



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 22, 2019 – 01:49 PM EST

PDB ID : 6E7R  
Title : Heterodimer of the GluN1b-GluN2B NMDA receptor amino-terminal domains bound to allosteric inhibitor 93-4  
Authors : Regan, M.C.; Furukawa, H.  
Deposited on : 2018-07-27  
Resolution : 2.10 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

<https://www.wwpdb.org/validation/2017/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 : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : rb-20031633  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20031633

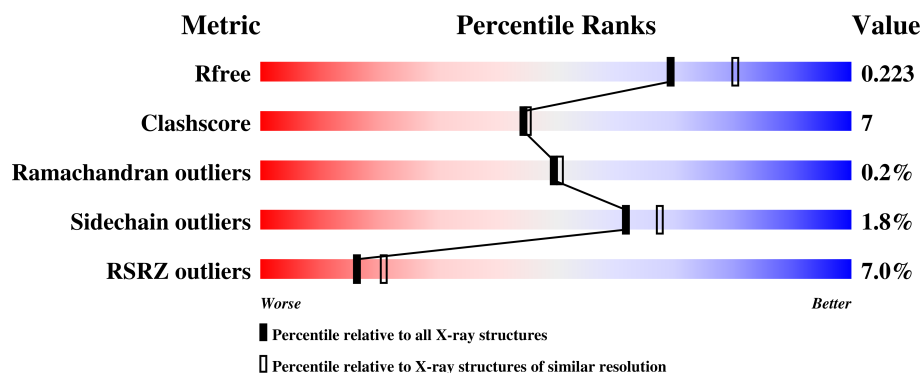
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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))
$R_{free}$	111664	4608 (2.10-2.10)
Clashscore	122126	5109 (2.10-2.10)
Ramachandran outliers	120053	5059 (2.10-2.10)
Sidechain outliers	120020	5060 (2.10-2.10)
RSRZ outliers	108989	4497 (2.10-2.10)

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	385	<div> <div>2%</div> <div>81% 12% 7%</div> </div>
1	C	385	<div> <div>5%</div> <div>78% 14% 7%</div> </div>
2	B	363	<div> <div>8%</div> <div>87% 12%</div> </div>
2	D	363	<div> <div>12%</div> <div>87% 11%</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	507	-	-	-	X
3	NAG	B	502	-	-	-	X
3	NAG	C	502	-	-	-	X
3	NAG	C	503	-	-	-	X
3	NAG	D	401	-	-	-	X
7	CL	A	510	-	-	X	-
7	CL	B	504	-	-	X	-
7	CL	B	507	-	-	X	-

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 11522 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 Glutamate receptor ionotropic, NMDA 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	358	Total	C	N	O	S	0	0	0
			2756	1759	479	508	10			
1	C	357	Total	C	N	O	S	0	0	0
			2714	1731	467	505	11			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	61	GLN	ASN	engineered mutation	UNP A0A1L8F5J9
A	371	GLN	ASN	engineered mutation	UNP A0A1L8F5J9
C	61	GLN	ASN	engineered mutation	UNP A0A1L8F5J9
C	371	GLN	ASN	engineered mutation	UNP A0A1L8F5J9

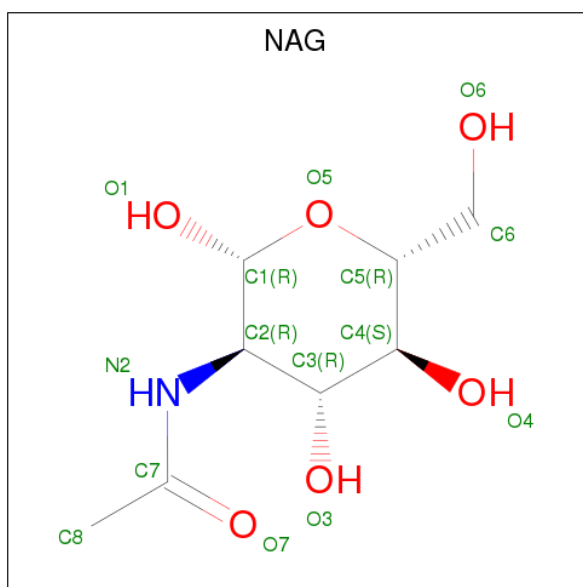
- Molecule 2 is a protein called Glutamate receptor ionotropic, NMDA 2B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	363	Total	C	N	O	S	0	0	0
			2775	1787	439	534	15			
2	D	358	Total	C	N	O	S	0	0	0
			2698	1737	428	517	16			

There are 2 discrepancies between the modelled and reference sequences:

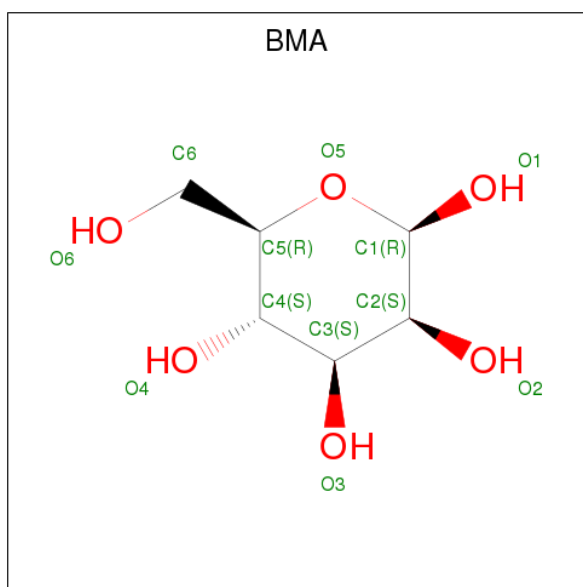
Chain	Residue	Modelled	Actual	Comment	Reference
B	348	ASP	ASN	engineered mutation	UNP Q00960
D	348	ASP	ASN	engineered mutation	UNP Q00960

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



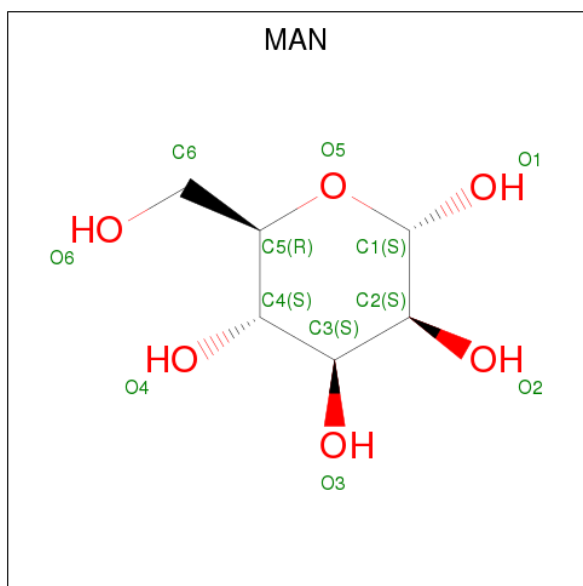
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			13	7	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is BETA-D-MANNOSE (three-letter code: BMA) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			11	6	5		

- Molecule 5 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula:  $C_6H_{12}O_6$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			11	6	5		
5	A	1	Total	C	O	0	0
			11	6	5		

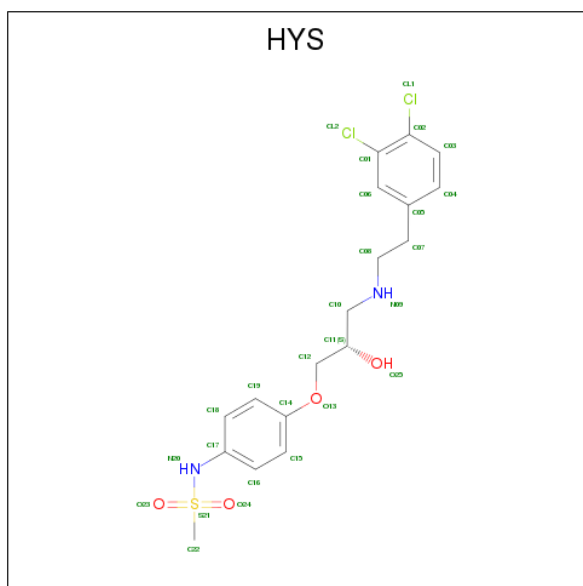
- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Na	0	0
			1	1		
6	C	1	Total	Na	0	0
			1	1		

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	4	Total	Cl	0	0
			4	4		
7	A	2	Total	Cl	0	0
			2	2		
7	D	4	Total	Cl	0	0
			4	4		
7	C	2	Total	Cl	0	0
			2	2		

- Molecule 8 is N-{4-[(2S)-3-{[2-(3,4-dichlorophenyl)ethyl]amino}-2-hydroxypropoxy]phenyl}methanesulfonamide (three-letter code: HYS) (formula: C<sub>18</sub>H<sub>22</sub>Cl<sub>2</sub>N<sub>2</sub>O<sub>4</sub>S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
8	B	1	Total	C	Cl	N	O	S	0	0
			27	18	2	2	4	1		
8	D	1	Total	C	Cl	N	O	S	0	0
			27	18	2	2	4	1		

- Molecule 9 is water.

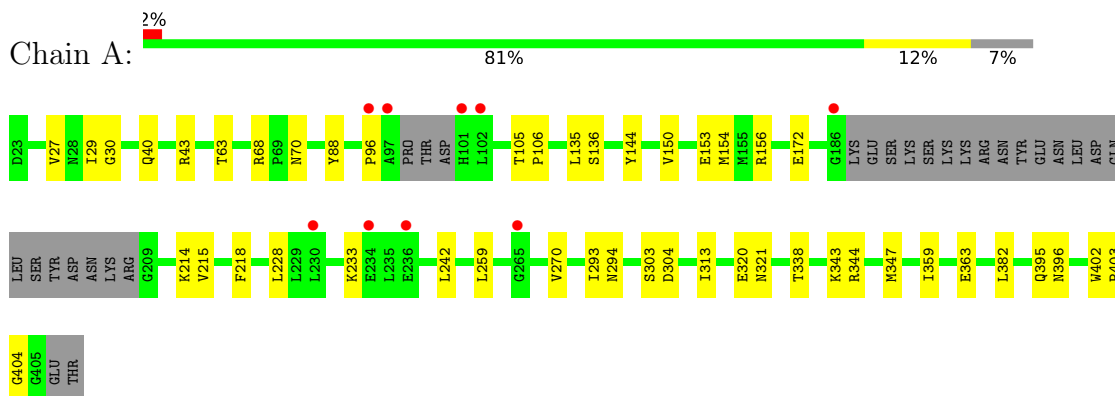
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	136	Total 136	O 136	0	0
9	B	80	Total 80	O 80	0	0
9	C	75	Total 75	O 75	0	0
9	D	48	Total 48	O 48	0	0



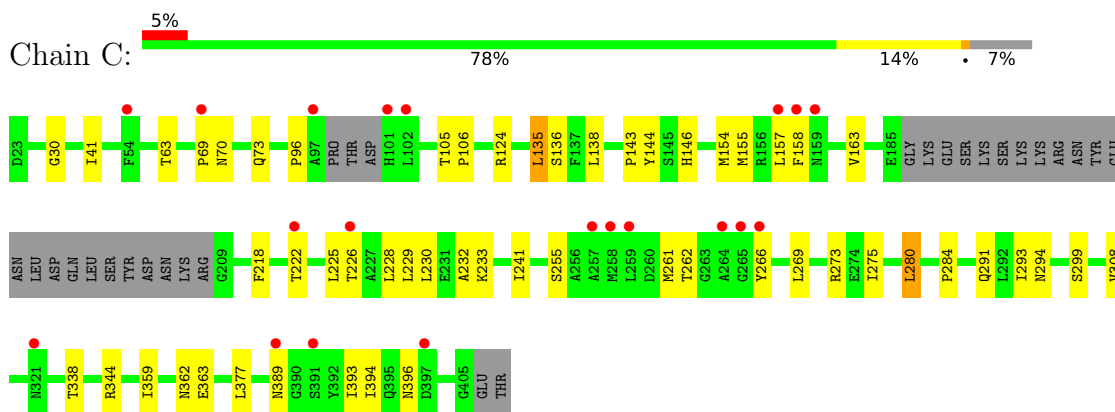
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

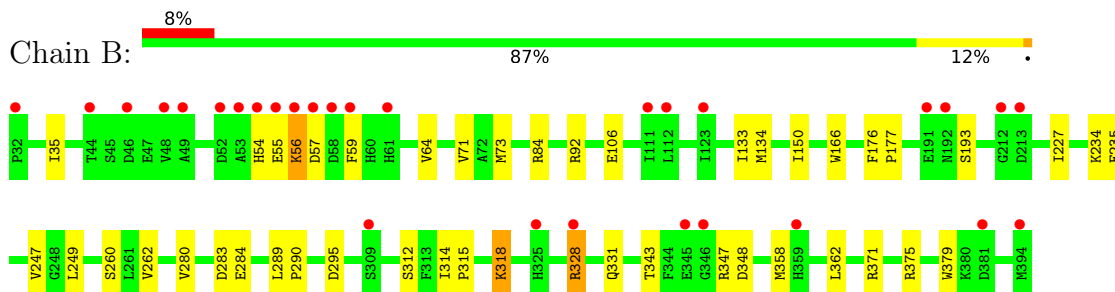
- Molecule 1: Glutamate receptor ionotropic, NMDA 1



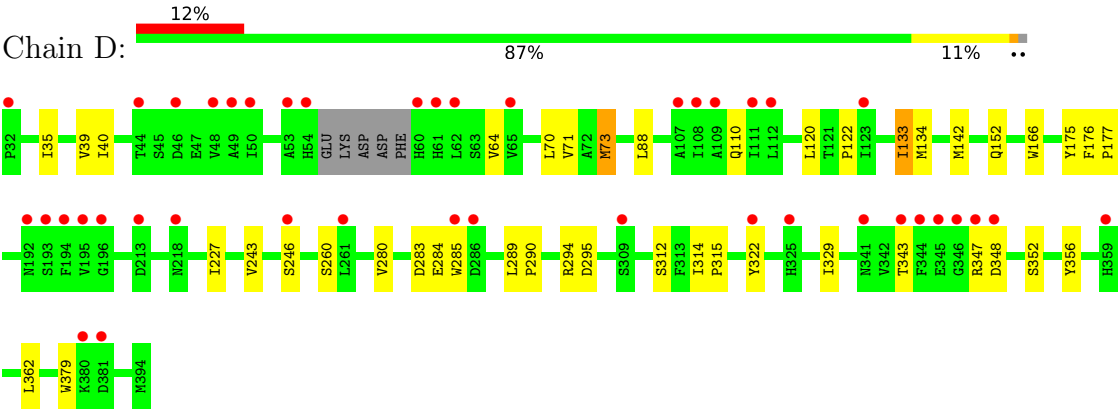
- Molecule 1: Glutamate receptor ionotropic, NMDA 1



- Molecule 2: Glutamate receptor ionotropic, NMDA 2B



- Molecule 2: Glutamate receptor ionotropic, NMDA 2B



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	267.95Å 59.90Å 145.29Å 90.00° 116.69° 90.00°	Depositor
Resolution (Å)	25.00 – 2.10 35.02 – 2.10	Depositor EDS
% Data completeness (in resolution range)	83.2 (25.00-2.10) 83.3 (35.02-2.10)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.11 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.189 , 0.218 0.197 , 0.223	Depositor DCC
$R_{free}$ test set	5146 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.0	Xtriage
Anisotropy	0.007	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 54.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	11522	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.59% 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, 0.333 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: BMA, NAG, CL, NA, HYS, MAN

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	0.37	0/2814	0.36	0/3826
1	C	0.32	0/2770	0.35	0/3772
2	B	0.35	0/2837	0.36	0/3873
2	D	0.31	0/2760	0.35	0/3773
All	All	0.34	0/11181	0.35	0/15244

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	404	GLY	Peptide

### 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	2756	0	2715	36	0
1	C	2714	0	2655	42	0
2	B	2775	0	2608	35	0
2	D	2698	0	2526	36	0
3	A	56	0	50	0	0
3	B	28	0	26	0	0
3	C	41	0	34	5	0
3	D	14	0	13	0	0
4	A	11	0	8	0	0
5	A	22	0	20	0	0
6	A	1	0	0	0	0
6	C	1	0	0	0	0
7	A	2	0	0	2	0
7	B	4	0	0	5	0
7	C	2	0	0	0	0
7	D	4	0	0	2	0
8	B	27	0	0	3	0
8	D	27	0	0	2	0
9	A	136	0	0	4	0
9	B	80	0	0	5	0
9	C	75	0	0	3	0
9	D	48	0	0	2	0
All	All	11522	0	10655	156	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 7.

All (156) 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:501:NAG:C8	3:C:501:NAG:O7	1.87	1.21
3:C:501:NAG:N2	3:C:501:NAG:O7	1.76	1.19
7:A:510:CL:CL	9:A:601:HOH:O	2.04	1.10
2:B:235:GLU:OE1	2:B:235:GLU:OE2	1.70	1.07
1:C:157:LEU:HD23	1:C:158:PHE:CE2	2.03	0.93
7:B:504:CL:CL	9:B:641:HOH:O	2.23	0.92
2:D:133:ILE:HG23	7:D:403:CL:CL	2.14	0.85
3:C:501:NAG:N2	3:C:501:NAG:C8	2.40	0.84
1:A:29:ILE:HD11	1:A:313:ILE:CD1	2.09	0.81
2:B:235:GLU:CG	2:B:235:GLU:OE2	2.32	0.78
2:B:318:LYS:HD2	2:B:331:GLN:OE1	1.84	0.78
2:B:235:GLU:OE1	2:B:235:GLU:CG	2.33	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:312:SER:O	9:B:601:HOH:O	2.02	0.76
1:C:157:LEU:HD23	1:C:158:PHE:CD2	2.20	0.76
2:B:375:ARG:NH1	9:B:603:HOH:O	2.17	0.76
2:D:120:LEU:C	2:D:142:MET:CE	2.56	0.74
1:C:222:THR:HB	1:C:225:LEU:HD21	1.72	0.71
1:A:218:PHE:HB3	1:A:228:LEU:HD13	1.71	0.71
2:B:193:SER:O	9:B:602:HOH:O	2.09	0.71
1:A:218:PHE:HB3	1:A:228:LEU:CD1	2.22	0.69
2:D:343:THR:HG22	2:D:348:ASP:HA	1.75	0.69
1:A:153:GLU:OE2	1:A:156:ARG:NH1	2.26	0.69
2:B:343:THR:HG22	2:B:348:ASP:HA	1.74	0.69
1:C:135:LEU:C	1:C:135:LEU:HD23	2.13	0.68
7:B:507:CL:CL	9:B:633:HOH:O	2.48	0.68
1:A:233:LYS:HE3	1:A:259:LEU:O	1.95	0.67
2:B:71:VAL:HG13	2:B:84:ARG:NH2	2.08	0.67
1:C:232:ALA:O	9:C:601:HOH:O	2.14	0.66
2:D:312:SER:O	9:D:501:HOH:O	2.12	0.66
1:A:68:ARG:HD2	9:A:712:HOH:O	1.95	0.65
1:A:29:ILE:HD11	1:A:313:ILE:HD11	1.79	0.65
2:B:328:ARG:O	9:D:501:HOH:O	2.15	0.64
1:C:41:ILE:HD13	1:C:299:SER:OG	1.98	0.64
2:D:283:ASP:O	2:D:285:TRP:CD1	2.51	0.64
2:D:289:LEU:HB3	2:D:290:PRO:HD3	1.80	0.64
1:C:229:LEU:HD12	1:C:255:SER:HB2	1.80	0.62
2:D:120:LEU:C	2:D:142:MET:HE2	2.19	0.62
1:C:69:PRO:HD2	1:C:73:GLN:OE1	1.99	0.62
1:C:262:THR:HB	1:C:284:PRO:HB3	1.81	0.62
1:A:150:VAL:O	1:A:154:MET:HG3	2.00	0.61
1:C:157:LEU:CD2	1:C:158:PHE:CE2	2.82	0.60
2:D:166:TRP:HB3	2:D:227:ILE:HG13	1.84	0.60
1:C:135:LEU:HD23	1:C:136:SER:N	2.17	0.60
2:B:133:ILE:HG23	7:B:504:CL:CL	2.39	0.60
2:B:55:GLU:C	2:B:57:ASP:H	2.05	0.60
1:C:218:PHE:HB3	1:C:228:LEU:CD1	2.33	0.59
2:D:40:ILE:HG12	2:D:71:VAL:CG2	2.34	0.57
2:D:176:PHE:CD1	2:D:177:PRO:HD2	2.39	0.57
1:A:395:GLN:NE2	7:A:510:CL:CL	2.74	0.57
1:C:273:ARG:HD3	9:C:640:HOH:O	2.04	0.57
1:C:218:PHE:HB3	1:C:228:LEU:HD13	1.88	0.56
1:C:229:LEU:CD1	1:C:255:SER:HB2	2.36	0.55
1:C:228:LEU:HD23	1:C:228:LEU:C	2.27	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:233:LYS:O	9:C:602:HOH:O	2.18	0.55
2:D:314:ILE:HB	2:D:315:PRO:HD2	1.88	0.55
2:B:362:LEU:HB2	2:B:379:TRP:HB3	1.88	0.55
1:A:68:ARG:CD	9:A:712:HOH:O	2.54	0.55
1:A:136:SER:HB3	9:A:665:HOH:O	2.06	0.55
2:D:39:VAL:HB	2:D:70:LEU:HD23	1.88	0.55
8:B:503:HYS:O25	8:B:503:HYS:C08	2.55	0.54
1:A:105:THR:N	1:A:106:PRO:CD	2.71	0.54
2:D:40:ILE:HG21	2:D:73:MET:HE2	1.90	0.54
1:C:396:ASN:C	1:C:396:ASN:OD1	2.46	0.53
2:B:35:ILE:HG23	2:B:64:VAL:HG21	1.91	0.53
1:C:261:MET:HA	1:C:266:TYR:CE2	2.44	0.52
1:A:135:LEU:HD12	1:A:135:LEU:C	2.30	0.52
2:D:283:ASP:O	2:D:285:TRP:HD1	1.93	0.52
2:B:289:LEU:HB3	2:B:290:PRO:HD3	1.90	0.52
2:B:176:PHE:CD1	2:B:177:PRO:HD2	2.45	0.52
2:D:243:VAL:O	2:D:246:SER:HB2	2.10	0.51
1:C:70:ASN:C	1:C:70:ASN:OD1	2.47	0.51
2:D:35:ILE:HG23	2:D:64:VAL:HG11	1.92	0.51
1:C:30:GLY:HA2	1:C:63:THR:O	2.10	0.51
2:D:329:ILE:HG12	2:D:329:ILE:O	2.10	0.51
1:A:40:GLN:OE1	1:A:43:ARG:NH1	2.43	0.51
2:B:133:ILE:HD12	2:B:150:ILE:HG12	1.92	0.51
2:D:295:ASP:OD2	2:D:347:ARG:NH2	2.43	0.51
2:B:57:ASP:C	2:B:59:PHE:H	2.13	0.51
2:D:120:LEU:O	2:D:142:MET:CE	2.58	0.51
2:B:234:LYS:HG3	2:B:262:VAL:O	2.11	0.51
2:D:73:MET:HG2	7:D:404:CL:CL	2.47	0.51
2:D:71:VAL:HG11	2:D:88:LEU:HD21	1.93	0.50
2:D:40:ILE:HA	2:D:71:VAL:HG23	1.94	0.50
1:C:293:ILE:O	1:C:294:ASN:HB2	2.11	0.50
1:A:304:ASP:HB3	1:A:359:ILE:CD1	2.42	0.50
2:D:284:GLU:O	2:D:284:GLU:HG3	2.13	0.49
1:C:105:THR:N	1:C:106:PRO:CD	2.75	0.49
2:D:314:ILE:HB	2:D:315:PRO:CD	2.42	0.49
1:A:242:LEU:HB3	1:A:270:VAL:HG12	1.94	0.49
1:C:389:ASN:C	1:C:389:ASN:OD1	2.50	0.49
2:D:362:LEU:HB2	2:D:379:TRP:HB3	1.93	0.48
1:C:308:VAL:HG21	1:C:359:ILE:HG21	1.95	0.48
2:B:54:HIS:CG	2:B:54:HIS:O	2.66	0.48
1:C:138:LEU:N	1:C:138:LEU:HD12	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:71:VAL:CG1	2:B:84:ARG:NH2	2.76	0.48
1:C:154:MET:HG2	1:C:393:ILE:HD11	1.95	0.48
2:D:260:SER:HA	2:D:280:VAL:O	2.13	0.48
1:C:229:LEU:HD12	1:C:255:SER:CB	2.43	0.47
2:D:40:ILE:HG12	2:D:71:VAL:HG21	1.95	0.47
1:A:30:GLY:HA2	1:A:63:THR:O	2.14	0.47
1:C:241:ILE:HA	1:C:269:LEU:O	2.15	0.47
1:C:363:GLU:CD	1:C:363:GLU:H	2.17	0.47
1:A:135:LEU:HD23	8:B:503:HYS:C14	2.44	0.47
2:B:260:SER:HA	2:B:280:VAL:O	2.15	0.47
2:D:110:GLN:CD	8:D:402:HYS:O25	2.52	0.47
2:D:122:PRO:HD3	2:D:142:MET:HE1	1.96	0.46
1:A:363:GLU:H	1:A:363:GLU:CD	2.17	0.46
1:A:68:ARG:NH1	1:A:68:ARG:HG2	2.30	0.46
1:C:124:ARG:O	1:C:143:PRO:HA	2.15	0.46
2:D:133:ILE:HB	2:D:356:TYR:OH	2.16	0.45
1:C:155:MET:HE1	1:C:163:VAL:HG21	1.98	0.45
1:A:293:ILE:O	1:A:294:ASN:HB2	2.16	0.45
1:A:214:LYS:HG3	1:A:215:VAL:N	2.32	0.45
3:C:501:NAG:O7	3:C:501:NAG:C2	2.61	0.45
1:A:338:THR:O	1:A:338:THR:HG22	2.17	0.45
2:D:35:ILE:HG23	2:D:64:VAL:CG1	2.47	0.44
1:C:73:GLN:HE21	2:D:322:TYR:CB	2.31	0.44
2:D:175:TYR:HB2	8:D:402:HYS:C22	2.47	0.44
1:A:29:ILE:CD1	1:A:313:ILE:HD11	2.47	0.44
2:B:284:GLU:HG2	2:B:284:GLU:O	2.18	0.44
2:B:55:GLU:C	2:B:57:ASP:N	2.69	0.44
1:C:394:ILE:HD11	3:C:502:NAG:H61	2.00	0.44
2:B:295:ASP:OD2	2:B:347:ARG:NH2	2.43	0.44
2:D:289:LEU:N	2:D:290:PRO:CD	2.81	0.44
1:A:304:ASP:HB3	1:A:359:ILE:HD11	2.00	0.44
2:B:247:VAL:HG23	2:B:249:LEU:HG	2.00	0.44
2:B:289:LEU:N	2:B:290:PRO:CD	2.80	0.44
1:A:70:ASN:OD1	1:A:70:ASN:C	2.56	0.43
1:C:154:MET:HG2	1:C:393:ILE:CD1	2.48	0.43
1:A:343:LYS:O	1:A:347:MET:HG2	2.18	0.43
2:D:39:VAL:HB	2:D:70:LEU:CD2	2.48	0.43
2:B:235:GLU:HB2	7:B:507:CL:CL	2.56	0.43
1:C:344:ARG:NH1	1:C:344:ARG:HG3	2.34	0.42
1:C:280:LEU:HA	1:C:280:LEU:HD23	1.84	0.42
2:B:35:ILE:HG23	2:B:64:VAL:CG2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:144:TYR:CE2	1:C:273:ARG:HD2	2.55	0.42
2:B:56:LYS:O	2:B:59:PHE:CB	2.68	0.42
2:B:166:TRP:HB3	2:B:227:ILE:HG13	2.01	0.42
2:D:120:LEU:CA	2:D:142:MET:HE2	2.49	0.42
1:C:275:ILE:O	1:C:280:LEU:HG	2.20	0.42
1:C:338:THR:O	1:C:338:THR:HG22	2.20	0.41
1:A:27:VAL:HG13	1:A:88:TYR:CD1	2.56	0.41
2:B:314:ILE:HB	2:B:315:PRO:CD	2.50	0.41
2:B:106:GLU:OE1	7:B:507:CL:CL	2.75	0.41
1:A:135:LEU:HD23	8:B:503:HYS:C19	2.51	0.41
1:A:320:GLU:O	1:A:321:ASN:HB2	2.20	0.41
1:A:402:TRP:HB3	1:A:403:PRO:HD2	2.03	0.41
2:B:283:ASP:O	2:B:284:GLU:C	2.59	0.41
1:A:344:ARG:NH1	1:A:344:ARG:HG3	2.36	0.41
1:A:68:ARG:HG2	1:A:68:ARG:HH11	1.85	0.41
1:A:382:LEU:HD23	1:A:382:LEU:HA	1.96	0.40
1:A:396:ASN:C	1:A:396:ASN:OD1	2.59	0.40
1:C:362:ASN:C	1:C:362:ASN:OD1	2.60	0.40
1:A:144:TYR:HB2	1:A:172:GLU:OE2	2.22	0.40
2:B:314:ILE:HB	2:B:315:PRO:HD2	2.04	0.40
1:C:154:MET:CE	1:C:158:PHE:HE2	2.35	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	352/385 (91%)	342 (97%)	9 (3%)	1 (0%)	43	43
1	C	351/385 (91%)	340 (97%)	10 (3%)	1 (0%)	43	43
2	B	361/363 (99%)	348 (96%)	12 (3%)	1 (0%)	43	43
2	D	354/363 (98%)	342 (97%)	12 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1418/1496 (95%)	1372 (97%)	43 (3%)	3 (0%)	49	51

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	56	LYS
1	C	96	PRO
1	A	96	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	288/331 (87%)	287 (100%)	1 (0%)	93	96
1	C	283/331 (86%)	276 (98%)	7 (2%)	50	55
2	B	288/326 (88%)	281 (98%)	7 (2%)	52	56
2	D	280/326 (86%)	274 (98%)	6 (2%)	56	62
All	All	1139/1314 (87%)	1118 (98%)	21 (2%)	62	67

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	303	SER
2	B	73	MET
2	B	92	ARG
2	B	134	MET
2	B	318	LYS
2	B	328	ARG
2	B	358	MET
2	B	371	ARG
1	C	135	LEU
1	C	146	HIS
1	C	226	THR
1	C	230	LEU

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Mol	Chain	Res	Type
1	C	280	LEU
1	C	291	GLN
1	C	377	LEU
2	D	73	MET
2	D	133	ILE
2	D	134	MET
2	D	152	GLN
2	D	294	ARG
2	D	352	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	152	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 29 ligands modelled in this entry, 14 are monoatomic - leaving 15 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	501	1	14,14,15	0.34	0	17,19,21	0.64	0
3	NAG	A	502	1,3	14,14,15	0.22	0	17,19,21	0.70	0
3	NAG	A	503	3,4	14,14,15	0.39	0	17,19,21	0.86	1 (5%)
4	BMA	A	504	3,5	11,11,12	0.25	0	15,15,17	0.65	0
5	MAN	A	505	4	11,11,12	0.28	0	15,15,17	0.60	0
5	MAN	A	506	4	11,11,12	0.21	0	15,15,17	0.66	0
3	NAG	A	507	1	14,14,15	0.37	0	17,19,21	0.74	0
3	NAG	B	501	2	14,14,15	0.39	0	17,19,21	0.78	0
3	NAG	B	502	2	14,14,15	0.58	0	17,19,21	0.95	1 (5%)
8	HYS	B	503	-	28,28,28	1.56	2 (7%)	36,38,38	2.16	2 (5%)
3	NAG	C	501	1	11,11,15	0.39	0	13,15,21	0.69	0
3	NAG	C	502	1,3	14,14,15	0.52	0	17,19,21	0.97	1 (5%)
3	NAG	C	503	3	14,14,15	0.31	0	17,19,21	0.71	0
3	NAG	D	401	2	14,14,15	0.30	0	17,19,21	0.67	0
8	HYS	D	402	-	28,28,28	1.56	2 (7%)	36,38,38	2.14	3 (8%)

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	501	1	-	0/6/23/26	0/1/1/1
3	NAG	A	502	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	503	3,4	-	0/6/23/26	0/1/1/1
4	BMA	A	504	3,5	-	0/2/19/22	0/1/1/1
5	MAN	A	505	4	-	0/2/19/22	0/1/1/1
5	MAN	A	506	4	-	0/2/19/22	0/1/1/1
3	NAG	A	507	1	-	0/6/23/26	0/1/1/1
3	NAG	B	501	2	-	0/6/23/26	0/1/1/1
3	NAG	B	502	2	-	0/6/23/26	0/1/1/1
8	HYS	B	503	-	-	0/17/17/17	0/2/2/2
3	NAG	C	501	1	-	0/2/19/26	0/1/1/1
3	NAG	C	502	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	503	3	-	0/6/23/26	0/1/1/1
3	NAG	D	401	2	-	0/6/23/26	0/1/1/1
8	HYS	D	402	-	-	0/17/17/17	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	402	HYS	C17-N20	2.24	1.46	1.43
8	B	503	HYS	C17-N20	2.57	1.47	1.43
8	B	503	HYS	S21-N20	5.88	1.71	1.63
8	D	402	HYS	S21-N20	6.01	1.71	1.63

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	503	HYS	O23-S21-O24	-11.44	101.67	118.79
8	D	402	HYS	O23-S21-O24	-11.37	101.77	118.79
3	A	503	NAG	O5-C1-C2	-2.42	108.18	111.52
3	B	502	NAG	C4-C3-C2	2.07	114.05	111.02
8	D	402	HYS	O23-S21-N20	2.11	111.45	107.12
3	C	502	NAG	C1-O5-C5	2.86	116.13	112.19
8	D	402	HYS	C22-S21-N20	2.88	110.08	106.66
8	B	503	HYS	C22-S21-N20	3.01	110.23	106.66

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	503	HYS	3	0
3	C	501	NAG	4	0
3	C	502	NAG	1	0
8	D	402	HYS	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	358/385 (92%)	-0.08	9 (2%) 57 63	11, 27, 60, 95	0
1	C	357/385 (92%)	0.20	20 (5%) 24 30	21, 40, 78, 102	0
2	B	363/363 (100%)	0.32	29 (7%) 12 16	11, 38, 78, 109	0
2	D	358/363 (98%)	0.49	42 (11%) 4 6	21, 42, 79, 125	0
All	All	1436/1496 (95%)	0.23	100 (6%) 16 21	11, 37, 75, 125	0

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	344	PHE	7.0
2	D	194	PHE	6.8
2	B	55	GLU	6.6
2	B	58	ASP	6.3
2	B	48	VAL	5.4
2	D	346	GLY	5.3
2	D	48	VAL	5.1
2	D	195	VAL	4.8
2	D	343	THR	4.8
2	B	44	THR	4.8
2	D	53	ALA	4.8
1	C	101	HIS	4.5
2	D	192	ASN	4.4
1	C	265	GLY	4.4
2	D	49	ALA	4.2
2	D	62	LEU	4.1
1	C	264	ALA	4.1
2	B	52	ASP	4.0
1	A	102	LEU	4.0
2	D	347	ARG	3.9
2	D	44	THR	3.9

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Mol	Chain	Res	Type	RSRZ
2	B	394	MET	3.8
2	D	348	ASP	3.7
2	D	46	ASP	3.7
2	B	49	ALA	3.7
1	C	158	PHE	3.7
1	A	97	ALA	3.7
2	D	381	ASP	3.6
2	D	32	PRO	3.4
1	A	234	GLU	3.4
1	C	321	ASN	3.3
1	A	186	GLY	3.2
1	C	397	ASP	3.1
2	D	61	HIS	3.1
2	D	325	HIS	3.1
2	B	54	HIS	3.1
2	B	61	HIS	3.1
2	D	359	HIS	3.1
2	D	380	LYS	3.1
2	D	345	GLU	3.1
1	C	258	MET	3.1
2	B	346	GLY	3.0
1	C	102	LEU	3.0
2	B	57	ASP	3.0
1	C	157	LEU	2.9
1	C	257	ALA	2.9
1	C	266	TYR	2.9
2	D	193	SER	2.9
1	C	97	ALA	2.9
1	A	230	LEU	2.9
2	D	60	HIS	2.8
2	D	65	VAL	2.8
1	C	54	PHE	2.8
2	B	59	PHE	2.8
2	D	111	ILE	2.8
1	A	101	HIS	2.8
2	D	123	ILE	2.7
1	A	96	PRO	2.7
2	B	213	ASP	2.6
2	B	212	GLY	2.6
2	B	192	ASN	2.6
1	C	69	PRO	2.5
2	D	109	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
2	D	108	ILE	2.5
2	B	381	ASP	2.5
1	A	236	GLU	2.5
2	B	46	ASP	2.4
2	D	50	ILE	2.4
2	B	56	LYS	2.4
2	B	53	ALA	2.4
2	D	246	SER	2.3
1	C	159	ASN	2.3
1	C	259	LEU	2.3
2	D	112	LEU	2.3
1	C	226	THR	2.3
2	B	325	HIS	2.3
2	D	286	ASP	2.3
2	D	341	ASN	2.3
2	B	359	HIS	2.2
2	B	111	ILE	2.2
2	B	191	GLU	2.2
2	B	345	GLU	2.2
1	C	222	THR	2.2
2	B	328	ARG	2.2
2	D	218	ASN	2.2
2	D	107	ALA	2.2
2	D	322	TYR	2.2
1	C	389	ASN	2.2
2	D	309	SER	2.1
1	C	391	SER	2.1
2	D	285	TRP	2.1
2	D	54	HIS	2.1
2	B	32	PRO	2.1
2	D	196	GLY	2.1
2	B	112	LEU	2.1
2	B	309	SER	2.1
2	D	261	LEU	2.1
1	A	265	GLY	2.1
2	D	213	ASP	2.0
2	B	123	ILE	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 ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	B-factors(Å <sup>2</sup> )	Q<0.9
3	NAG	A	507	14/15	0.47	0.59	86,104,127,140	0
3	NAG	B	502	14/15	0.50	0.55	95,113,118,123	0
3	NAG	C	503	14/15	0.62	0.72	113,143,161,182	0
3	NAG	B	501	14/15	0.64	0.34	69,86,92,95	0
3	NAG	C	502	14/15	0.68	0.48	86,111,128,141	0
3	NAG	D	401	14/15	0.70	0.48	95,102,112,115	0
7	CL	D	404	1/1	0.74	0.26	77,77,77,77	0
7	CL	D	406	1/1	0.75	0.12	75,75,75,75	0
7	CL	C	505	1/1	0.78	0.21	71,71,71,71	0
7	CL	B	506	1/1	0.80	0.14	53,53,53,53	0
5	MAN	A	506	11/12	0.80	0.27	103,108,114,125	0
4	BMA	A	504	11/12	0.89	0.17	57,67,76,97	0
7	CL	B	505	1/1	0.90	0.11	68,68,68,68	0
7	CL	D	405	1/1	0.90	0.13	71,71,71,71	0
3	NAG	A	503	14/15	0.91	0.13	49,55,60,70	0
3	NAG	C	501	13/15	0.91	0.16	43,52,59,64	0
3	NAG	A	501	14/15	0.91	0.17	31,40,45,54	0
5	MAN	A	505	11/12	0.92	0.12	46,50,55,56	0
3	NAG	A	502	14/15	0.92	0.13	37,42,48,51	0
7	CL	D	403	1/1	0.93	0.21	58,58,58,58	0
8	HYS	B	503	27/27	0.94	0.18	19,31,51,57	0
7	CL	A	509	1/1	0.94	0.06	53,53,53,53	0
8	HYS	D	402	27/27	0.95	0.13	29,40,53,65	0
7	CL	B	507	1/1	0.97	0.08	57,57,57,57	0
6	NA	C	504	1/1	0.97	0.08	25,25,25,25	0
6	NA	A	508	1/1	0.98	0.11	18,18,18,18	0
7	CL	C	506	1/1	0.98	0.06	47,47,47,47	0
7	CL	B	504	1/1	0.98	0.05	46,46,46,46	0
7	CL	A	510	1/1	0.98	0.14	42,42,42,42	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.