B:350:PHE:HB3	2.22	0.40
1:A:10:ASN:HB3	1:A:52:TRP:CZ3	2.56	0.40
1:A:348:LYS:HG3	1:A:348:LYS:H	1.73	0.40
1:A:259:GLU:HG2	1:A:262:LYS:HD2	2.04	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:528:LYS:NZ	5:A:603:SO4:O2[4_545]	2.18	0.02

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	526/574 (92%)	463 (88%)	50 (10%)	13 (2%)	7 24
1	B	526/574 (92%)	454 (86%)	59 (11%)	13 (2%)	7 24
All	All	1052/1148 (92%)	917 (87%)	109 (10%)	26 (2%)	7 24

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	105	LYS
1	A	379	ASP
1	B	105	LYS
1	B	106	ASN
1	B	252	CYS
1	B	486	GLN
1	A	117	GLY
1	A	485	ASN
1	A	507	SER
1	B	39	GLY
1	B	198	SER
1	B	485	ASN
1	A	256	ASN
1	A	486	GLN
1	B	93	LEU
1	B	533	THR
1	A	9	LYS
1	A	54	ASP
1	A	298	PHE
1	A	451	GLU
1	B	89	SER
1	B	347	ARG
1	B	384	ASN
1	A	342	ASN
1	B	507	SER

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Mol	Chain	Res	Type
1	A	281	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	454/494 (92%)	417 (92%)	37 (8%)	15	39
1	B	454/494 (92%)	416 (92%)	38 (8%)	14	37
All	All	908/988 (92%)	833 (92%)	75 (8%)	14	38

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ILE
1	A	16	MET
1	A	35	GLN
1	A	51	LYS
1	A	53	SER
1	A	72	SER
1	A	103	LYS
1	A	105	LYS
1	A	108	THR
1	A	110	LEU
1	A	127	VAL
1	A	139	VAL
1	A	182	ILE
1	A	188	ASN
1	A	195	PHE
1	A	249	LEU
1	A	270	GLN
1	A	271	GLU
1	A	323	LYS
1	A	343	SER
1	A	375	ASP
1	A	376	TRP

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Mol	Chain	Res	Type
1	A	377	VAL
1	A	378	ASP
1	A	428	LEU
1	A	429	PRO
1	A	443	GLU
1	A	452	ARG
1	A	466	SER
1	A	469	LYS
1	A	471	TRP
1	A	495	SER
1	A	497	GLU
1	A	506	GLU
1	A	518	GLN
1	A	523	THR
1	A	533	THR
1	B	4	ILE
1	B	16	MET
1	B	19	THR
1	B	40	ARG
1	B	49	LEU
1	B	50	THR
1	B	51	LYS
1	B	69	ILE
1	B	71	GLN
1	B	72	SER
1	B	87	ASP
1	B	99	ILE
1	B	105	LYS
1	B	108	THR
1	B	156	LEU
1	B	195	PHE
1	B	234	THR
1	B	235	SER
1	B	237	TYR
1	B	253	SER
1	B	256	ASN
1	B	257	GLU
1	B	274	LEU
1	B	286	LEU
1	B	287	SER
1	B	304	ASP
1	B	343	SER

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Mol	Chain	Res	Type
1	B	377	VAL
1	B	378	ASP
1	B	379	ASP
1	B	414	ASN
1	B	428	LEU
1	B	452	ARG
1	B	482	GLU
1	B	496	THR
1	B	497	GLU
1	B	506	GLU
1	B	517	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	ASN
1	A	119	GLN
1	A	126	HIS
1	A	176	GLN
1	A	188	ASN
1	A	270	GLN
1	A	275	ASN
1	A	351	GLN
1	A	397	ASN
1	A	517	GLN
1	A	518	GLN
1	B	83	ASN
1	B	159	ASN
1	B	172	GLN
1	B	176	GLN
1	B	188	ASN
1	B	256	ASN
1	B	270	GLN
1	B	275	ASN
1	B	341	ASN
1	B	397	ASN
1	B	414	ASN
1	B	485	ASN
1	B	517	GLN
1	B	518	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

2 carbohydrates 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	C	781	1,2	14,14,15	0.76	0	15,19,21	1.97	2 (13%)
2	NAG	C	782	2	14,14,15	0.78	0	15,19,21	1.36	1 (6%)

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	C	781	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	782	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	781	NAG	C4-C3-C2	2.50	115.11	111.23
2	C	782	NAG	C3-C4-C5	4.02	117.20	110.20
2	C	781	NAG	C2-N2-C7	6.03	130.79	123.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	781	NAG	2	0
2	C	782	NAG	1	0

5.6 Ligand geometry (i)

17 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	$\#\|Z\| > 2$
5	SO4	A	601	-	4,4,4	0.29	0	6,6,6	0.58	0
5	SO4	A	602	-	4,4,4	0.54	0	6,6,6	0.98	0
5	SO4	A	603	-	4,4,4	1.01	0	6,6,6	0.88	0
5	SO4	A	604	-	4,4,4	0.57	0	6,6,6	0.49	0
5	SO4	A	606	-	4,4,4	0.50	0	6,6,6	1.24	1 (16%)
4	NDG	A	678	1	14,14,15	0.82	1 (7%)	15,19,21	2.19	1 (6%)
6	GOL	A	774	-	5,5,5	0.34	0	5,5,5	0.28	0
6	GOL	A	777	-	5,5,5	0.41	0	5,5,5	0.97	0
3	NAG	A	791	1	14,14,15	0.66	0	15,19,21	1.44	3 (20%)
3	NAG	A	798	1	14,14,15	0.54	0	15,19,21	1.90	3 (20%)
6	GOL	A	999	-	5,5,5	0.30	0	5,5,5	0.58	0
5	SO4	B	601	-	4,4,4	0.18	0	6,6,6	0.18	0
5	SO4	B	602	-	4,4,4	0.47	0	6,6,6	0.74	0
6	GOL	B	774	-	5,5,5	0.34	0	5,5,5	0.40	0
6	GOL	B	777	-	5,5,5	0.35	0	5,5,5	0.20	0
3	NAG	B	781	-	14,14,15	0.53	0	15,19,21	1.49	3 (20%)
3	NAG	B	791	1	14,14,15	0.55	0	15,19,21	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
5	SO4	A	601	-	-	0/0/0/0	0/0/0/0
5	SO4	A	602	-	-	0/0/0/0	0/0/0/0
5	SO4	A	603	-	-	0/0/0/0	0/0/0/0
5	SO4	A	604	-	-	0/0/0/0	0/0/0/0
5	SO4	A	606	-	-	0/0/0/0	0/0/0/0
4	NDG	A	678	1	1/1/5/7	0/6/23/26	0/1/1/1
6	GOL	A	774	-	-	0/4/4/4	0/0/0/0
6	GOL	A	777	-	-	0/4/4/4	0/0/0/0
3	NAG	A	791	1	-	0/6/23/26	0/1/1/1
3	NAG	A	798	1	-	0/6/23/26	0/1/1/1
6	GOL	A	999	-	-	0/4/4/4	0/0/0/0
5	SO4	B	601	-	-	0/0/0/0	0/0/0/0
5	SO4	B	602	-	-	0/0/0/0	0/0/0/0
6	GOL	B	774	-	-	0/4/4/4	0/0/0/0
6	GOL	B	777	-	-	0/4/4/4	0/0/0/0
3	NAG	B	781	-	-	0/6/23/26	0/1/1/1
3	NAG	B	791	1	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	678	NDG	C1-C2	2.42	1.55	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	606	SO4	O2-S-O1	-2.96	100.12	109.50
3	B	781	NAG	C3-C4-C5	-2.81	105.30	110.20
3	B	781	NAG	O7-C7-C8	-2.42	117.62	122.06
3	A	791	NAG	O7-C7-C8	-2.10	118.21	122.06
3	A	798	NAG	O5-C5-C6	2.70	113.19	107.35
3	B	781	NAG	C2-N2-C7	2.70	126.51	123.04
3	A	791	NAG	O4-C4-C5	2.77	116.57	109.24
3	A	791	NAG	C1-O5-C5	3.21	116.32	112.25
3	A	798	NAG	C3-C4-C5	3.71	116.67	110.20
3	A	798	NAG	C4-C3-C2	4.87	118.80	111.23
4	A	678	NDG	C1-O-C5	7.55	121.82	112.25

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	678	NDG	C1

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	602	SO4	1	0
5	A	603	SO4	1	1
5	A	604	SO4	1	0
5	A	606	SO4	3	0
6	A	774	GOL	1	0
6	B	774	GOL	1	0
3	B	781	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, 95^{th} 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	530/574 (92%)	-0.02	21 (3%)	42	30	31, 50, 74, 86	0
1	B	530/574 (92%)	0.06	16 (3%)	54	41	39, 59, 82, 95	0
All	All	1060/1148 (92%)	0.02	37 (3%)	48	35	31, 56, 79, 95	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	377	VAL	4.6
1	B	378	ASP	4.2
1	B	53	SER	4.0
1	A	258	THR	3.8
1	A	282	TYR	3.7
1	A	53	SER	3.7
1	A	259	GLU	3.6
1	B	377	VAL	3.5
1	B	380	GLN	3.5
1	B	379	ASP	3.4
1	A	266	ASN	3.1
1	A	281	PRO	2.8
1	B	348	LYS	2.6
1	A	359	PRO	2.6
1	B	507	SER	2.5
1	A	252	CYS	2.5
1	A	251	GLY	2.5
1	B	376	TRP	2.5
1	A	244	LEU	2.5
1	A	260	ILE	2.5
1	B	244	LEU	2.5
1	A	52	TRP	2.4
1	A	346	THR	2.4
1	B	16	MET	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	340	ASP	2.4
1	A	12	LYS	2.3
1	A	257	GLU	2.3
1	B	237	TYR	2.3
1	A	237	TYR	2.2
1	A	54	ASP	2.2
1	B	256	ASN	2.2
1	B	375	ASP	2.1
1	A	256	ASN	2.1
1	B	19	THR	2.0
1	A	378	ASP	2.0
1	A	278	PHE	2.0
1	B	282	TYR	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)

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^{th} 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^2)	Q<0.9
2	NAG	C	781	14/15	0.90	0.17	-0.89	54,56,57,61	0
2	NAG	C	782	14/15	0.86	0.33	-	66,68,70,70	0

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^{th} 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^2)	Q<0.9
6	GOL	B	774	6/6	0.77	0.28	4.36	58,60,61,61	0
6	GOL	A	777	6/6	0.89	0.28	2.71	45,48,53,54	0
6	GOL	A	774	6/6	0.83	0.25	2.31	54,62,62,62	0
6	GOL	A	999	6/6	0.86	0.24	2.06	61,62,62,63	0
4	NDG	A	678	14/15	0.90	0.17	0.69	64,71,72,72	0
5	SO4	A	603	5/5	0.99	0.17	0.20	19,21,24,27	0
5	SO4	A	604	5/5	0.98	0.17	0.15	33,34,35,36	0
5	SO4	A	606	5/5	0.99	0.12	-1.23	33,33,34,37	0
5	SO4	A	602	5/5	0.99	0.13	-1.30	34,34,37,39	0
5	SO4	B	602	5/5	0.98	0.14	-2.05	41,42,43,45	0
3	NAG	B	781	14/15	0.85	0.16	-2.89	69,71,74,76	0
3	NAG	B	791	14/15	0.83	0.21	-	62,64,67,68	0
6	GOL	B	777	6/6	0.62	0.51	-	84,86,87,87	0
3	NAG	A	798	14/15	0.73	0.37	-	71,74,76,77	0
5	SO4	A	601	5/5	0.99	0.12	-	50,50,51,51	0
3	NAG	A	791	14/15	0.85	0.23	-	54,55,56,56	0
5	SO4	B	601	5/5	0.98	0.12	-	44,44,45,45	0

6.5 Other polymers

There are no such residues in this entry.