



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 13, 2016 – 02:25 PM EDT

PDB ID : 5L1E  
Title : AMPA subtype ionotropic glutamate receptor GluA2 in complex with non-competitive inhibitor CP465022  
Authors : Yelshanskaya, M.V.; Singh, A.K.; Sampson, J.M.; Sobolevsky, A.I.  
Deposited on : 2016-07-29  
Resolution : 4.37 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027939  
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) : rb-20027939

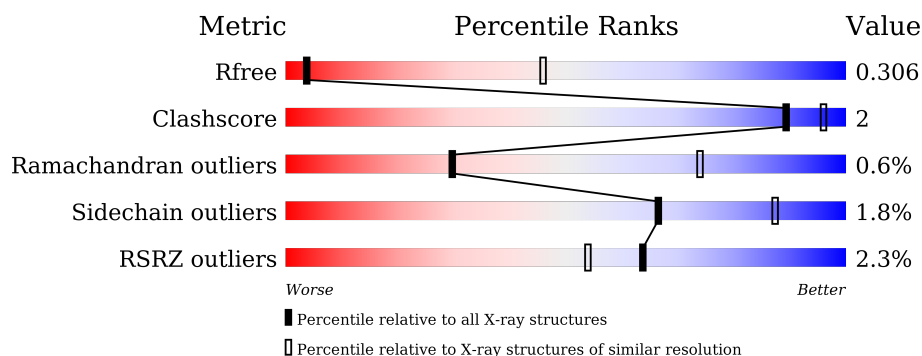
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.37 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	1063 (5.08-3.60)
Clashscore	102246	1171 (5.08-3.60)
Ramachandran outliers	100387	1110 (5.08-3.60)
Sidechain outliers	100360	1093 (5.08-3.60)
RSRZ outliers	91569	1067 (5.08-3.60)

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

Mol	Chain	Length	Quality of chain
1	A	803	<div> <div>2%</div> <div>91% 6% .</div> </div>
1	B	803	<div> <div>2%</div> <div>86% 10% .</div> </div>
1	C	803	<div> <div>3%</div> <div>88% 7% . .</div> </div>
1	D	803	<div> <div>2%</div> <div>92% 5% .</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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	C	901	-	-	-	X
3	6ZQ	A	902	-	-	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 24092 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 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	777	Total	C	N	O	S	0	0	0
			5986	3847	992	1118	29			
1	B	773	Total	C	N	O	S	0	0	0
			5993	3846	989	1129	29			
1	C	773	Total	C	N	O	S	0	0	0
			5952	3825	985	1114	28			
1	D	777	Total	C	N	O	S	0	0	0
			5972	3835	990	1120	27			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	241	GLU	ASN	engineered mutation	UNP P19491
A	?	-	VAL	deletion	UNP P19491
A	?	-	THR	deletion	UNP P19491
A	?	-	LEU	deletion	UNP P19491
A	?	-	PRO	deletion	UNP P19491
A	?	-	SER	deletion	UNP P19491
A	?	-	GLY	deletion	UNP P19491
A	385	ASP	ASN	engineered mutation	UNP P19491
A	392	GLN	ASN	engineered mutation	UNP P19491
A	564	ASP	-	linker	UNP P19491
A	565	THR	-	linker	UNP P19491
A	566	ASP	-	linker	UNP P19491
A	589	ALA	CYS	engineered mutation	UNP P19491
A	827	GLY	-	cloning artifact	UNP P19491
A	828	LEU	-	cloning artifact	UNP P19491
A	829	VAL	-	cloning artifact	UNP P19491
A	830	PRO	-	cloning artifact	UNP P19491
A	831	ARG	-	cloning artifact	UNP P19491
B	241	GLU	ASN	engineered mutation	UNP P19491
B	?	-	VAL	deletion	UNP P19491
B	?	-	THR	deletion	UNP P19491

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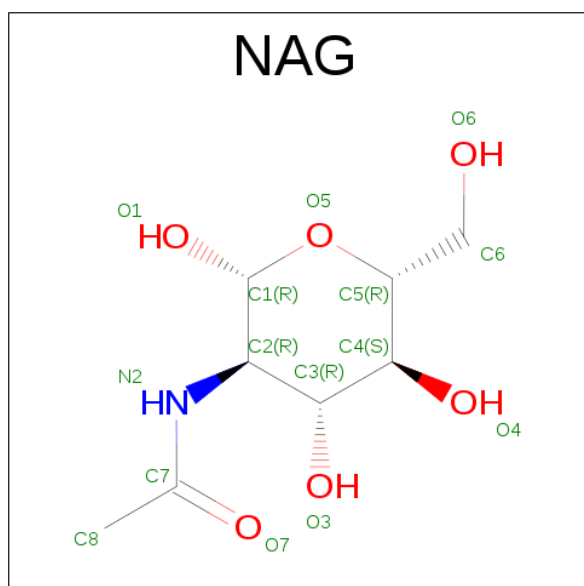
Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	LEU	deletion	UNP P19491
B	?	-	PRO	deletion	UNP P19491
B	?	-	SER	deletion	UNP P19491
B	?	-	GLY	deletion	UNP P19491
B	385	ASP	ASN	engineered mutation	UNP P19491
B	392	GLN	ASN	engineered mutation	UNP P19491
B	564	ASP	-	linker	UNP P19491
B	565	THR	-	linker	UNP P19491
B	566	ASP	-	linker	UNP P19491
B	589	ALA	CYS	engineered mutation	UNP P19491
B	827	GLY	-	cloning artifact	UNP P19491
B	828	LEU	-	cloning artifact	UNP P19491
B	829	VAL	-	cloning artifact	UNP P19491
B	830	PRO	-	cloning artifact	UNP P19491
B	831	ARG	-	cloning artifact	UNP P19491
C	241	GLU	ASN	engineered mutation	UNP P19491
C	?	-	VAL	deletion	UNP P19491
C	?	-	THR	deletion	UNP P19491
C	?	-	LEU	deletion	UNP P19491
C	?	-	PRO	deletion	UNP P19491
C	?	-	SER	deletion	UNP P19491
C	?	-	GLY	deletion	UNP P19491
C	385	ASP	ASN	engineered mutation	UNP P19491
C	392	GLN	ASN	engineered mutation	UNP P19491
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C	565	THR	-	linker	UNP P19491
C	566	ASP	-	linker	UNP P19491
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C	827	GLY	-	cloning artifact	UNP P19491
C	828	LEU	-	cloning artifact	UNP P19491
C	829	VAL	-	cloning artifact	UNP P19491
C	830	PRO	-	cloning artifact	UNP P19491
C	831	ARG	-	cloning artifact	UNP P19491
D	241	GLU	ASN	engineered mutation	UNP P19491
D	?	-	VAL	deletion	UNP P19491
D	?	-	THR	deletion	UNP P19491
D	?	-	LEU	deletion	UNP P19491
D	?	-	PRO	deletion	UNP P19491
D	?	-	SER	deletion	UNP P19491
D	?	-	GLY	deletion	UNP P19491
D	385	ASP	ASN	engineered mutation	UNP P19491
D	392	GLN	ASN	engineered mutation	UNP P19491

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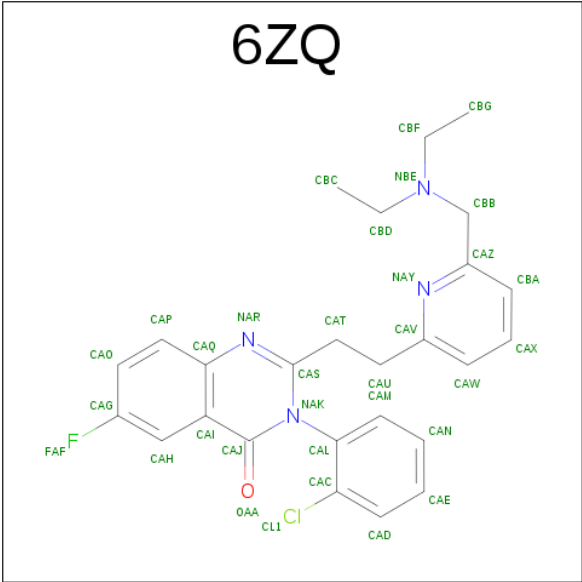
Chain	Residue	Modelled	Actual	Comment	Reference
D	564	ASP	-	linker	UNP P19491
D	565	THR	-	linker	UNP P19491
D	566	ASP	-	linker	UNP P19491
D	589	ALA	CYS	engineered mutation	UNP P19491
D	827	GLY	-	cloning artifact	UNP P19491
D	828	LEU	-	cloning artifact	UNP P19491
D	829	VAL	-	cloning artifact	UNP P19491
D	830	PRO	-	cloning artifact	UNP P19491
D	831	ARG	-	cloning artifact	UNP P19491

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			15	8	1	6		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is 3-(2-chlorophenyl)-2-(2-{6-[(diethylamino)methyl]pyridin-2-yl}ethyl)-6-fluoroquinazolin-4(3H)-one (three-letter code: 6ZQ) (formula:  $C_{26}H_{26}ClFN_4O$ ).

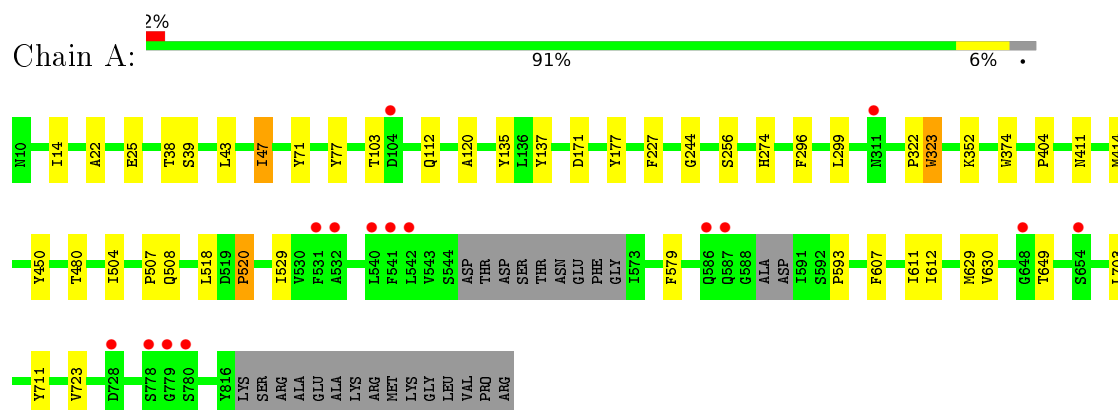


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	Cl	F	N	O	0	0
			33	26	1	1	4	1		
3	B	1	Total	C	Cl	F	N	O	0	0
			33	26	1	1	4	1		
3	C	1	Total	C	Cl	F	N	O	0	0
			33	26	1	1	4	1		
3	D	1	Total	C	Cl	F	N	O	0	0
			33	26	1	1	4	1		

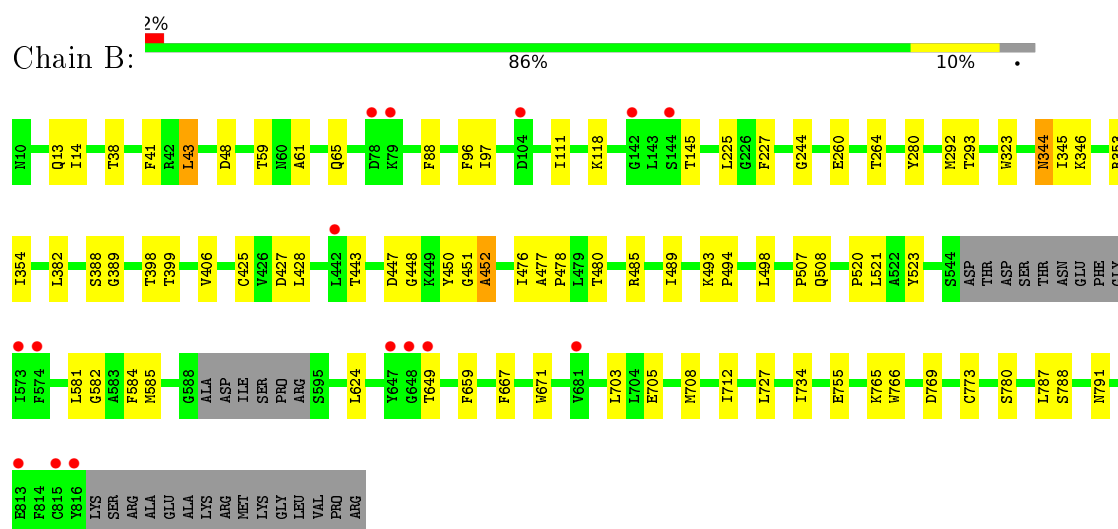
### 3 Residue-property plots

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.

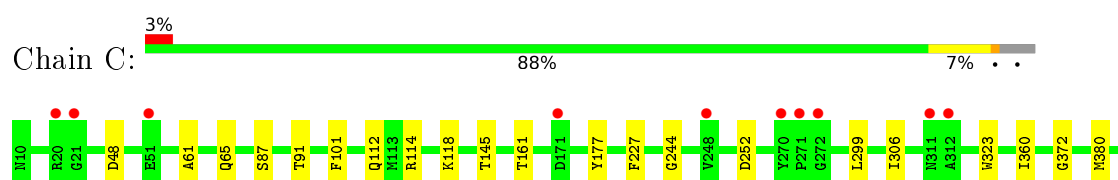
#### • Molecule 1: Glutamate receptor 2



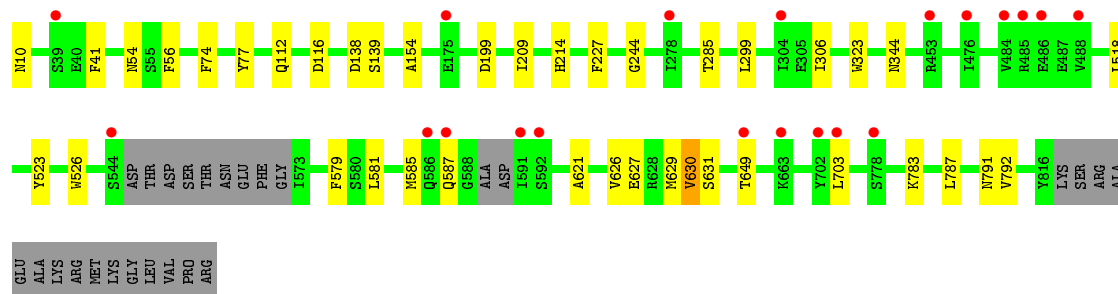
#### • Molecule 1: Glutamate receptor 2



#### • Molecule 1: Glutamate receptor 2







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	92.68Å 109.86Å 602.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.02 – 4.37 49.02 – 4.37	Depositor EDS
% Data completeness (in resolution range)	97.9 (49.02-4.37) 98.5 (49.02-4.37)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.52 (at 4.45Å)	Xtriage
Refinement program	PHENIX (1.10.1 _2155: ???)	Depositor
R, $R_{free}$	0.239 , 0.292 0.262 , 0.306	Depositor DCC
$R_{free}$ test set	2025 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	238.0	Xtriage
Anisotropy	0.187	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.22 , 224.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.35$ , $\langle L^2 \rangle = 0.18$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.85	EDS
Total number of atoms	24092	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	275.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.12% 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: 6ZQ, NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.24	0/6109	0.41	0/8269
1	B	0.25	0/6115	0.43	0/8274
1	C	0.31	1/6074 (0.0%)	0.45	3/8225 (0.0%)
1	D	0.24	0/6095	0.41	0/8255
All	All	0.26	1/24393 (0.0%)	0.42	3/33023 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	629	MET	C-N	14.61	1.67	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	629	MET	C-N-CA	7.13	139.53	121.70
1	C	388	SER	CA-C-N	5.21	126.62	116.20
1	C	632	PRO	CA-C-N	5.00	128.21	117.20

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5986	0	5886	20	0
1	B	5993	0	5913	42	0
1	C	5952	0	5839	40	0
1	D	5972	0	5848	22	0
2	A	15	0	15	0	0
2	B	14	0	13	0	0
2	C	14	0	13	0	0
2	D	14	0	13	0	0
3	A	33	0	0	1	0
3	B	33	0	0	1	0
3	C	33	0	0	2	0
3	D	33	0	0	3	0
All	All	24092	0	23540	115	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 2.

All (115) 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:C:629:MET:C	1:C:630:VAL:N	1.67	1.45
1:C:631:SER:OG	1:C:632:PRO:C	2.06	0.93
1:D:630:VAL:HG23	3:D:902:6ZQ:CBG	2.02	0.89
1:C:626:VAL:HG11	1:D:783:LYS:O	1.82	0.79
1:C:631:SER:OG	1:C:632:PRO:O	2.01	0.78
1:D:630:VAL:CG2	3:D:902:6ZQ:CBG	2.61	0.78
1:B:451:GLY:HA2	1:B:452:ALA:HB3	1.67	0.77
1:C:630:VAL:HG12	1:C:632:PRO:HA	1.70	0.71
1:C:631:SER:OG	1:C:632:PRO:CA	2.41	0.68
1:C:629:MET:CA	1:C:630:VAL:N	2.59	0.65
1:C:388:SER:CB	1:C:389:GLY:HA2	2.27	0.64
1:C:360:ILE:HB	1:C:372:GLY:HA3	1.81	0.61
1:B:97:ILE:HD13	1:B:292:MET:HG2	1.83	0.61
1:C:87:SER:OG	1:D:54:ASN:OD1	2.20	0.59
1:D:629:MET:O	1:D:631:SER:N	2.36	0.58
1:B:447:ASP:N	1:B:448:GLY:HA2	2.19	0.57
1:A:649:THR:HG22	1:A:703:LEU:HB2	1.86	0.56
1:C:649:THR:HG22	1:C:703:LEU:HB2	1.89	0.55
1:D:518:LEU:H	1:D:518:LEU:HD23	1.72	0.55
1:C:630:VAL:HG12	1:C:632:PRO:CA	2.41	0.51
1:D:227:PHE:CD2	1:D:244:GLY:HA3	2.45	0.51
1:B:476:ILE:HG22	1:B:734:ILE:HG12	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:346:LYS:HG3	1:B:354:ILE:HG13	1.93	0.51
1:C:118:LYS:HG2	1:C:145:THR:HG22	1.93	0.50
1:B:14:ILE:HD12	1:B:43:LEU:HB3	1.94	0.50
1:B:43:LEU:HD21	1:B:293:THR:HG22	1.93	0.50
1:B:227:PHE:CD1	1:B:244:GLY:HA3	2.47	0.50
1:A:135:TYR:CE1	1:A:137:TYR:HB3	2.46	0.50
1:A:47:ILE:HD13	1:A:47:ILE:H	1.76	0.50
1:C:632:PRO:HD2	1:C:633:ILE:HB	1.94	0.49
1:C:630:VAL:HG12	1:C:631:SER:N	2.26	0.49
1:B:521:LEU:HD12	1:C:787:LEU:HD21	1.93	0.49
1:C:631:SER:OG	1:C:632:PRO:HA	2.11	0.49
1:A:411:ASN:HB2	1:A:414:MET:HE2	1.94	0.49
1:A:14:ILE:HD13	1:A:43:LEU:HD23	1.95	0.49
1:D:299:LEU:HD13	1:D:306:ILE:HG21	1.95	0.49
1:C:618:ALA:HA	1:D:621:ALA:HB2	1.95	0.48
1:A:227:PHE:CD1	1:A:244:GLY:HA3	2.49	0.48
1:C:520:PRO:HD3	3:C:902:6ZQ:NAR	2.28	0.48
1:A:103:THR:O	1:A:352:LYS:NZ	2.46	0.48
1:B:581:LEU:HA	1:B:584:PHE:HB3	1.96	0.48
1:C:627:GLU:O	1:C:630:VAL:HG23	2.14	0.47
1:B:48:ASP:OD1	1:B:65:GLN:NE2	2.47	0.47
1:C:161:THR:HG23	1:D:154:ALA:HB2	1.96	0.47
1:B:667:PHE:HE1	1:B:727:LEU:HD13	1.80	0.47
1:A:71:TYR:HA	1:A:323:TRP:HH2	1.80	0.47
1:A:607:PHE:O	1:A:611:ILE:HG12	2.15	0.47
1:B:649:THR:HG22	1:B:703:LEU:HB2	1.97	0.47
1:A:529:ILE:HD13	1:A:612:ILE:HD12	1.97	0.46
1:B:260:GLU:O	1:B:264:THR:OG1	2.34	0.46
1:D:626:VAL:HG12	1:D:627:GLU:N	2.29	0.46
1:B:498:LEU:HD13	1:B:705:GLU:HB2	1.98	0.46
1:B:755:GLU:OE2	1:C:483:LEU:N	2.44	0.46
1:A:22:ALA:HB1	1:A:25:GLU:HB2	1.98	0.46
1:B:398:THR:HA	1:B:443:THR:O	2.16	0.45
1:C:474:ILE:HG13	1:C:736:THR:HG22	1.97	0.45
1:B:582:GLY:HA2	1:B:585:MET:HE3	1.97	0.45
1:B:118:LYS:HB3	1:B:145:THR:HG22	1.99	0.45
1:A:171:ASP:N	1:A:171:ASP:OD1	2.46	0.45
1:C:101:PHE:HA	1:C:114:ARG:HD2	1.98	0.45
1:C:754:SER:HB2	1:C:759:LEU:HD12	1.97	0.45
1:D:649:THR:HG22	1:D:703:LEU:HB2	1.98	0.45
1:A:520:PRO:HD3	3:A:902:6ZQ:NAR	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:518:LEU:HB2	1:D:526:TRP:CD1	2.52	0.45
1:B:388:SER:HA	1:B:389:GLY:HA3	1.77	0.44
1:B:708:MET:O	1:B:712:ILE:HG12	2.17	0.44
1:C:620:LEU:HD11	3:C:902:6ZQ:CL1	2.54	0.44
1:C:600:ILE:HG22	1:D:581:LEU:HD23	2.00	0.44
1:B:477:ALA:HB1	1:B:478:PRO:HD2	2.00	0.43
1:A:120:ALA:HB2	1:A:374:TRP:NE1	2.33	0.43
1:B:225:LEU:HB2	1:B:280:TYR:CD2	2.53	0.43
1:B:61:ALA:O	1:B:65:GLN:HG2	2.18	0.43
1:C:494:PRO:HA	1:C:732:TYR:O	2.18	0.43
1:B:427:ASP:OD2	1:B:766:TRP:NE1	2.41	0.43
1:C:227:PHE:CD2	1:C:244:GLY:HA3	2.53	0.43
1:D:787:LEU:HD21	1:D:792:VAL:HG21	1.99	0.43
1:B:765:LYS:O	1:B:769:ASP:HB2	2.19	0.43
1:B:96:PHE:O	1:B:111:ILE:N	2.43	0.43
1:C:299:LEU:HD13	1:C:306:ILE:HG21	2.01	0.43
1:A:507:PRO:HA	1:A:508:GLN:CB	2.49	0.43
1:C:91:THR:HG21	1:D:56:PHE:CE1	2.54	0.43
1:D:138:ASP:OD1	1:D:139:SER:N	2.52	0.43
1:D:10:ASN:HB2	1:D:41:PHE:HA	2.01	0.43
1:B:787:LEU:HD22	1:B:788:SER:H	1.85	0.42
1:C:403:SER:HA	1:C:404:PRO:HA	1.82	0.42
1:C:607:PHE:O	1:C:611:ILE:HG12	2.19	0.42
1:D:209:ILE:HA	1:D:214:HIS:CD2	2.54	0.42
1:B:344:ASN:O	1:B:353:ARG:NH2	2.50	0.42
1:C:630:VAL:CG1	1:C:631:SER:N	2.82	0.42
1:B:624:LEU:HD11	3:B:902:6ZQ:CL1	2.56	0.42
1:A:411:ASN:OD1	1:A:411:ASN:N	2.51	0.42
1:C:529:ILE:HD13	1:C:612:ILE:HD12	2.02	0.42
1:B:485:ARG:O	1:B:489:ILE:HG13	2.20	0.42
1:C:61:ALA:O	1:C:65:GLN:HG2	2.19	0.42
1:B:344:ASN:HD22	1:B:345:ILE:N	2.17	0.41
1:B:507:PRO:N	1:B:508:GLN:HA	2.35	0.41
1:B:399:THR:HG21	1:B:406:VAL:HG21	2.02	0.41
1:C:447:ASP:N	1:C:447:ASP:OD1	2.52	0.41
1:D:74:PHE:CZ	1:D:285:THR:HG23	2.55	0.41
1:A:404:PRO:HB3	1:A:711:TYR:CZ	2.56	0.41
1:B:507:PRO:HD2	1:B:508:GLN:HA	2.01	0.41
1:B:494:PRO:HG3	1:C:494:PRO:HG3	2.02	0.41
1:A:38:THR:OG1	1:A:39:SER:N	2.54	0.41
1:B:425:CYS:HA	1:B:428:LEU:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:THR:HG23	1:B:41:PHE:H	1.85	0.41
1:B:659:PHE:HB3	1:B:671:TRP:HB2	2.02	0.41
1:A:296:PHE:HA	1:A:299:LEU:HD12	2.03	0.41
1:C:477:ALA:HB1	1:C:478:PRO:HD2	2.03	0.41
1:B:507:PRO:CD	1:B:508:GLN:HA	2.51	0.41
1:B:493:LYS:HB3	1:B:494:PRO:HD2	2.03	0.41
1:C:518:LEU:HB2	1:C:526:TRP:CD1	2.56	0.41
1:B:59:THR:HG23	1:B:88:PHE:CZ	2.57	0.40
1:D:626:VAL:CG1	1:D:627:GLU:N	2.84	0.40
1:D:630:VAL:HG21	3:D:902:6ZQ:CBG	2.50	0.40
1:A:504:ILE:HD11	1:A:723:VAL:HG11	2.03	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	771/803 (96%)	723 (94%)	44 (6%)	4 (0%)	34	77
1	B	767/803 (96%)	714 (93%)	50 (6%)	3 (0%)	39	80
1	C	767/803 (96%)	718 (94%)	41 (5%)	8 (1%)	19	65
1	D	771/803 (96%)	722 (94%)	47 (6%)	2 (0%)	46	83
All	All	3076/3212 (96%)	2877 (94%)	182 (6%)	17 (1%)	30	74

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	388	SER
1	C	630	VAL
1	C	743	GLY
1	C	786	ALA

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Mol	Chain	Res	Type
1	D	587	GLN
1	A	520	PRO
1	B	780	SER
1	C	587	GLN
1	B	452	ALA
1	B	520	PRO
1	A	630	VAL
1	C	380	MET
1	C	520	PRO
1	A	322	PRO
1	C	633	ILE
1	D	630	VAL
1	A	593	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	627/683 (92%)	615 (98%)	12 (2%)	65	86
1	B	636/683 (93%)	626 (98%)	10 (2%)	70	88
1	C	622/683 (91%)	610 (98%)	12 (2%)	65	86
1	D	623/683 (91%)	613 (98%)	10 (2%)	70	88
All	All	2508/2732 (92%)	2464 (98%)	44 (2%)	66	87

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	ILE
1	A	77	TYR
1	A	112	GLN
1	A	177	TYR
1	A	256	SER
1	A	274	HIS
1	A	323	TRP
1	A	450	TYR

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Mol	Chain	Res	Type
1	A	480	THR
1	A	518	LEU
1	A	579	PHE
1	A	629	MET
1	B	13	GLN
1	B	43	LEU
1	B	323	TRP
1	B	344	ASN
1	B	382	LEU
1	B	450	TYR
1	B	480	THR
1	B	523	TYR
1	B	773	CYS
1	B	791	ASN
1	C	48	ASP
1	C	112	GLN
1	C	177	TYR
1	C	252	ASP
1	C	323	TRP
1	C	394	THR
1	C	480	THR
1	C	518	LEU
1	C	523	TYR
1	C	585	MET
1	C	629	MET
1	C	638	ASP
1	D	77	TYR
1	D	112	GLN
1	D	116	ASP
1	D	199	ASP
1	D	323	TRP
1	D	344	ASN
1	D	523	TYR
1	D	579	PHE
1	D	585	MET
1	D	791	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	344	ASN
1	C	344	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
2	NAG	A	901	-	15,15,15	0.12	0	17,21,21	0.20	0
3	6ZQ	A	902	-	36,36,36	1.44	5 (13%)	37,50,50	1.59	7 (18%)
2	NAG	B	901	-	14,14,15	0.32	0	15,19,21	0.40	0
3	6ZQ	B	902	-	36,36,36	1.44	5 (13%)	37,50,50	1.50	6 (16%)
2	NAG	C	901	-	14,14,15	0.38	0	15,19,21	0.52	0
3	6ZQ	C	902	-	36,36,36	1.47	5 (13%)	37,50,50	1.54	6 (16%)
2	NAG	D	901	-	14,14,15	0.28	0	15,19,21	0.25	0
3	6ZQ	D	902	-	36,36,36	1.43	4 (11%)	37,50,50	1.56	8 (21%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	901	-	-	0/6/26/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	6ZQ	A	902	-	-	0/17/17/17	0/4/4/4
2	NAG	B	901	-	-	0/6/23/26	0/1/1/1
3	6ZQ	B	902	-	-	0/17/17/17	0/4/4/4
2	NAG	C	901	-	-	0/6/23/26	0/1/1/1
3	6ZQ	C	902	-	-	0/17/17/17	0/4/4/4
2	NAG	D	901	-	-	0/6/23/26	0/1/1/1
3	6ZQ	D	902	-	-	0/17/17/17	0/4/4/4

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	902	6ZQ	CAJ-NAK	-2.57	1.33	1.37
3	B	902	6ZQ	CAJ-NAK	-2.49	1.33	1.37
3	D	902	6ZQ	CAJ-NAK	-2.38	1.33	1.37
3	A	902	6ZQ	CAI-CAQ	-2.27	1.36	1.41
3	D	902	6ZQ	CAI-CAQ	-2.26	1.36	1.41
3	B	902	6ZQ	CAI-CAQ	-2.24	1.36	1.41
3	C	902	6ZQ	CAI-CAQ	-2.22	1.36	1.41
3	C	902	6ZQ	CAJ-NAK	-2.09	1.34	1.37
3	A	902	6ZQ	CAH-CAG	2.02	1.39	1.35
3	B	902	6ZQ	CAH-CAG	2.03	1.39	1.35
3	B	902	6ZQ	CAC-CL1	2.03	1.78	1.73
3	A	902	6ZQ	CAC-CL1	2.04	1.78	1.73
3	D	902	6ZQ	CAC-CL1	2.05	1.79	1.73
3	C	902	6ZQ	CAC-CL1	2.07	1.79	1.73
3	C	902	6ZQ	CAH-CAG	2.27	1.40	1.35
3	A	902	6ZQ	OAA-CAJ	6.09	1.39	1.24
3	B	902	6ZQ	OAA-CAJ	6.20	1.40	1.24
3	D	902	6ZQ	OAA-CAJ	6.21	1.40	1.24
3	C	902	6ZQ	OAA-CAJ	6.42	1.40	1.24

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	902	6ZQ	CAI-CAQ-NAR	-3.97	118.66	123.22
3	D	902	6ZQ	CAI-CAQ-NAR	-3.93	118.70	123.22
3	C	902	6ZQ	CAI-CAQ-NAR	-3.88	118.76	123.22
3	B	902	6ZQ	CAI-CAQ-NAR	-3.80	118.85	123.22
3	A	902	6ZQ	CAT-CAU-CAV	-2.71	107.26	112.76
3	B	902	6ZQ	CAO-CAG-CAH	-2.34	120.04	123.26
3	A	902	6ZQ	CAO-CAG-CAH	-2.32	120.07	123.26
3	D	902	6ZQ	CAO-CAG-CAH	-2.27	120.13	123.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	902	6ZQ	CAT-CAU-CAV	-2.12	108.47	112.76
3	D	902	6ZQ	CAW-CAX-CBA	-2.09	117.22	120.25
3	C	902	6ZQ	CAT-CAU-CAV	-2.03	108.64	112.76
3	D	902	6ZQ	CBB-CAZ-NAY	2.26	119.59	115.85
3	A	902	6ZQ	CAD-CAC-CAL	2.47	119.93	118.60
3	C	902	6ZQ	CBB-CAZ-NAY	2.49	119.98	115.85
3	A	902	6ZQ	CBB-CAZ-NAY	2.52	120.03	115.85
3	B	902	6ZQ	CBB-CAZ-NAY	2.57	120.11	115.85
3	A	902	6ZQ	CAV-NAY-CAZ	2.60	121.32	118.15
3	D	902	6ZQ	CAV-NAY-CAZ	2.60	121.32	118.15
3	B	902	6ZQ	CAD-CAC-CAL	2.75	120.08	118.60
3	C	902	6ZQ	CAV-NAY-CAZ	2.76	121.51	118.15
3	B	902	6ZQ	CAV-NAY-CAZ	2.82	121.58	118.15
3	C	902	6ZQ	CAD-CAC-CAL	3.06	120.25	118.60
3	D	902	6ZQ	CAU-CAV-NAY	3.12	120.45	115.71
3	B	902	6ZQ	CAU-CAV-NAY	3.12	120.46	115.71
3	C	902	6ZQ	CAU-CAV-NAY	3.29	120.71	115.71
3	D	902	6ZQ	CAD-CAC-CAL	3.49	120.48	118.60
3	A	902	6ZQ	CAU-CAV-NAY	3.63	121.23	115.71

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	902	6ZQ	1	0
3	B	902	6ZQ	1	0
3	C	902	6ZQ	2	0
3	D	902	6ZQ	3	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	629:MET	C	630:VAL	N	1.67

## 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	777/803 (96%)	-0.24	15 (1%) 70 61	141, 251, 384, 431	0
1	B	773/803 (96%)	-0.18	15 (1%) 70 61	128, 237, 362, 483	0
1	C	773/803 (96%)	-0.06	21 (2%) 58 48	160, 288, 389, 435	0
1	D	777/803 (96%)	-0.15	20 (2%) 59 49	176, 299, 395, 443	0
All	All	3100/3212 (96%)	-0.16	71 (2%) 64 54	128, 272, 387, 483	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	816	TYR	6.8
1	D	702	TYR	5.2
1	C	20	ARG	5.1
1	A	778	SER	5.0
1	C	544	SER	5.0
1	A	779	GLY	4.9
1	D	703	LEU	4.3
1	C	510	SER	4.1
1	A	780	SER	4.1
1	C	21	GLY	4.0
1	C	647	TYR	3.9
1	B	104	ASP	3.9
1	B	648	GLY	3.8
1	C	311	ASN	3.7
1	D	649	THR	3.6
1	C	587	GLN	3.6
1	B	649	THR	3.3
1	C	509	LYS	3.2
1	D	663	LYS	3.2
1	B	573	ILE	3.2
1	B	813	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	540	LEU	3.1
1	A	311	ASN	3.1
1	C	51	GLU	3.1
1	D	485	ARG	3.0
1	A	648	GLY	3.0
1	D	778	SER	3.0
1	C	272	GLY	3.0
1	C	270	TYR	2.9
1	C	646	ALA	2.9
1	B	442	LEU	2.8
1	C	724	GLY	2.8
1	D	544	SER	2.8
1	C	588	GLY	2.7
1	D	486	GLU	2.7
1	D	587	GLN	2.7
1	D	476	ILE	2.7
1	D	591	ILE	2.7
1	A	532	ALA	2.7
1	C	536	VAL	2.7
1	D	39	SER	2.6
1	B	142	GLY	2.6
1	B	144	SER	2.6
1	D	484	VAL	2.5
1	D	304	ILE	2.5
1	D	488	VAL	2.5
1	A	587	GLN	2.4
1	A	586	GLN	2.4
1	D	175	GLU	2.4
1	C	271	PRO	2.3
1	A	654	SER	2.3
1	B	815	CYS	2.3
1	D	592	SER	2.3
1	A	541	PHE	2.2
1	B	681	VAL	2.2
1	D	278	ILE	2.2
1	C	171	ASP	2.2
1	D	586	GLN	2.2
1	C	408	MET	2.1
1	A	728	ASP	2.1
1	B	574	PHE	2.1
1	C	248	VAL	2.1
1	A	531	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	78	ASP	2.1
1	B	79	LYS	2.1
1	D	453	ARG	2.1
1	B	647	TYR	2.1
1	C	312	ALA	2.1
1	C	725	GLY	2.0
1	A	104	ASP	2.0
1	A	542	LEU	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](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAG	C	901	14/15	0.96	0.39	2.92	264,288,305,316	0
3	6ZQ	A	902	33/33	0.89	0.45	1.11	233,285,399,416	0
3	6ZQ	C	902	33/33	0.92	0.40	0.40	244,354,442,442	0
3	6ZQ	B	902	33/33	0.90	0.26	0.27	295,323,434,439	0
3	6ZQ	D	902	33/33	0.80	0.23	-0.43	240,314,354,385	0
2	NAG	A	901	15/15	0.94	0.15	-	72,132,149,152	0
2	NAG	D	901	14/15	0.71	0.57	-	228,316,336,339	0
2	NAG	B	901	14/15	0.97	0.22	-	196,210,271,277	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.