



# Full wwPDB X-ray Structure Validation Report

Oct 15, 2014 – 02:58 PM EDT

PDB ID : 4U4G  
Title : Structure of GluA2\* in complex with competitive antagonist ZK 200775  
Authors : Yelshanskaya, M.V.; Li, M.; Sobolevsky, A.I.  
Deposited on : 2014-07-23  
Resolution : 4.49 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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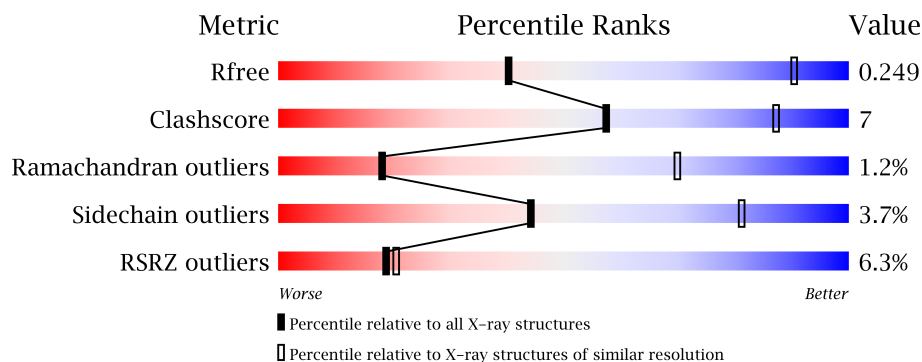
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.16 November 2013  
Xtriage (Phenix) : dev-1439  
EDS : trunk24003  
Percentile statistics : 23426  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk24003

# 1 Overall quality at a glance

The reported resolution of this entry is 4.49 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))
$R_{free}$	77520	1000 (5.46-3.52)
Clashscore	88313	1006 (5.30-3.60)
Ramachandran outliers	86584	1043 (5.46-3.52)
C $\alpha$ geometry	86677	1000 (5.30-3.58)
Sidechain outliers	86556	1023 (5.46-3.52)
RSRZ outliers	77580	1335 (5.50-3.50)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	827	
1	B	827	
1	C	827	
1	D	827	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 23812 atoms, of which 0 are hydrogen and 0 are deuterium.

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 2.

Mol	Chain	Residues	Atoms								ZeroOcc	AltConf	Trace
1	A	773	Total	C	F	N	O	P	S		0	0	0
			5966	3823	3	976	1135	1	28				
1	B	773	Total	C	F	N	O	P	S		0	0	0
			5946	3809	3	966	1139	1	28				
1	C	773	Total	C	F	N	O	P	S		0	0	0
			5940	3805	3	968	1135	1	28				
1	D	773	Total	C	F	N	O	P	S		0	0	0
			5960	3818	3	971	1139	1	28				

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	241	GLU	ASN	conflict	UNP P19491
A	382	LEU	VAL	conflict	UNP P19491
A	?	-	LEU	deletion	UNP P19491
A	?	-	THR	deletion	UNP P19491
A	?	-	GLU	deletion	UNP P19491
A	?	-	LEU	deletion	UNP P19491
A	?	-	PRO	deletion	UNP P19491
A	?	-	SER	deletion	UNP P19491
A	384	GLU	GLY	conflict	UNP P19491
A	385	ASP	ASN	conflict	UNP P19491
A	392	GLN	ASN	conflict	UNP P19491
A	828	GLY	-	expression tag	UNP P19491
A	829	LEU	-	expression tag	UNP P19491
A	830	VAL	-	expression tag	UNP P19491
A	831	PRO	-	expression tag	UNP P19491
A	832	ARG	-	expression tag	UNP P19491
A	833	ZK1	-	expression tag	UNP P19491
A	834	NAG	-	expression tag	UNP P19491
A	835	NAG	-	expression tag	UNP P19491
A	836	BMA	-	expression tag	UNP P19491
A	837	BMA	-	expression tag	UNP P19491

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Chain	Residue	Modelled	Actual	Comment	Reference
B	241	GLU	ASN	conflict	UNP P19491
B	382	LEU	VAL	conflict	UNP P19491
B	?	-	LEU	deletion	UNP P19491
B	?	-	THR	deletion	UNP P19491
B	?	-	GLU	deletion	UNP P19491
B	?	-	LEU	deletion	UNP P19491
B	?	-	PRO	deletion	UNP P19491
B	?	-	SER	deletion	UNP P19491
B	384	GLU	GLY	conflict	UNP P19491
B	385	ASP	ASN	conflict	UNP P19491
B	392	GLN	ASN	conflict	UNP P19491
B	828	GLY	-	expression tag	UNP P19491
B	829	LEU	-	expression tag	UNP P19491
B	830	VAL	-	expression tag	UNP P19491
B	831	PRO	-	expression tag	UNP P19491
B	832	ARG	-	expression tag	UNP P19491
B	833	ZK1	-	expression tag	UNP P19491
B	834	NAG	-	expression tag	UNP P19491
B	835	NAG	-	expression tag	UNP P19491
B	836	BMA	-	expression tag	UNP P19491
B	837	BMA	-	expression tag	UNP P19491
C	241	GLU	ASN	conflict	UNP P19491
C	382	LEU	VAL	conflict	UNP P19491
C	?	-	LEU	deletion	UNP P19491
C	?	-	THR	deletion	UNP P19491
C	?	-	GLU	deletion	UNP P19491
C	?	-	LEU	deletion	UNP P19491
C	?	-	PRO	deletion	UNP P19491
C	?	-	SER	deletion	UNP P19491
C	384	GLU	GLY	conflict	UNP P19491
C	385	ASP	ASN	conflict	UNP P19491
C	392	GLN	ASN	conflict	UNP P19491
C	828	GLY	-	expression tag	UNP P19491
C	829	LEU	-	expression tag	UNP P19491
C	830	VAL	-	expression tag	UNP P19491
C	831	PRO	-	expression tag	UNP P19491
C	832	ARG	-	expression tag	UNP P19491
C	833	ZK1	-	expression tag	UNP P19491
C	834	NAG	-	expression tag	UNP P19491
C	835	NAG	-	expression tag	UNP P19491
C	836	BMA	-	expression tag	UNP P19491
C	837	BMA	-	expression tag	UNP P19491

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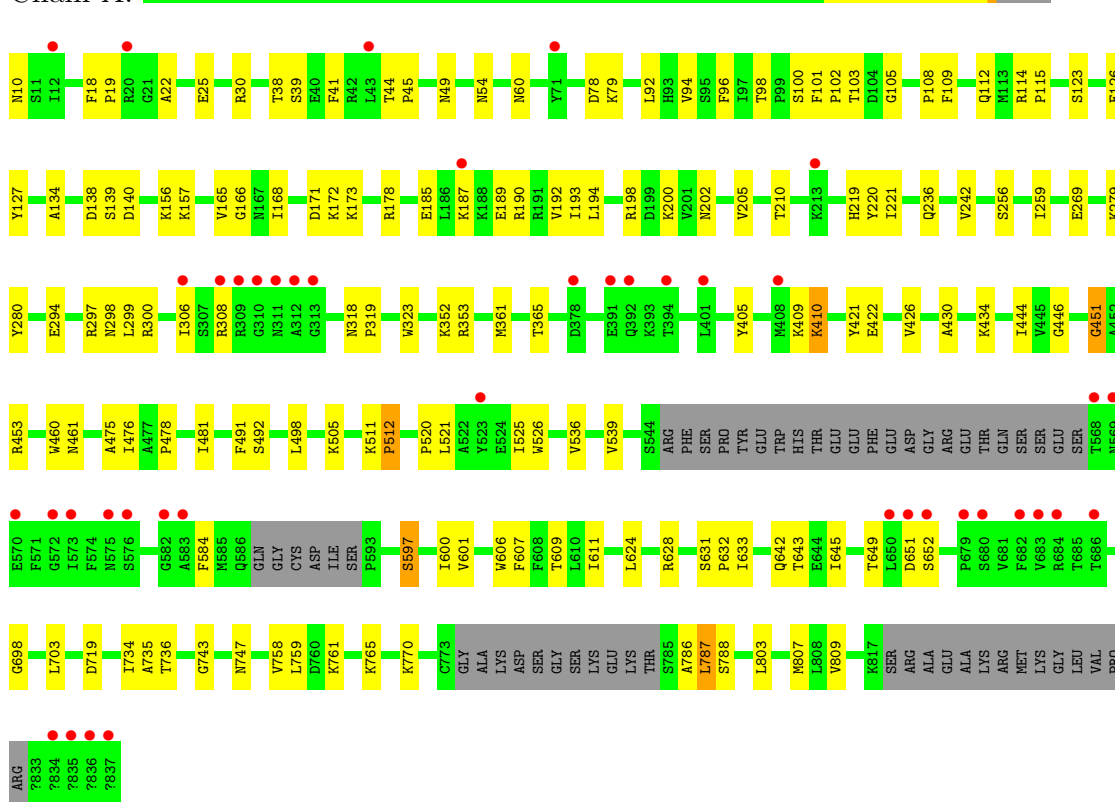
Chain	Residue	Modelled	Actual	Comment	Reference
D	241	GLU	ASN	conflict	UNP P19491
D	382	LEU	VAL	conflict	UNP P19491
D	?	-	LEU	deletion	UNP P19491
D	?	-	THR	deletion	UNP P19491
D	?	-	GLU	deletion	UNP P19491
D	?	-	LEU	deletion	UNP P19491
D	?	-	PRO	deletion	UNP P19491
D	?	-	SER	deletion	UNP P19491
D	384	GLU	GLY	conflict	UNP P19491
D	385	ASP	ASN	conflict	UNP P19491
D	392	GLN	ASN	conflict	UNP P19491
D	828	GLY	-	expression tag	UNP P19491
D	829	LEU	-	expression tag	UNP P19491
D	830	VAL	-	expression tag	UNP P19491
D	831	PRO	-	expression tag	UNP P19491
D	832	ARG	-	expression tag	UNP P19491
D	833	ZK1	-	expression tag	UNP P19491
D	834	NAG	-	expression tag	UNP P19491
D	835	NAG	-	expression tag	UNP P19491
D	836	BMA	-	expression tag	UNP P19491
D	837	BMA	-	expression tag	UNP P19491

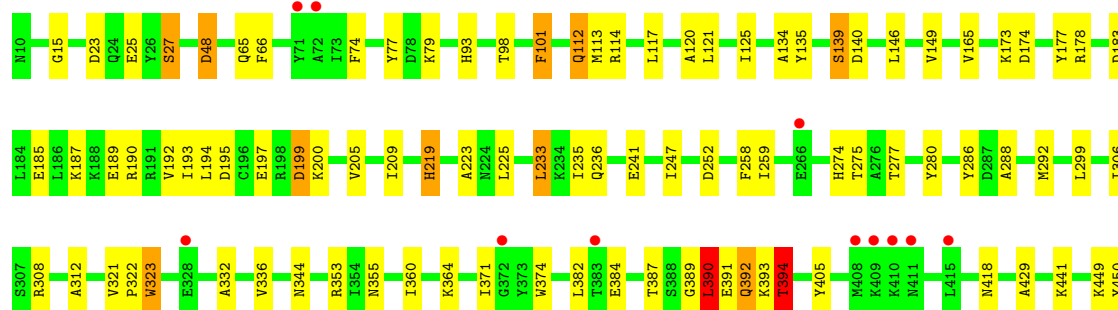
### 3 Residue-property plots

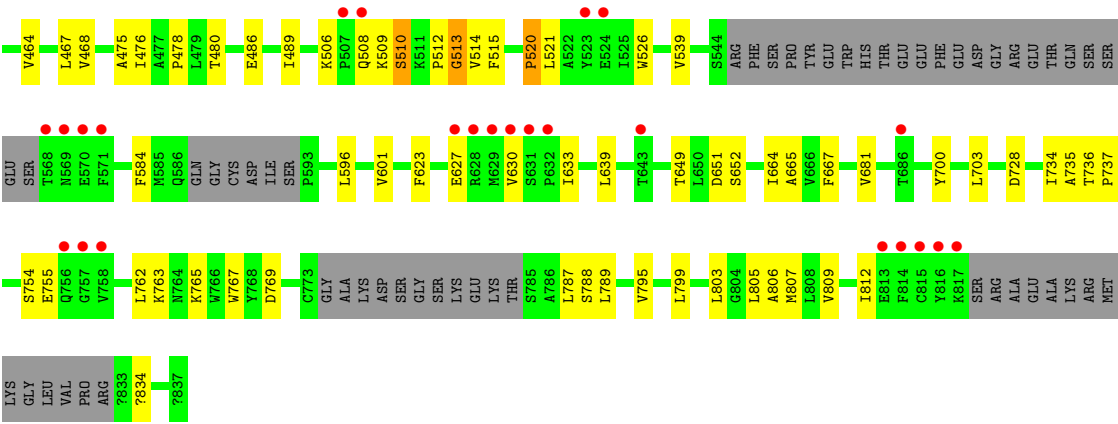
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: Glutamate receptor 2

Chain A:









## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	92.00Å 310.36Å 109.50Å 90.00° 94.82° 90.00°	Depositor
Resolution (Å)	50.00 – 4.49 48.72 – 4.49	Depositor EDS
% Data completeness (in resolution range)	98.7 (50.00-4.49) 98.7 (48.72-4.49)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.66 (at 4.45Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8-1069)	Depositor
R, $R_{free}$	0.217 , 0.248 0.218 , 0.249	Depositor DCC
$R_{free}$ test set	1796 reflections (4.99%)	DCC
Wilson B-factor (Å <sup>2</sup> )	206.6	Xtriage
Anisotropy	0.230	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.21 , 65.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 36039 reflections	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	23812	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	160.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.75% 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 ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, ZK1

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	0.23	0/6010	0.39	0/8148
1	B	0.23	0/5990	0.39	0/8128
1	C	0.23	0/5984	0.40	0/8121
1	D	0.23	0/6004	0.40	0/8143
All	All	0.23	0/23988	0.40	0/32540

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	2	0
1	B	2	0
All	All	4	0

There are no bond length outliers.

There are no bond angle outliers.

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	834	NAG	C1
1	A	836	BMA	C1
1	B	834	NAG	C1
1	B	835	NAG	C1

There are no planarity outliers.

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5966	0	5794	87	0
1	B	5946	0	5736	85	0
1	C	5940	0	5728	85	0
1	D	5960	0	5769	84	0
All	All	23812	0	23027	307	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 7.

All (307) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:510:SER:H	1:D:512:PRO:HD3	1.48	0.79
1:B:102:PRO:HD3	1:B:114:ARG:HD2	1.63	0.78
1:B:649:THR:HG22	1:B:703:LEU:HB2	1.72	0.71
1:A:736:THR:HG21	1:A:743:GLY:HA2	1.72	0.71
1:B:255:VAL:HG13	1:B:341:LEU:HD22	1.73	0.70
1:B:536:VAL:HG22	1:C:803:LEU:HD21	1.73	0.70
1:C:536:VAL:HG22	1:D:803:LEU:HD21	1.72	0.70
1:A:166:GLY:HA2	1:A:200:LYS:HE2	1.72	0.70
1:B:114:ARG:NH1	1:B:280:TYR:OH	2.25	0.69
1:C:166:GLY:HA2	1:C:200:LYS:HE2	1.75	0.69
1:A:409:LYS:HD3	1:A:422:GLU:HG3	1.74	0.69
1:C:154:ALA:HB1	1:D:183:ASP:HB3	1.76	0.68
1:A:649:THR:HG22	1:A:703:LEU:HB2	1.77	0.67
1:C:642:GLN:HE22	1:C:645:ILE:HB	1.60	0.66
1:A:475:ALA:HB3	1:A:735:ALA:HB3	1.77	0.65
1:D:23:ASP:O	1:D:27:SER:OG	2.14	0.65
1:B:611:ILE:HG21	1:C:795:VAL:HG21	1.77	0.65
1:B:525:ILE:HG12	1:C:789:LEU:HD13	1.78	0.65
1:B:601:VAL:HG23	1:C:806:ALA:HB3	1.78	0.64
1:C:170:ASN:HA	1:C:173:LYS:HB2	1.78	0.64
1:B:628:ARG:NH2	1:C:628:ARG:O	2.31	0.63
1:B:48:ASP:OD2	1:B:65:GLN:NE2	2.32	0.63
1:B:17:LEU:HG	1:B:50:LEU:HD21	1.80	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:220:TYR:HB2	1:A:242:VAL:HG22	1.80	0.62
1:B:528:CYS:HA	1:B:531:PHE:HB2	1.80	0.62
1:B:366:ASN:OD1	1:B:366:ASN:N	2.31	0.62
1:C:758:VAL:HA	1:C:761:LYS:HB3	1.81	0.62
1:A:294:GLU:OE2	1:A:297:ARG:NH1	2.33	0.62
1:B:475:ALA:HB3	1:B:735:ALA:HB3	1.81	0.62
1:C:236:GLN:NE2	1:C:365:THR:O	2.31	0.62
1:D:114:ARG:NH1	1:D:280:TYR:OH	2.33	0.62
1:A:525:ILE:HG12	1:B:789:LEU:HD13	1.80	0.62
1:D:112:GLN:H	1:D:112:GLN:HE21	1.48	0.62
1:A:536:VAL:HG22	1:B:803:LEU:HD21	1.82	0.61
1:D:475:ALA:HB3	1:D:735:ALA:HB3	1.82	0.61
1:A:10:ASN:HB3	1:A:300:ARG:HH22	1.66	0.60
1:A:185:GLU:HG3	1:A:190:ARG:HH22	1.66	0.60
1:D:418:ASN:HD21	1:D:441:LYS:HA	1.66	0.60
1:B:489:ILE:HD12	1:B:735:ALA:HB1	1.83	0.60
1:B:63:CYS:O	1:B:67:SER:OG	2.19	0.59
1:A:102:PRO:HD3	1:A:114:ARG:HD2	1.85	0.59
1:C:506:LYS:HD2	1:C:507:PRO:HD2	1.85	0.59
1:D:185:GLU:HG3	1:D:190:ARG:HH12	1.66	0.59
1:B:517:PHE:HB2	1:B:791:ASN:HD21	1.69	0.58
1:D:233:LEU:HA	1:D:236:GLN:HB2	1.85	0.58
1:C:525:ILE:HG12	1:D:789:LEU:HD13	1.86	0.57
1:C:334:LYS:NZ	1:C:349:GLN:O	2.32	0.57
1:B:613:ILE:O	1:B:617:THR:OG1	2.17	0.57
1:A:78:ASP:OD1	1:A:79:LYS:N	2.32	0.57
1:D:513:GLY:O	1:D:515:PHE:N	2.38	0.56
1:A:236:GLN:NE2	1:A:365:THR:O	2.36	0.56
1:C:101:PHE:HA	1:C:114:ARG:HD3	1.88	0.56
1:A:409:LYS:HG2	1:A:410:LYS:H	1.68	0.56
1:C:464:VAL:HG13	1:C:489:ILE:HD13	1.87	0.55
1:D:633:ILE:HG21	1:D:639:LEU:HG	1.88	0.55
1:C:220:TYR:HB2	1:C:242:VAL:HG22	1.88	0.55
1:B:299:LEU:HD13	1:B:306:ILE:HG21	1.87	0.55
1:C:490:ASP:HB2	1:C:736:THR:HG23	1.89	0.55
1:B:601:VAL:HG22	1:C:803:LEU:HD23	1.90	0.54
1:C:702:TYR:HE2	1:C:704:LEU:HD13	1.73	0.54
1:D:728:ASP:OD1	1:D:728:ASP:N	2.39	0.54
1:A:642:GLN:HE22	1:A:645:ILE:HB	1.72	0.54
1:A:758:VAL:HA	1:A:761:LYS:HB3	1.89	0.54
1:B:521:LEU:HD22	1:B:526:TRP:CD2	2.42	0.54
1:A:134:ALA:HB3	1:A:192:VAL:HG22	1.88	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:451:GLY:O	1:C:485:ARG:NH2	2.38	0.53
1:C:294:GLU:HG3	1:C:338:VAL:HG11	1.90	0.53
1:D:467:LEU:HD22	1:D:737:PRO:HD3	1.89	0.53
1:C:611:ILE:HG21	1:D:795:VAL:HG21	1.90	0.53
1:B:728:ASP:OD1	1:B:728:ASP:N	2.40	0.53
1:D:165:VAL:O	1:D:200:LYS:NZ	2.34	0.53
1:B:261:ARG:NH2	1:B:261:ARG:O	2.42	0.53
1:C:521:LEU:HD22	1:C:526:TRP:CD2	2.44	0.53
1:A:606:TRP:HA	1:A:609:THR:HG22	1.91	0.53
1:A:803:LEU:HD22	1:D:539:VAL:HG11	1.90	0.52
1:D:344:ASN:O	1:D:353:ARG:NH2	2.43	0.52
1:B:411:ASN:N	1:B:411:ASN:OD1	2.42	0.52
1:C:135:TYR:OH	1:C:195:ASP:OD2	2.25	0.52
1:C:174:ASP:OD1	1:C:207:GLN:NE2	2.44	0.51
1:A:624:LEU:O	1:A:628:ARG:HG2	2.09	0.51
1:D:308:ARG:HG2	1:D:323:TRP:HZ3	1.75	0.51
1:B:521:LEU:HD23	1:B:525:ILE:HB	1.91	0.51
1:A:511:LYS:HG2	1:A:512:PRO:HD2	1.92	0.51
1:B:388:SER:OG	1:B:391:GLU:OE1	2.29	0.51
1:C:186:LEU:HD23	1:C:187:LYS:HG3	1.92	0.51
1:B:115:PRO:HG2	1:B:247:ILE:HD11	1.92	0.51
1:D:77:TYR:CE2	1:D:98:THR:HG21	2.46	0.51
1:C:330:GLU:HG2	1:C:334:LYS:HE2	1.93	0.51
1:C:284:LEU:O	1:C:288:ALA:N	2.43	0.50
1:D:101:PHE:HA	1:D:114:ARG:HD2	1.93	0.50
1:D:174:ASP:O	1:D:178:ARG:NH1	2.45	0.50
1:A:633:ILE:HD11	1:A:645:ILE:HD12	1.93	0.50
1:A:809:VAL:HG11	1:D:596:LEU:HD23	1.94	0.50
1:A:601:VAL:HG22	1:B:803:LEU:HD23	1.92	0.50
1:D:332:ALA:O	1:D:336:VAL:HG23	2.11	0.50
1:C:13:GLN:HG2	1:C:70:VAL:HG12	1.93	0.50
1:D:135:TYR:OH	1:D:195:ASP:OD2	2.25	0.50
1:C:409:LYS:HG2	1:C:410:LYS:H	1.77	0.49
1:D:809:VAL:HA	1:D:812:ILE:HG12	1.93	0.49
1:C:401:LEU:HD23	1:C:406:VAL:HG12	1.93	0.49
1:A:787:LEU:HD13	1:A:788:SER:H	1.76	0.49
1:A:171:ASP:OD1	1:A:172:LYS:N	2.45	0.49
1:B:477:ALA:O	1:B:479:LEU:N	2.43	0.49
1:B:608:PHE:CG	1:C:799:LEU:HD22	2.47	0.49
1:D:429:ALA:HA	1:D:476:ILE:HD13	1.94	0.49
1:C:476:ILE:HG12	1:C:734:ILE:HD12	1.93	0.49
1:D:788:SER:OG	1:D:789:LEU:N	2.45	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:255:VAL:HG22	1:B:341:LEU:HA	1.94	0.49
1:C:38:THR:OG1	1:C:39:SER:N	2.45	0.49
1:D:355:ASN:HB3	1:D:834:NAG:H82	1.95	0.49
1:A:505:LYS:HB3	1:A:698:GLY:HA2	1.94	0.49
1:B:231:ASP:HB3	1:B:234:LYS:HE2	1.95	0.49
1:C:514:VAL:HG13	1:C:794:GLY:HA3	1.94	0.48
1:A:108:PRO:HB2	1:A:109:PHE:HD1	1.78	0.48
1:A:30:ARG:NH2	1:A:269:GLU:OE2	2.47	0.48
1:A:22:ALA:HB1	1:A:25:GLU:HB2	1.94	0.48
1:C:116:ASP:OD1	1:C:117:LEU:N	2.45	0.48
1:D:199:ASP:N	1:D:199:ASP:OD1	2.46	0.48
1:B:532:ALA:O	1:B:536:VAL:HG23	2.13	0.48
1:C:651:ASP:OD1	1:C:652:SER:N	2.47	0.48
1:A:138:ASP:OD1	1:A:139:SER:N	2.45	0.48
1:A:103:THR:OG1	1:A:352:LYS:NZ	2.47	0.48
1:B:535:GLY:O	1:B:539:VAL:HG23	2.14	0.48
1:C:97:ILE:HG13	1:C:111:ILE:HB	1.96	0.48
1:D:464:VAL:HG13	1:D:489:ILE:HD13	1.96	0.48
1:A:597:SER:O	1:A:600:ILE:HG12	2.14	0.47
1:B:659:PHE:HB3	1:B:671:TRP:HB2	1.96	0.47
1:D:299:LEU:HD13	1:D:306:ILE:HG21	1.96	0.47
1:A:96:PHE:HE1	1:A:98:THR:HB	1.79	0.47
1:B:760:ASP:HB3	1:C:664:ILE:HD11	1.96	0.47
1:D:205:VAL:O	1:D:209:ILE:HG13	2.14	0.47
1:A:787:LEU:HB2	1:D:520:PRO:O	2.15	0.47
1:C:642:GLN:OE1	1:C:644:GLU:N	2.47	0.47
1:D:754:SER:OG	1:D:755:GLU:N	2.47	0.47
1:C:157:LYS:HE2	1:D:187:LYS:HG3	1.95	0.47
1:D:288:ALA:O	1:D:292:MET:HG3	2.14	0.47
1:C:412:HIS:CE1	1:C:413:GLU:HG3	2.50	0.47
1:D:25:GLU:N	1:D:25:GLU:OE1	2.46	0.47
1:B:227:PHE:CD1	1:B:244:GLY:HA3	2.49	0.47
1:D:258:PHE:HE2	1:D:286:TYR:CZ	2.33	0.47
1:B:536:VAL:HG21	1:B:605:TRP:CE3	2.49	0.47
1:B:626:VAL:HB	1:C:628:ARG:NH1	2.30	0.47
1:D:765:LYS:HA	1:D:769:ASP:HB2	1.96	0.47
1:A:115:PRO:HA	1:A:353:ARG:HB2	1.96	0.47
1:C:31:VAL:HG21	1:C:262:TRP:HZ3	1.80	0.47
1:C:754:SER:HB3	1:C:759:LEU:HD12	1.96	0.47
1:B:38:THR:OG1	1:B:39:SER:N	2.48	0.47
1:A:651:ASP:OD1	1:A:652:SER:N	2.48	0.46
1:D:275:THR:OG1	1:D:277:THR:O	2.33	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:681:VAL:O	1:D:700:TYR:OH	2.20	0.46
1:D:382:LEU:H	1:D:382:LEU:HD23	1.80	0.46
1:A:193:ILE:HG12	1:A:221:ILE:HB	1.95	0.46
1:A:405:TYR:CG	1:A:478:PRO:HG3	2.51	0.46
1:C:77:TYR:HE2	1:C:98:THR:HG21	1.80	0.46
1:A:453:ARG:HD2	1:A:460:TRP:CZ2	2.51	0.46
1:A:597:SER:HA	1:B:809:VAL:HB	1.98	0.46
1:C:521:LEU:HD23	1:C:525:ILE:HB	1.97	0.46
1:D:405:TYR:CG	1:D:478:PRO:HG3	2.50	0.46
1:A:430:ALA:O	1:A:434:LYS:N	2.48	0.46
1:B:711:TYR:O	1:B:715:ARG:HG2	2.16	0.46
1:D:146:LEU:HA	1:D:149:VAL:HG22	1.98	0.46
1:B:664:ILE:HB	1:B:667:PHE:HD2	1.80	0.46
1:A:409:LYS:HD3	1:A:422:GLU:CG	2.45	0.46
1:B:135:TYR:OH	1:B:195:ASP:OD2	2.33	0.46
1:C:488:VAL:HG23	1:C:489:ILE:HG23	1.97	0.46
1:C:171:ASP:OD1	1:C:172:LYS:N	2.49	0.45
1:D:219:HIS:ND1	1:D:241:GLU:O	2.47	0.45
1:D:763:LYS:O	1:D:767:TRP:HB2	2.16	0.45
1:B:539:VAL:HG11	1:B:601:VAL:HG21	1.98	0.45
1:C:346:LYS:HD2	1:C:354:ILE:HD11	1.97	0.45
1:C:601:VAL:HG23	1:D:806:ALA:HB3	1.98	0.45
1:C:464:VAL:HG22	1:C:479:LEU:HD21	1.97	0.45
1:D:48:ASP:OD2	1:D:65:GLN:NE2	2.49	0.45
1:B:539:VAL:HG22	1:C:807:MET:HG2	1.97	0.45
1:D:195:ASP:HA	1:D:223:ALA:HB3	1.98	0.45
1:B:29:PHE:O	1:B:33:MET:HG2	2.16	0.45
1:D:805:LEU:O	1:D:809:VAL:HG23	2.15	0.45
1:A:481:ILE:HG22	1:A:491:PHE:CG	2.52	0.45
1:B:529:ILE:O	1:B:533:TYR:HB2	2.17	0.45
1:C:510:SER:HB3	1:C:511:LYS:HG3	1.99	0.45
1:B:115:PRO:HA	1:B:353:ARG:HB2	1.98	0.45
1:A:178:ARG:HH11	1:A:210:THR:HG21	1.82	0.44
1:D:117:LEU:HD12	1:D:120:ALA:HB3	1.99	0.44
1:B:539:VAL:O	1:B:543:VAL:HG23	2.17	0.44
1:C:113:MET:HG3	1:C:288:ALA:HB2	1.97	0.44
1:D:664:ILE:HB	1:D:667:PHE:HD2	1.82	0.44
1:D:649:THR:HG22	1:D:703:LEU:HB2	1.98	0.44
1:A:405:TYR:CD2	1:A:478:PRO:HG3	2.52	0.44
1:D:521:LEU:HD22	1:D:526:TRP:CD2	2.52	0.44
1:A:299:LEU:HD13	1:A:306:ILE:HD13	1.99	0.44
1:B:514:VAL:HG11	1:B:794:GLY:HA3	1.98	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:65:GLN:HE21	1:C:65:GLN:HA	1.81	0.44
1:A:114:ARG:NH1	1:A:280:TYR:OH	2.50	0.44
1:B:612:ILE:HD11	1:C:796:PHE:CE1	2.52	0.44
1:A:18:PHE:HA	1:A:19:PRO:HD3	1.87	0.44
1:B:113:MET:O	1:B:353:ARG:NH1	2.49	0.44
1:D:464:VAL:O	1:D:468:VAL:HG23	2.18	0.44
1:A:765:LYS:O	1:A:770:LYS:HB2	2.18	0.44
1:B:511:LYS:HE3	1:B:511:LYS:HB2	1.75	0.44
1:B:651:ASP:OD1	1:B:652:SER:N	2.51	0.44
1:A:294:GLU:O	1:A:298:ASN:ND2	2.36	0.43
1:A:318:ASN:HA	1:A:319:PRO:HA	1.89	0.43
1:B:647:TYR:HB3	1:B:701:ALA:HB3	1.99	0.43
1:B:719:ASP:OD1	1:B:719:ASP:N	2.41	0.43
1:A:194:LEU:HD23	1:A:194:LEU:HA	1.76	0.43
1:B:250:TYR:OH	1:B:278:ILE:N	2.37	0.43
1:D:392:GLN:O	1:D:394:THR:N	2.51	0.43
1:B:498:LEU:HD13	1:B:707:THR:HG23	2.00	0.43
1:C:608:PHE:CG	1:D:799:LEU:HD22	2.53	0.43
1:A:108:PRO:HB2	1:A:109:PHE:CD1	2.54	0.43
1:D:173:LYS:HG2	1:D:177:TYR:HE2	1.84	0.43
1:A:539:VAL:HG21	1:B:803:LEU:HB3	2.00	0.43
1:B:619:ASN:HB2	1:C:624:LEU:HD13	2.00	0.43
1:A:198:ARG:HD3	1:A:279:LYS:HE3	2.01	0.43
1:A:38:THR:HG23	1:A:41:PHE:H	1.83	0.43
1:A:492:SER:HB2	1:A:747:ASN:HA	2.00	0.43
1:A:607:PHE:O	1:A:611:ILE:HG12	2.19	0.43
1:B:135:TYR:CE2	1:B:137:TYR:HB3	2.54	0.43
1:B:789:LEU:HD12	1:B:792:VAL:HB	1.99	0.43
1:C:132:LYS:HE2	1:C:189:GLU:HG2	2.00	0.43
1:D:651:ASP:OD1	1:D:652:SER:N	2.51	0.43
1:B:521:LEU:HD22	1:B:526:TRP:CE2	2.54	0.43
1:B:710:GLU:O	1:B:714:GLN:HG2	2.18	0.43
1:C:101:PHE:HA	1:C:102:PRO:HD3	1.89	0.43
1:C:467:LEU:HD22	1:C:737:PRO:HD3	2.01	0.43
1:A:105:GLY:O	1:A:352:LYS:NZ	2.48	0.43
1:A:38:THR:OG1	1:A:39:SER:N	2.50	0.43
1:C:36:PHE:CZ	1:C:290:GLN:HB2	2.54	0.43
1:C:297:ARG:HG2	1:C:301:LYS:HE3	2.00	0.43
1:D:633:ILE:HD13	1:D:639:LEU:HD21	2.00	0.43
1:B:530:VAL:HA	1:B:533:TYR:HB3	2.01	0.43
1:C:593:PRO:HB2	1:C:594:ARG:H	1.64	0.43
1:A:631:SER:HA	1:A:632:PRO:HD3	1.92	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:54:ASN:OD1	1:B:87:SER:OG	2.36	0.43
1:D:134:ALA:HB3	1:D:192:VAL:HG22	2.00	0.43
1:B:416:GLU:HA	1:B:420:ARG:HD3	1.99	0.42
1:B:619:ASN:HD22	1:C:624:LEU:HD13	1.82	0.42
1:C:728:ASP:N	1:C:728:ASP:OD1	2.51	0.42
1:D:321:VAL:HA	1:D:322:PRO:HD3	1.85	0.42
1:D:449:LYS:HG2	1:D:450:TYR:H	1.84	0.42
1:C:14:ILE:HD13	1:C:43:LEU:HD23	2.00	0.42
1:D:225:LEU:HD22	1:D:247:ILE:HD13	2.00	0.42
1:A:422:GLU:HA	1:A:426:VAL:HG11	2.01	0.42
1:A:476:ILE:HG12	1:A:734:ILE:HG23	2.01	0.42
1:A:803:LEU:O	1:A:807:MET:HG2	2.19	0.42
1:D:79:LYS:HE3	1:D:139:SER:HB2	2.00	0.42
1:B:626:VAL:O	1:B:627:GLU:HG2	2.20	0.42
1:C:194:LEU:HG	1:C:222:ILE:HD13	2.01	0.42
1:C:511:LYS:HG2	1:C:512:PRO:HD2	2.01	0.42
1:C:762:LEU:O	1:C:766:TRP:HD1	2.03	0.42
1:D:476:ILE:HG12	1:D:734:ILE:HD12	2.02	0.42
1:B:424:TYR:CE1	1:B:762:LEU:HB3	2.55	0.42
1:A:259:ILE:HD13	1:A:259:ILE:HA	1.82	0.42
1:D:66:PHE:CE2	1:D:312:ALA:HB1	2.54	0.42
1:A:187:LYS:HZ1	1:B:157:LYS:HB3	1.85	0.42
1:C:209:ILE:HA	1:C:214:HIS:ND1	2.35	0.42
1:C:29:PHE:O	1:C:33:MET:HG2	2.20	0.42
1:D:308:ARG:HG2	1:D:323:TRP:CZ3	2.52	0.42
1:D:360:ILE:HG22	1:D:371:ILE:HG12	2.00	0.42
1:A:202:ASN:HA	1:A:205:VAL:HB	2.01	0.42
1:A:44:THR:HA	1:A:45:PRO:HD3	1.82	0.42
1:A:759:LEU:HD23	1:A:759:LEU:HA	1.91	0.42
1:C:539:VAL:HG13	1:D:807:MET:HG2	2.02	0.42
1:D:120:ALA:HA	1:D:374:TRP:CE2	2.55	0.42
1:A:521:LEU:HD22	1:A:526:TRP:CD2	2.55	0.41
1:B:332:ALA:O	1:B:336:VAL:HG23	2.20	0.41
1:B:494:PRO:HA	1:B:732:TYR:O	2.20	0.41
1:B:526:TRP:HA	1:B:529:ILE:HG22	2.02	0.41
1:C:601:VAL:HG22	1:D:803:LEU:HD23	2.01	0.41
1:D:389:GLY:O	1:D:391:GLU:N	2.53	0.41
1:A:101:PHE:HA	1:A:114:ARG:HD2	2.01	0.41
1:A:92:LEU:HB2	1:A:94:VAL:HG23	2.01	0.41
1:D:390:LEU:H	1:D:390:LEU:HG	1.58	0.41
1:C:110:VAL:HG12	1:C:112:GLN:HG3	2.02	0.41
1:D:121:LEU:HD11	1:D:193:ILE:HD13	2.02	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:121:LEU:O	1:D:125:ILE:HG13	2.20	0.41
1:A:30:ARG:HH22	1:A:269:GLU:HG3	1.85	0.41
1:A:476:ILE:HG12	1:A:734:ILE:HD12	2.02	0.41
1:A:178:ARG:NH1	1:A:210:THR:HG21	2.36	0.41
1:D:15:GLY:O	1:D:74:PHE:N	2.50	0.41
1:B:98:THR:HA	1:B:99:PRO:HD3	1.83	0.41
1:C:18:PHE:O	1:C:49:ASN:HA	2.21	0.41
1:C:227:PHE:CD1	1:C:244:GLY:HA3	2.55	0.41
1:A:126:GLU:HG3	1:A:156:LYS:HE3	2.02	0.41
1:A:168:ILE:HD13	1:A:173:LYS:HG3	2.02	0.41
1:A:123:SER:O	1:A:127:TYR:N	2.49	0.41
1:A:157:LYS:HD3	1:A:157:LYS:HA	1.87	0.41
1:B:619:ASN:HD22	1:C:624:LEU:HB3	1.86	0.41
1:D:113:MET:HG3	1:D:288:ALA:HB2	2.03	0.41
1:D:364:LYS:HD3	1:D:364:LYS:HA	1.80	0.41
1:A:421:TYR:CE1	1:A:444:ILE:HD11	2.55	0.41
1:B:763:LYS:O	1:B:767:TRP:HB2	2.21	0.41
1:C:195:ASP:HA	1:C:223:ALA:HB3	2.02	0.41
1:A:719:ASP:N	1:A:719:ASP:OD1	2.54	0.41
1:B:246:GLN:HB2	1:B:361:MET:HG3	2.03	0.41
1:B:25:GLU:N	1:B:25:GLU:OE1	2.52	0.41
1:B:299:LEU:HA	1:B:299:LEU:HD23	1.95	0.41
1:B:77:TYR:CE2	1:B:98:THR:HG21	2.55	0.41
1:C:259:ILE:HA	1:C:259:ILE:HD13	1.91	0.41
1:C:98:THR:HA	1:C:99:PRO:HD3	1.84	0.41
1:C:425:CYS:HB3	1:C:476:ILE:HG22	2.02	0.40
1:A:18:PHE:O	1:A:49:ASN:HA	2.21	0.40
1:B:136:LEU:HB2	1:B:194:LEU:HD12	2.04	0.40
1:A:803:LEU:HD23	1:D:601:VAL:HG22	2.04	0.40
1:D:405:TYR:CD1	1:D:478:PRO:HG3	2.56	0.40
1:A:451:GLY:HA2	1:A:461:ASN:O	2.21	0.40
1:D:762:LEU:HD23	1:D:762:LEU:HA	1.97	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	760/827 (92%)	694 (91%)	57 (8%)	9 (1%)	18	70
1	B	760/827 (92%)	701 (92%)	52 (7%)	7 (1%)	23	74
1	C	760/827 (92%)	683 (90%)	70 (9%)	7 (1%)	23	74
1	D	760/827 (92%)	689 (91%)	58 (8%)	13 (2%)	13	64
All	All	3040/3308 (92%)	2767 (91%)	237 (8%)	36 (1%)	18	70

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	140	ASP
1	A	410	LYS
1	A	512	PRO
1	A	597	SER
1	D	514	VAL
1	A	786	ALA
1	B	157	LYS
1	B	520	PRO
1	B	584	PHE
1	B	597	SER
1	C	389	GLY
1	C	584	PHE
1	D	140	ASP
1	D	390	LEU
1	D	393	LYS
1	D	394	THR
1	A	520	PRO
1	A	584	PHE
1	C	410	LYS
1	C	630	VAL
1	D	510	SER
1	D	584	PHE
1	C	390	LEU
1	D	384	GLU
1	D	665	ALA
1	B	478	PRO
1	C	507	PRO
1	C	597	SER
1	D	392	GLN
1	D	506	LYS

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Mol	Chain	Res	Type
1	D	513	GLY
1	A	451	GLY
1	B	451	GLY
1	A	446	GLY
1	D	520	PRO
1	B	743	GLY

### 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	615/702 (88%)	602 (98%)	13 (2%)	64	89
1	B	611/702 (87%)	584 (96%)	27 (4%)	37	77
1	C	609/702 (87%)	587 (96%)	22 (4%)	45	82
1	D	614/702 (88%)	585 (95%)	29 (5%)	35	76
All	All	2449/2808 (87%)	2358 (96%)	91 (4%)	44	81

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	ASN
1	A	100	SER
1	A	112	GLN
1	A	165	VAL
1	A	189	GLU
1	A	219	HIS
1	A	256	SER
1	A	308	ARG
1	A	323	TRP
1	A	361	MET
1	A	498	LEU
1	A	643	THR
1	A	787	LEU
1	B	37	SER
1	B	38	THR
1	B	60	ASN

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Mol	Chain	Res	Type
1	B	67	SER
1	B	112	GLN
1	B	194	LEU
1	B	197	GLU
1	B	210	THR
1	B	235	ILE
1	B	247	ILE
1	B	259	ILE
1	B	314	ASP
1	B	323	TRP
1	B	325	GLN
1	B	327	VAL
1	B	357	THR
1	B	361	MET
1	B	366	ASN
1	B	511	LYS
1	B	525	ILE
1	B	537	SER
1	B	627	GLU
1	B	633	ILE
1	B	708	MET
1	B	719	ASP
1	B	760	ASP
1	B	762	LEU
1	C	65	GLN
1	C	87	SER
1	C	88	PHE
1	C	93	HIS
1	C	112	GLN
1	C	139	SER
1	C	194	LEU
1	C	211	ILE
1	C	219	HIS
1	C	247	ILE
1	C	248	VAL
1	C	253	SER
1	C	274	HIS
1	C	307	SER
1	C	393	LYS
1	C	498	LEU
1	C	510	SER
1	C	521	LEU

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Mol	Chain	Res	Type
1	C	601	VAL
1	C	635	SER
1	C	709	ASN
1	C	815	CYS
1	D	27	SER
1	D	48	ASP
1	D	93	HIS
1	D	101	PHE
1	D	112	GLN
1	D	139	SER
1	D	189	GLU
1	D	194	LEU
1	D	197	GLU
1	D	199	ASP
1	D	219	HIS
1	D	233	LEU
1	D	235	ILE
1	D	252	ASP
1	D	259	ILE
1	D	274	HIS
1	D	323	TRP
1	D	387	THR
1	D	390	LEU
1	D	394	THR
1	D	480	THR
1	D	486	GLU
1	D	508	GLN
1	D	509	LYS
1	D	623	PHE
1	D	627	GLU
1	D	630	VAL
1	D	736	THR
1	D	787	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	337	GLN
1	B	619	ASN
1	C	13	GLN
1	C	65	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

16 non-standard protein/DNA/RNA residues 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$
1	NAG	A	834	1	14,14,15	0.53	0	19,19,21	1.25	1 (5%)
1	NAG	A	835	1	14,14,15	0.47	0	19,19,21	0.86	0
1	BMA	A	836	1	11,11,12	0.60	0	15,15,17	0.81	0
1	BMA	A	837	1	11,11,12	0.61	0	15,15,17	0.87	0
1	NAG	B	834	1	14,14,15	0.53	0	19,19,21	1.07	1 (5%)
1	NAG	B	835	1	14,14,15	0.43	0	19,19,21	1.08	2 (10%)
1	BMA	B	836	1	11,11,12	0.60	0	15,15,17	0.87	0
1	BMA	B	837	1	11,11,12	0.58	0	15,15,17	0.89	0
1	NAG	C	834	1	14,14,15	0.55	0	19,19,21	0.99	2 (10%)
1	NAG	C	835	1	14,14,15	0.50	0	19,19,21	0.90	1 (5%)
1	BMA	C	836	1	11,11,12	0.59	0	15,15,17	0.86	0
1	BMA	C	837	1	11,11,12	0.65	0	15,15,17	0.84	0
1	NAG	D	834	1	14,14,15	0.65	0	19,19,21	1.80	4 (21%)
1	NAG	D	835	1	14,14,15	0.49	0	19,19,21	0.84	0
1	BMA	D	836	1	11,11,12	0.56	0	15,15,17	0.82	0
1	BMA	D	837	1	11,11,12	0.64	0	15,15,17	0.85	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
1	NAG	A	834	1	1/1/5/7	0/6/23/26	0/1/1/1
1	NAG	A	835	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	BMA	A	836	1	1/1/4/5	0/2/19/22	0/1/1/1
1	BMA	A	837	1	-	0/2/19/22	0/1/1/1
1	NAG	B	834	1	1/1/5/7	0/6/23/26	0/1/1/1
1	NAG	B	835	1	1/1/5/7	2/6/23/26	0/1/1/1
1	BMA	B	836	1	-	0/2/19/22	0/1/1/1
1	BMA	B	837	1	-	0/2/19/22	0/1/1/1
1	NAG	C	834	1	-	0/6/23/26	0/1/1/1
1	NAG	C	835	1	-	0/6/23/26	0/1/1/1
1	BMA	C	836	1	-	0/2/19/22	0/1/1/1
1	BMA	C	837	1	-	0/2/19/22	0/1/1/1
1	NAG	D	834	1	-	0/6/23/26	0/1/1/1
1	NAG	D	835	1	-	0/6/23/26	0/1/1/1
1	BMA	D	836	1	-	0/2/19/22	0/1/1/1
1	BMA	D	837	1	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	834	NAG	C2-N2-C7	-5.28	116.65	123.42
1	A	834	NAG	C1-C2-C3	3.57	114.80	109.15
1	D	834	NAG	C1-C2-C3	3.16	114.14	109.15
1	B	834	NAG	C1-C2-C3	3.04	113.96	109.15
1	B	835	NAG	C1-O5-C5	2.78	115.71	112.13
1	C	834	NAG	C1-C2-C3	2.50	113.10	109.15
1	B	835	NAG	C2-N2-C7	-2.48	120.24	123.42
1	C	835	NAG	C1-C2-C3	2.39	112.93	109.15
1	D	834	NAG	C1-O5-C5	2.37	115.17	112.13
1	C	834	NAG	C1-O5-C5	2.08	114.80	112.13
1	D	834	NAG	O5-C5-C6	2.03	110.47	106.97

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	834	NAG	C1
1	A	834	NAG	C1
1	B	835	NAG	C1
1	A	836	BMA	C1

All (2) torsion outliers are listed below:



Mol	Chain	Res	Type	Atoms
1	B	835	NAG	O7-C7-N2-C2
1	B	835	NAG	C8-C7-N2-C2

There are no ring outliers.

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

There are no ligands in this entry.

## 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	772/827 (93%)	0.29	42 (5%) 24 23	58, 156, 267, 497	0
1	B	772/827 (93%)	0.42	61 (7%) 12 16	41, 167, 300, 506	0
1	C	772/827 (93%)	0.42	57 (7%) 14 17	45, 148, 265, 547	0
1	D	772/827 (93%)	0.32	35 (4%) 31 29	27, 135, 292, 515	0
All	All	3088/3308 (93%)	0.36	195 (6%) 19 21	27, 151, 277, 547	0

All (195) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	571	PHE	11.3
1	C	572	GLY	10.6
1	C	570	GLU	10.5
1	A	309	ARG	9.6
1	A	837	BMA	9.1
1	C	391	GLU	8.9
1	A	310	GLY	8.8
1	C	389	GLY	8.3
1	D	629	MET	8.2
1	C	573	ILE	8.1
1	C	392	GLN	7.4
1	D	816	TYR	7.0
1	C	575	ASN	6.8
1	C	577	LEU	6.8
1	C	568	THR	6.7
1	A	311	ASN	6.4
1	D	817	LYS	6.2
1	C	574	PHE	6.1
1	A	308	ARG	6.1
1	D	569	ASN	5.9
1	B	389	GLY	5.9

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Mol	Chain	Res	Type	RSRZ
1	B	568	THR	5.8
1	B	390	LEU	5.7
1	D	815	CYS	5.7
1	A	71	TYR	5.6
1	B	391	GLU	5.6
1	B	392	GLN	5.4
1	D	568	THR	5.4
1	D	628	ARG	5.4
1	D	570	GLU	5.3
1	C	386	ASP	5.2
1	D	71	TYR	5.2
1	C	569	ASN	5.1
1	C	388	SER	4.9
1	B	393	LYS	4.9
1	B	444	ILE	4.9
1	D	756	GLN	4.8
1	A	306	ILE	4.7
1	B	442	LEU	4.7
1	C	816	TYR	4.7
1	D	814	PHE	4.6
1	C	543	VAL	4.6
1	A	684	ARG	4.6
1	C	815	CYS	4.6
1	C	306	ILE	4.4
1	A	679	PRO	4.4
1	C	390	LEU	4.3
1	C	436	CYS	4.3
1	B	518	LEU	4.3
1	B	521	LEU	4.2
1	C	813	GLU	4.2
1	C	435	HIS	4.2
1	B	388	SER	4.2
1	D	627	GLU	4.1
1	D	410	LYS	4.1
1	B	385	ASP	3.9
1	C	576	SER	3.8
1	B	523	TYR	3.8
1	D	631	SER	3.7
1	C	385	ASP	3.7
1	B	175	GLU	3.7
1	D	630	VAL	3.7
1	A	583	ALA	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	683	VAL	3.7
1	B	659	PHE	3.6
1	A	312	ALA	3.6
1	C	578	TRP	3.5
1	B	438	PHE	3.5
1	B	519	ASP	3.5
1	A	651	ASP	3.4
1	B	387	THR	3.4
1	B	512	PRO	3.4
1	B	593	PRO	3.4
1	C	585	MET	3.3
1	D	328	GLU	3.3
1	A	408	MET	3.2
1	B	72	ALA	3.2
1	B	394	THR	3.2
1	D	524	GLU	3.1
1	A	213	LYS	3.1
1	B	421	TYR	3.1
1	C	584	PHE	3.1
1	B	511	LYS	3.1
1	D	409	LYS	3.1
1	B	815	CYS	3.1
1	C	387	THR	3.1
1	B	667	PHE	3.0
1	B	685	THR	3.0
1	D	408	MET	3.0
1	C	511	LYS	3.0
1	C	633	ILE	3.0
1	C	812	ILE	3.0
1	C	544	SER	3.0
1	B	665	ALA	3.0
1	C	810	ALA	3.0
1	B	811	LEU	3.0
1	A	835	NAG	3.0
1	C	384	GLU	3.0
1	D	632	PRO	3.0
1	A	523	TYR	3.0
1	B	664	ILE	3.0
1	A	836	BMA	2.9
1	C	393	LYS	2.9
1	B	666	VAL	2.9
1	B	520	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	399	THR	2.9
1	B	684	ARG	2.9
1	B	522	ALA	2.8
1	B	636	ALA	2.8
1	D	507	PRO	2.8
1	C	307	SER	2.8
1	B	20	ARG	2.8
1	D	508	GLN	2.8
1	A	568	THR	2.7
1	C	509	LYS	2.7
1	B	33	MET	2.7
1	C	432	ILE	2.7
1	C	785	SER	2.7
1	C	460	TRP	2.7
1	D	411	ASN	2.7
1	B	71	TYR	2.7
1	A	834	NAG	2.7
1	A	401	LEU	2.7
1	B	569	ASN	2.7
1	D	72	ALA	2.7
1	A	392	GLN	2.7
1	C	510	SER	2.7
1	C	688	GLU	2.6
1	D	757	GLY	2.6
1	B	400	ILE	2.6
1	C	581	LEU	2.6
1	B	39	SER	2.6
1	A	391	GLU	2.6
1	A	682	PHE	2.6
1	B	816	TYR	2.6
1	A	686	THR	2.6
1	A	582	GLY	2.6
1	C	814	PHE	2.5
1	A	12	ILE	2.5
1	B	440	TYR	2.5
1	B	510	SER	2.5
1	C	689	GLY	2.5
1	C	811	LEU	2.5
1	A	569	ASN	2.4
1	B	251	ASP	2.4
1	A	576	SER	2.4
1	B	686	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	836	BMA	2.4
1	C	645	ILE	2.4
1	B	386	ASP	2.4
1	A	652	SER	2.4
1	A	187	LYS	2.4
1	D	266	GLU	2.4
1	B	526	TRP	2.3
1	D	813	GLU	2.3
1	B	92	LEU	2.3
1	B	814	PHE	2.3
1	C	308	ARG	2.3
1	B	401	LEU	2.3
1	A	20	ARG	2.3
1	A	313	GLY	2.3
1	A	650	LEU	2.3
1	D	643	THR	2.3
1	A	573	ILE	2.2
1	C	71	TYR	2.2
1	B	168	ILE	2.2
1	B	515	PHE	2.2
1	B	570	GLU	2.2
1	C	817	LYS	2.2
1	C	787	LEU	2.2
1	A	680	SER	2.2
1	A	394	THR	2.2
1	C	421	TYR	2.2
1	B	662	SER	2.1
1	A	570	GLU	2.1
1	A	43	LEU	2.1
1	D	686	THR	2.1
1	C	159	GLN	2.1
1	C	453	ARG	2.1
1	B	687	ALA	2.1
1	D	571	PHE	2.1
1	A	575	ASN	2.1
1	A	572	GLY	2.1
1	D	383	THR	2.1
1	B	436	CYS	2.1
1	B	416	GLU	2.1
1	C	786	ALA	2.0
1	D	523	TYR	2.0
1	D	372	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	415	LEU	2.0
1	B	196	CYS	2.0
1	A	378	ASP	2.0
1	C	408	MET	2.0
1	B	395	VAL	2.0
1	D	758	VAL	2.0

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

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	NAG	A	834	14/15	0.64	16.67	227,227,227,227	0
1	BMA	B	837	11/12	0.44	4.50	231,231,231,231	0
1	NAG	D	835	14/15	0.26	3.44	294,294,294,294	0
1	NAG	B	834	14/15	0.52	2.65	167,167,167,167	0
1	NAG	C	834	14/15	0.53	2.47	211,211,211,211	0
1	NAG	D	834	14/15	0.30	1.52	336,336,336,336	0
1	BMA	B	836	11/12	0.40	-	232,232,232,232	0
1	BMA	D	836	11/12	0.22	-	233,233,233,233	0
1	BMA	D	837	11/12	0.24	-	264,264,264,264	0
1	BMA	A	837	11/12	1.82	-	269,269,269,269	0
1	BMA	C	837	11/12	0.54	-	287,287,287,287	0
1	NAG	A	835	14/15	0.68	-	269,269,269,269	0
1	BMA	C	836	11/12	0.70	-	254,254,254,254	0
1	NAG	C	835	14/15	0.43	-	225,225,225,225	0
1	NAG	B	835	14/15	0.26	-	180,180,180,180	0
1	BMA	A	836	11/12	0.79	-	280,280,280,280	0

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.