



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 15, 2016 – 05:10 PM EST

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 X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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-20028442
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-20028442

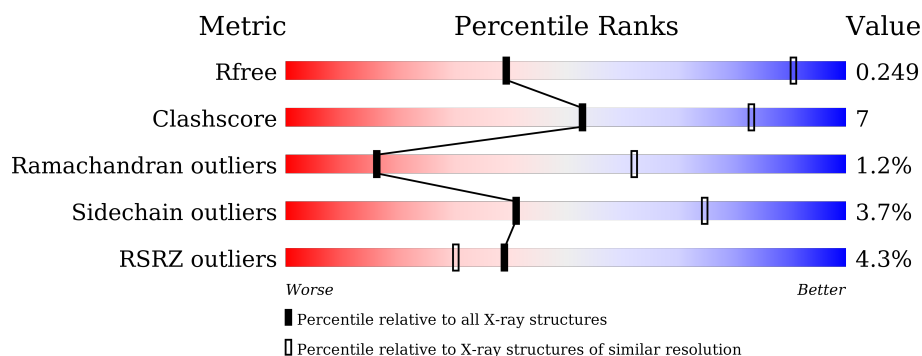
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.49 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}	91344	1071 (5.40-3.60)
Clashscore	102246	1003 (5.30-3.62)
Ramachandran outliers	100387	1117 (5.40-3.60)
Sidechain outliers	100360	1099 (5.40-3.60)
RSRZ outliers	91569	1075 (5.40-3.60)

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 ≥ 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	822	<div> <div>3%</div> <div> <div></div> <div>75%</div> <div>18%</div> <div>• 7%</div> </div> </div>
1	B	822	<div> <div>5%</div> <div> <div></div> <div>77%</div> <div>15%</div> <div>• 7%</div> </div> </div>
1	C	822	<div> <div>5%</div> <div> <div></div> <div>75%</div> <div>17%</div> <div>• 7%</div> </div> </div>
1	D	822	<div> <div>3%</div> <div> <div></div> <div>75%</div> <div>17%</div> <div>• 7%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	A	902	X	-	-	-
3	NAG	B	902	X	-	-	-
3	NAG	B	903	X	-	-	-
3	NAG	C	902	-	-	-	X
4	BMA	A	904	X	-	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 23812 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	768	Total	C	N	O	S	0	0	0
			5889	3781	971	1109	28			
1	B	768	Total	C	N	O	S	0	0	0
			5869	3767	961	1113	28			
1	C	768	Total	C	N	O	S	0	0	0
			5863	3763	963	1109	28			
1	D	768	Total	C	N	O	S	0	0	0
			5883	3776	966	1113	28			

There are 64 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	827	GLY	-	expression tag	UNP P19491
A	828	LEU	-	expression tag	UNP P19491
A	829	VAL	-	expression tag	UNP P19491
A	830	PRO	-	expression tag	UNP P19491
A	831	ARG	-	expression tag	UNP P19491
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

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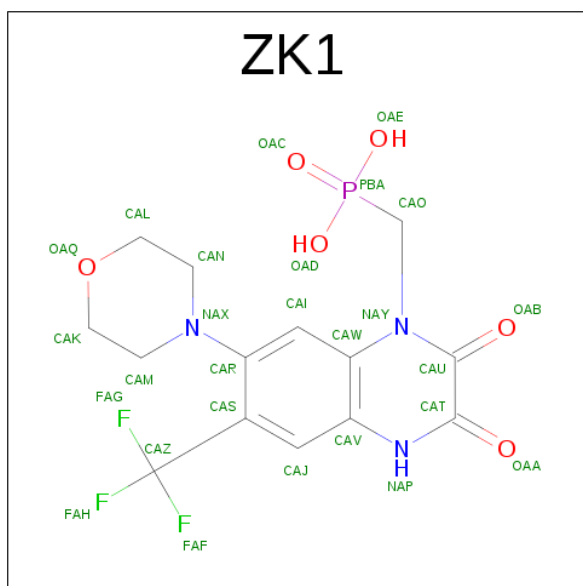
Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	LEU	deletion	UNP P19491
B	?	-	PRO	deletion	UNP P19491
B	?	-	SER	deletion	UNP P19491
B	384	GLU	GLY	conflict	UNP P19491
B	385	ASP	ASN	conflict	UNP P19491
B	392	GLN	ASN	conflict	UNP P19491
B	827	GLY	-	expression tag	UNP P19491
B	828	LEU	-	expression tag	UNP P19491
B	829	VAL	-	expression tag	UNP P19491
B	830	PRO	-	expression tag	UNP P19491
B	831	ARG	-	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	827	GLY	-	expression tag	UNP P19491
C	828	LEU	-	expression tag	UNP P19491
C	829	VAL	-	expression tag	UNP P19491
C	830	PRO	-	expression tag	UNP P19491
C	831	ARG	-	expression tag	UNP P19491
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	827	GLY	-	expression tag	UNP P19491
D	828	LEU	-	expression tag	UNP P19491
D	829	VAL	-	expression tag	UNP P19491
D	830	PRO	-	expression tag	UNP P19491

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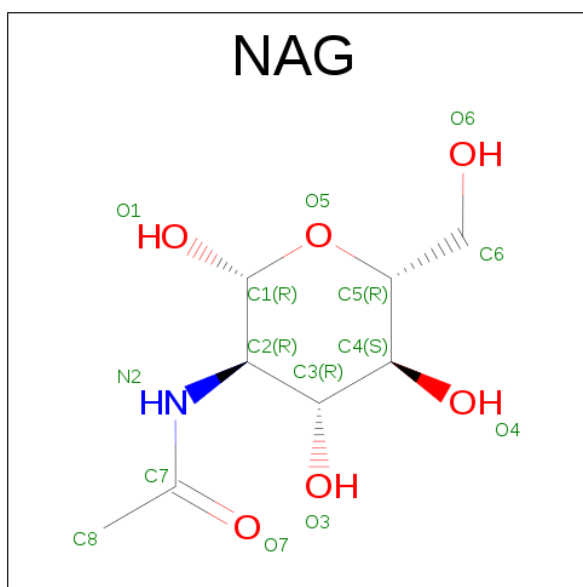
Chain	Residue	Modelled	Actual	Comment	Reference
D	831	ARG	-	expression tag	UNP P19491

- Molecule 2 is {[7-morpholin-4-yl-2,3-dioxo-6-(trifluoromethyl)-3,4-dihydroquinoxalin-1(2H)-yl]methyl}phosphonic acid (three-letter code: ZK1) (formula: C₁₄H₁₅F₃N₃O₆P).



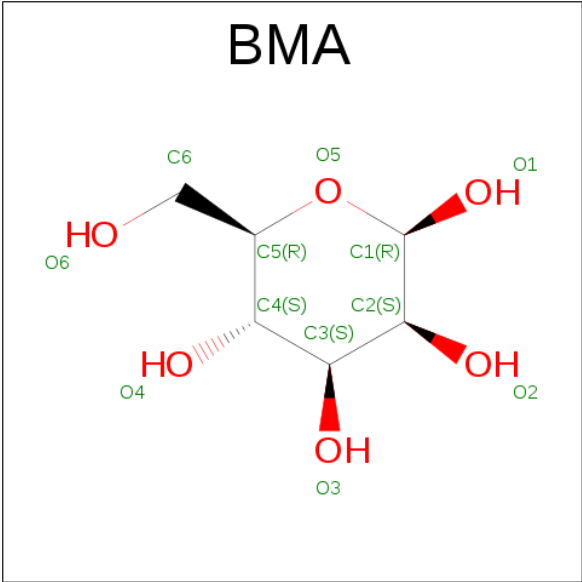
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	P	0	0
			27	14	3	3	6	1		
2	B	1	Total	C	F	N	O	P	0	0
			27	14	3	3	6	1		
2	C	1	Total	C	F	N	O	P	0	0
			27	14	3	3	6	1		
2	D	1	Total	C	F	N	O	P	0	0
			27	14	3	3	6	1		

- Molecule 3 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C₈H₁₅NO₆).

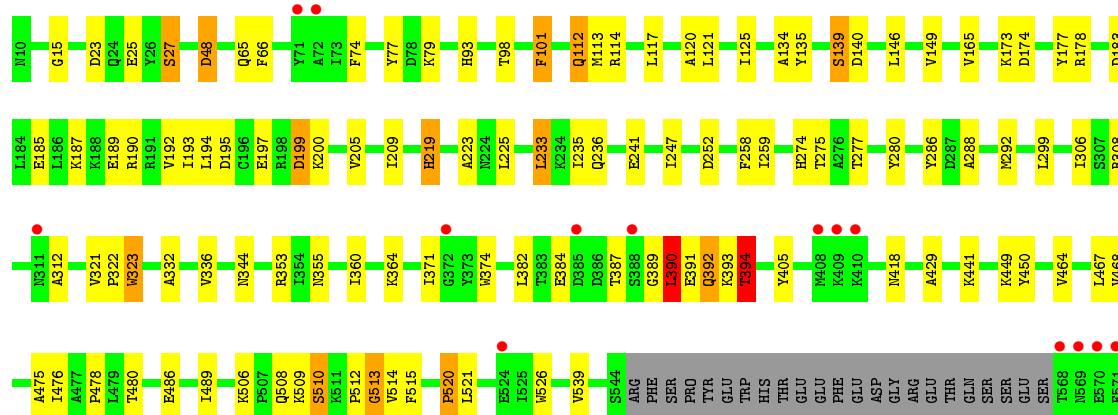


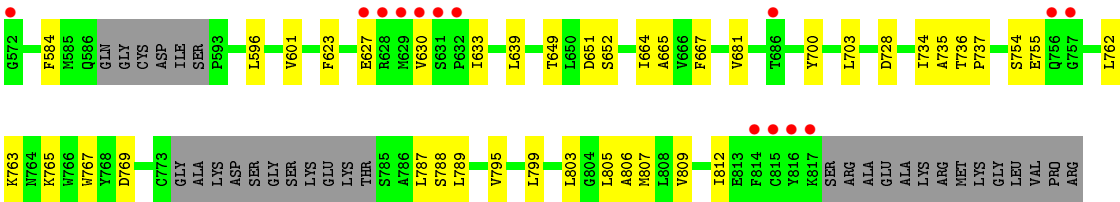
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1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

- Molecule 4 is BETA-D-MANNOSE (three-letter code: BMA) (formula: C₆H₁₂O₆).



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





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	92.00 Å 310.36 Å 109.50 Å 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
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 4.45 Å)	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 ²)	206.6	Xtriage
Anisotropy	0.230	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.21 , 94.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	23812	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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, 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

There are no bond length outliers.

There are no bond angle outliers.

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	5889	0	5738	87	0
1	B	5869	0	5680	85	0
1	C	5863	0	5672	85	0
1	D	5883	0	5713	84	0
2	A	27	0	13	0	0
2	B	27	0	13	0	0
2	C	27	0	13	0	0
2	D	27	0	13	0	0
3	A	28	0	24	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	28	0	24	0	0
3	C	28	0	24	0	0
3	D	28	0	24	1	0
4	A	22	0	19	0	0
4	B	22	0	19	0	0
4	C	22	0	19	0	0
4	D	22	0	19	0	0
All	All	23812	0	23027	307	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 (307) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:255:VAL:HG22	1:B:341:LEU:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:38:THR:OG1	1:C:39:SER:N	2.45	0.49
1:D:355:ASN:HB3	3:D:902: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	Interatomic distance (Å)	Clash overlap (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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:514:VAL:HG11	1:B:794:GLY:HA3	1.98	0.44
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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	760/822 (92%)	694 (91%)	57 (8%)	9 (1%)	16	62
1	B	760/822 (92%)	701 (92%)	52 (7%)	7 (1%)	21	67
1	C	760/822 (92%)	683 (90%)	70 (9%)	7 (1%)	21	67
1	D	760/822 (92%)	689 (91%)	58 (8%)	13 (2%)	11	56
All	All	3040/3288 (92%)	2767 (91%)	237 (8%)	36 (1%)	16	62

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

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Mol	Chain	Res	Type
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
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%)	61	85
1	B	611/702 (87%)	584 (96%)	27 (4%)	35	71
1	C	609/702 (87%)	587 (96%)	22 (4%)	42	75
1	D	614/702 (88%)	585 (95%)	29 (5%)	32	69
All	All	2449/2808 (87%)	2358 (96%)	91 (4%)	41	75

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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 [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](#)

20 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	ZK1	A	901	-	28,29,29	3.21	14 (50%)	35,45,45	1.89	5 (14%)
3	NAG	A	902	1,3	14,14,15	0.53	0	15,19,21	0.80	0
3	NAG	A	903	3,4	14,14,15	0.47	0	15,19,21	0.69	0
4	BMA	A	904	3,4	11,11,12	0.60	0	15,15,17	0.75	0
4	BMA	A	905	4	11,11,12	0.62	0	15,15,17	0.81	0
2	ZK1	B	901	-	28,29,29	3.19	14 (50%)	35,45,45	1.91	4 (11%)
3	NAG	B	902	1,3	14,14,15	0.53	0	15,19,21	0.65	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	B	903	3,4	14,14,15	0.44	0	15,19,21	1.08	2 (13%)
4	BMA	B	904	3,4	11,11,12	0.61	0	15,15,17	0.81	0
4	BMA	B	905	4	11,11,12	0.59	0	15,15,17	0.84	0
2	ZK1	C	901	-	28,29,29	3.17	12 (42%)	35,45,45	1.88	5 (14%)
3	NAG	C	902	1,3	14,14,15	0.56	0	15,19,21	0.77	0
3	NAG	C	903	3,4	14,14,15	0.51	0	15,19,21	0.66	0
4	BMA	C	904	3,4	11,11,12	0.60	0	15,15,17	0.79	0
4	BMA	C	905	4	11,11,12	0.65	0	15,15,17	0.78	0
2	ZK1	D	901	-	28,29,29	3.12	12 (42%)	35,45,45	1.92	4 (11%)
3	NAG	D	902	1,3	14,14,15	0.66	0	15,19,21	1.66	2 (13%)
3	NAG	D	903	3,4	14,14,15	0.50	0	15,19,21	0.70	0
4	BMA	D	904	3,4	11,11,12	0.57	0	15,15,17	0.75	0
4	BMA	D	905	4	11,11,12	0.65	0	15,15,17	0.78	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
2	ZK1	A	901	-	-	0/13/23/23	0/3/3/3
3	NAG	A	902	1,3	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	A	903	3,4	-	0/6/23/26	0/1/1/1
4	BMA	A	904	3,4	1/1/4/5	0/2/19/22	0/1/1/1
4	BMA	A	905	4	-	0/2/19/22	0/1/1/1
2	ZK1	B	901	-	-	0/13/23/23	0/3/3/3
3	NAG	B	902	1,3	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	B	903	3,4	1/1/5/7	2/6/23/26	0/1/1/1
4	BMA	B	904	3,4	-	0/2/19/22	0/1/1/1
4	BMA	B	905	4	-	0/2/19/22	0/1/1/1
2	ZK1	C	901	-	-	0/13/23/23	0/3/3/3
3	NAG	C	902	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	903	3,4	-	0/6/23/26	0/1/1/1
4	BMA	C	904	3,4	-	0/2/19/22	0/1/1/1
4	BMA	C	905	4	-	0/2/19/22	0/1/1/1
2	ZK1	D	901	-	-	0/13/23/23	0/3/3/3
3	NAG	D	902	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	903	3,4	-	0/6/23/26	0/1/1/1
4	BMA	D	904	3,4	-	0/2/19/22	0/1/1/1
4	BMA	D	905	4	-	0/2/19/22	0/1/1/1

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	901	ZK1	CAN-NAX	-7.66	1.35	1.46
2	A	901	ZK1	CAN-NAX	-7.65	1.35	1.46
2	B	901	ZK1	CAN-NAX	-7.64	1.35	1.46
2	C	901	ZK1	CAM-NAX	-7.60	1.35	1.46
2	A	901	ZK1	CAM-NAX	-7.54	1.35	1.46
2	C	901	ZK1	CAN-NAX	-7.54	1.35	1.46
2	D	901	ZK1	CAM-NAX	-7.46	1.35	1.46
2	B	901	ZK1	CAM-NAX	-7.42	1.35	1.46
2	A	901	ZK1	PBA-OAE	-2.05	1.49	1.54
2	B	901	ZK1	PBA-OAE	-2.04	1.49	1.54
2	C	901	ZK1	PBA-OAE	-2.03	1.49	1.54
2	D	901	ZK1	PBA-CAO	2.02	1.86	1.81
2	B	901	ZK1	PBA-OAC	2.07	1.54	1.50
2	A	901	ZK1	PBA-CAO	2.08	1.86	1.81
2	B	901	ZK1	PBA-CAO	2.12	1.86	1.81
2	D	901	ZK1	CAT-NAP	2.23	1.37	1.33
2	D	901	ZK1	CAR-CAS	2.26	1.43	1.40
2	C	901	ZK1	CAT-NAP	2.28	1.37	1.33
2	C	901	ZK1	CAI-CAR	2.30	1.40	1.37
2	B	901	ZK1	CAT-NAP	2.31	1.37	1.33
2	A	901	ZK1	CAT-NAP	2.32	1.37	1.33
2	C	901	ZK1	CAR-CAS	2.38	1.44	1.40
2	D	901	ZK1	CAI-CAR	2.39	1.41	1.37
2	A	901	ZK1	CAI-CAR	2.39	1.41	1.37
2	B	901	ZK1	CAR-CAS	2.44	1.44	1.40
2	A	901	ZK1	CAR-CAS	2.44	1.44	1.40
2	B	901	ZK1	CAI-CAR	2.49	1.41	1.37
2	D	901	ZK1	CAR-NAX	2.71	1.47	1.41
2	A	901	ZK1	CAR-NAX	2.75	1.47	1.41
2	C	901	ZK1	CAR-NAX	2.79	1.47	1.41
2	B	901	ZK1	CAR-NAX	2.82	1.47	1.41
2	A	901	ZK1	CAI-CAW	2.88	1.47	1.40
2	C	901	ZK1	CAI-CAW	2.89	1.47	1.40
2	D	901	ZK1	CAI-CAW	2.94	1.47	1.40
2	B	901	ZK1	CAI-CAW	2.98	1.47	1.40
2	C	901	ZK1	CAJ-CAS	3.12	1.42	1.37
2	B	901	ZK1	CAJ-CAS	3.14	1.42	1.37
2	D	901	ZK1	CAJ-CAS	3.17	1.42	1.37
2	A	901	ZK1	CAJ-CAS	3.20	1.42	1.37
2	A	901	ZK1	PBA-OAC	3.37	1.57	1.50
2	A	901	ZK1	CAV-NAP	3.88	1.41	1.35
2	D	901	ZK1	CAV-NAP	3.93	1.41	1.35
2	C	901	ZK1	CAV-NAP	4.03	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	901	ZK1	CAV-NAP	4.10	1.41	1.35
2	D	901	ZK1	OAB-CAU	6.50	1.40	1.24
2	C	901	ZK1	OAB-CAU	6.53	1.40	1.24
2	A	901	ZK1	OAB-CAU	6.55	1.41	1.24
2	B	901	ZK1	OAB-CAU	6.56	1.41	1.24
2	B	901	ZK1	OAA-CAT	6.61	1.41	1.24
2	D	901	ZK1	OAA-CAT	6.62	1.41	1.24
2	A	901	ZK1	OAA-CAT	6.65	1.41	1.24
2	C	901	ZK1	OAA-CAT	6.67	1.41	1.24

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	902	NAG	C2-N2-C7	-4.96	116.65	123.11
2	A	901	ZK1	CAI-CAR-NAX	-3.83	117.22	122.62
2	C	901	ZK1	CAI-CAR-NAX	-3.66	117.46	122.62
2	D	901	ZK1	CAI-CAR-NAX	-3.33	117.92	122.62
2	B	901	ZK1	CAI-CAR-NAX	-3.28	118.00	122.62
2	A	901	ZK1	FAG-CAZ-CAS	-2.24	108.86	112.67
3	B	903	NAG	C2-N2-C7	-2.21	120.24	123.11
2	C	901	ZK1	FAG-CAZ-CAS	-2.05	109.18	112.67
3	D	902	NAG	C1-O5-C5	2.06	115.17	112.14
2	B	901	ZK1	CAK-CAM-NAX	2.18	113.89	109.94
2	D	901	ZK1	CAL-CAN-NAX	2.19	113.91	109.94
3	B	903	NAG	C1-O5-C5	2.43	115.71	112.14
2	C	901	ZK1	CAS-CAR-NAX	2.47	122.79	120.15
2	A	901	ZK1	CAS-CAR-NAX	2.68	123.01	120.15
2	A	901	ZK1	CAO-NAY-CAW	2.81	123.99	120.09
2	D	901	ZK1	CAO-NAY-CAW	2.82	124.00	120.09
2	C	901	ZK1	CAO-NAY-CAW	2.85	124.05	120.09
2	B	901	ZK1	CAO-NAY-CAW	3.10	124.40	120.09
2	A	901	ZK1	CAN-NAX-CAM	7.95	128.00	111.54
2	C	901	ZK1	CAN-NAX-CAM	8.09	128.30	111.54
2	B	901	ZK1	CAN-NAX-CAM	8.35	128.83	111.54
2	D	901	ZK1	CAN-NAX-CAM	8.44	129.01	111.54

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	B	902	NAG	C1
4	A	904	BMA	C1
3	B	903	NAG	C1

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Mol	Chain	Res	Type	Atom
3	A	902	NAG	C1

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	903	NAG	O7-C7-N2-C2
3	B	903	NAG	C8-C7-N2-C2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	902	NAG	1	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	768/822 (93%)	-0.10	28 (3%)	46	37	58, 155, 265, 497	0
1	B	768/822 (93%)	0.00	40 (5%)	31	24	41, 167, 300, 506	0
1	C	768/822 (93%)	-0.04	37 (4%)	34	26	45, 148, 265, 547	0
1	D	768/822 (93%)	-0.09	28 (3%)	46	37	27, 135, 288, 515	0
All	All	3072/3288 (93%)	-0.05	133 (4%)	39	30	27, 151, 276, 547	0

All (133) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	310	GLY	9.1
1	C	571	PHE	8.6
1	A	311	ASN	8.4
1	D	569	ASN	8.0
1	D	568	THR	7.3
1	A	309	ARG	7.2
1	C	570	GLU	7.2
1	C	391	GLU	6.9
1	C	392	GLN	6.3
1	C	572	GLY	6.1
1	C	389	GLY	5.9
1	A	308	ARG	5.8
1	C	575	ASN	5.7
1	D	570	GLU	5.0
1	B	568	THR	4.8
1	D	629	MET	4.8
1	B	444	ILE	4.6
1	D	816	TYR	4.2
1	A	306	ILE	4.1
1	B	442	LEU	4.1
1	A	684	ARG	4.0

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Mol	Chain	Res	Type	RSRZ
1	C	568	THR	4.0
1	B	393	LYS	3.9
1	D	817	LYS	3.9
1	B	421	TYR	3.9
1	C	306	ILE	3.9
1	C	543	VAL	3.9
1	C	569	ASN	3.9
1	A	213	LYS	3.8
1	A	312	ALA	3.8
1	C	574	PHE	3.8
1	D	815	CYS	3.7
1	A	683	VAL	3.7
1	D	631	SER	3.7
1	A	71	TYR	3.7
1	C	573	ILE	3.7
1	C	386	ASP	3.7
1	A	583	ALA	3.6
1	B	392	GLN	3.6
1	A	569	ASN	3.6
1	D	628	ARG	3.6
1	D	814	PHE	3.5
1	D	311	ASN	3.5
1	D	71	TYR	3.5
1	C	813	GLU	3.5
1	B	438	PHE	3.4
1	D	756	GLN	3.4
1	B	391	GLU	3.4
1	C	815	CYS	3.3
1	C	816	TYR	3.3
1	C	307	SER	3.3
1	B	39	SER	3.2
1	B	593	PRO	3.2
1	A	568	THR	3.1
1	A	679	PRO	3.1
1	B	385	ASP	3.1
1	B	512	PRO	3.0
1	B	399	THR	3.0
1	C	308	ARG	3.0
1	B	684	ARG	2.9
1	C	577	LEU	2.9
1	B	659	PHE	2.9
1	C	388	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	572	GLY	2.9
1	A	651	ASP	2.8
1	C	460	TRP	2.8
1	C	810	ALA	2.8
1	C	390	LEU	2.7
1	A	576	SER	2.7
1	C	785	SER	2.7
1	B	510	SER	2.7
1	B	519	ASP	2.7
1	B	389	GLY	2.7
1	B	416	GLU	2.7
1	B	667	PHE	2.7
1	D	686	THR	2.7
1	B	521	LEU	2.7
1	D	630	VAL	2.6
1	C	584	PHE	2.6
1	D	410	LYS	2.6
1	B	390	LEU	2.6
1	A	392	GLN	2.6
1	C	393	LYS	2.6
1	A	682	PHE	2.5
1	B	388	SER	2.5
1	C	593	PRO	2.5
1	B	511	LYS	2.5
1	A	575	ASN	2.5
1	B	418	ASN	2.5
1	D	571	PHE	2.5
1	A	582	GLY	2.5
1	B	569	ASN	2.5
1	A	686	THR	2.5
1	B	685	THR	2.5
1	C	576	SER	2.4
1	B	394	THR	2.4
1	B	420	ARG	2.4
1	C	411	ASN	2.4
1	C	578	TRP	2.4
1	B	411	ASN	2.4
1	A	391	GLU	2.3
1	B	417	GLY	2.3
1	C	510	SER	2.3
1	B	666	VAL	2.3
1	B	816	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	409	LYS	2.3
1	B	523	TYR	2.3
1	C	585	MET	2.3
1	A	680	SER	2.3
1	C	435	HIS	2.3
1	B	814	PHE	2.3
1	C	814	PHE	2.3
1	A	570	GLU	2.2
1	D	72	ALA	2.2
1	B	518	LEU	2.2
1	D	408	MET	2.2
1	B	815	CYS	2.2
1	A	323	TRP	2.2
1	D	627	GLU	2.1
1	D	372	GLY	2.1
1	D	632	PRO	2.1
1	C	385	ASP	2.1
1	D	757	GLY	2.1
1	C	812	ILE	2.1
1	B	724	GLY	2.1
1	B	811	LEU	2.1
1	D	385	ASP	2.1
1	A	572	GLY	2.1
1	A	21	GLY	2.0
1	D	524	GLU	2.0
1	D	388	SER	2.0
1	B	443	THR	2.0
1	A	313	GLY	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	NAG	C	902	14/15	0.94	0.44	3.50	211,211,211,211	0
3	NAG	D	902	14/15	0.70	0.33	1.95	336,336,336,336	0
2	ZK1	C	901	27/27	0.86	0.30	0.76	137,137,137,137	0
2	ZK1	B	901	27/27	0.80	0.34	0.59	236,236,236,236	0
2	ZK1	D	901	27/27	0.79	0.31	0.07	136,136,136,136	0
2	ZK1	A	901	27/27	0.80	0.35	0.02	138,138,138,138	0
4	BMA	D	904	11/12	0.72	0.20	-	233,233,233,233	0
4	BMA	D	905	11/12	0.85	0.29	-	264,264,264,264	0
3	NAG	B	902	14/15	0.84	0.36	-	167,167,167,167	0
4	BMA	A	904	11/12	0.15	0.77	-	280,280,280,280	0
4	BMA	C	905	11/12	0.77	0.51	-	287,287,287,287	0
3	NAG	C	903	14/15	0.87	0.41	-	225,225,225,225	0
4	BMA	B	904	11/12	0.61	0.38	-	232,232,232,232	0
3	NAG	D	903	14/15	0.76	0.31	-	294,294,294,294	0
3	NAG	B	903	14/15	0.86	0.24	-	180,180,180,180	0
3	NAG	A	902	14/15	0.91	0.64	-	227,227,227,227	0
4	BMA	A	905	11/12	0.40	1.79	-	269,269,269,269	0
4	BMA	B	905	11/12	0.87	0.42	-	231,231,231,231	0
3	NAG	A	903	14/15	0.82	0.68	-	269,269,269,269	0
4	BMA	C	904	11/12	0.64	0.61	-	254,254,254,254	0

6.5 Other polymers [i](#)

There are no such residues in this entry.