



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 01:04 PM BST

PDB ID : 4U2P
Title : Full-length AMPA subtype ionotropic glutamate receptor GluA2 in the apo state
Authors : Duerr, K.L.; Gouaux, E.
Deposited on : 2014-07-17
Resolution : 3.24 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

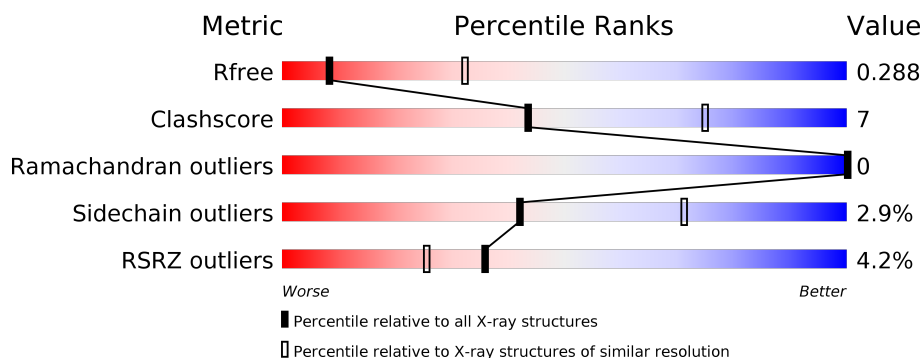
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.24 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}	130704	1619 (3.28-3.20)
Clashscore	141614	1755 (3.28-3.20)
Ramachandran outliers	138981	1728 (3.28-3.20)
Sidechain outliers	138945	1727 (3.28-3.20)
RSRZ outliers	127900	1567 (3.28-3.20)

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 respectively. 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	824	<div> <div>5%</div> <div> <div></div> <div>78%</div> <div>13%</div> <div>8%</div> </div> </div>
1	B	824	<div> <div>3%</div> <div> <div></div> <div>76%</div> <div>16%</div> <div>8%</div> </div> </div>
1	C	824	<div> <div>4%</div> <div> <div></div> <div>76%</div> <div>15%</div> <div>8%</div> </div> </div>
1	D	824	<div> <div>4%</div> <div> <div></div> <div>76%</div> <div>15%</div> <div>9%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 22388 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	755	Total	C	N	O	S	0	0	0
			5496	3519	909	1045	23			
1	B	761	Total	C	N	O	S	0	0	0
			5653	3626	933	1070	24			
1	D	751	Total	C	N	O	S	0	0	0
			5548	3548	912	1062	26			
1	C	755	Total	C	N	O	S	0	0	0
			5587	3578	934	1051	24			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	239	GLU	ASN	conflict	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	conflict	UNP P19491
A	392	GLN	ASN	conflict	UNP P19491
A	528	ALA	CYS	conflict	UNP P19491
A	585	PHE	MET	conflict	UNP P19491
A	589	ALA	CYS	conflict	UNP P19491
A	598	ALA	GLY	conflict	UNP P19491
A	602	ALA	GLY	conflict	UNP P19491
A	815	ALA	CYS	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	239	GLU	ASN	conflict	UNP P19491
B	?	-	LEU	deletion	UNP P19491
B	?	-	PRO	deletion	UNP P19491

Continued on next page...

Continued from previous page...

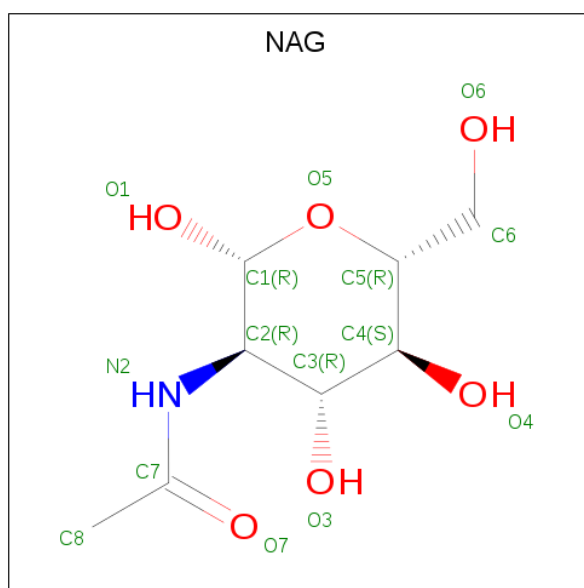
Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	SER	deletion	UNP P19491
B	?	-	GLY	deletion	UNP P19491
B	385	ASP	ASN	conflict	UNP P19491
B	392	GLN	ASN	conflict	UNP P19491
B	528	ALA	CYS	conflict	UNP P19491
B	585	PHE	MET	conflict	UNP P19491
B	589	ALA	CYS	conflict	UNP P19491
B	598	ALA	GLY	conflict	UNP P19491
B	602	ALA	GLY	conflict	UNP P19491
B	815	ALA	CYS	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
D	239	GLU	ASN	conflict	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	conflict	UNP P19491
D	392	GLN	ASN	conflict	UNP P19491
D	528	ALA	CYS	conflict	UNP P19491
D	585	PHE	MET	conflict	UNP P19491
D	589	ALA	CYS	conflict	UNP P19491
D	598	ALA	GLY	conflict	UNP P19491
D	602	ALA	GLY	conflict	UNP P19491
D	815	ALA	CYS	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
D	831	ARG	-	expression tag	UNP P19491
C	239	GLU	ASN	conflict	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	conflict	UNP P19491
C	392	GLN	ASN	conflict	UNP P19491
C	528	ALA	CYS	conflict	UNP P19491
C	585	PHE	MET	conflict	UNP P19491

Continued on next page...

Continued from previous page...

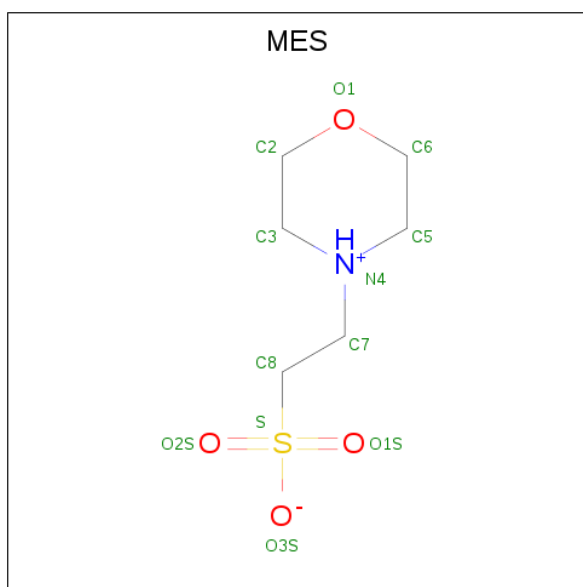
Chain	Residue	Modelled	Actual	Comment	Reference
C	589	ALA	CYS	conflict	UNP P19491
C	598	ALA	GLY	conflict	UNP P19491
C	602	ALA	GLY	conflict	UNP P19491
C	815	ALA	CYS	conflict	UNP P19491
C	827	GLY	-	expression tag	UNP P19491
C	828	LEU	-	expression tag	UNP P19491
C	829	VAL	-	expression tag	UNP P19491
C	830	PRO	-	expression tag	UNP P19491
C	831	ARG	-	expression tag	UNP P19491

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (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
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).

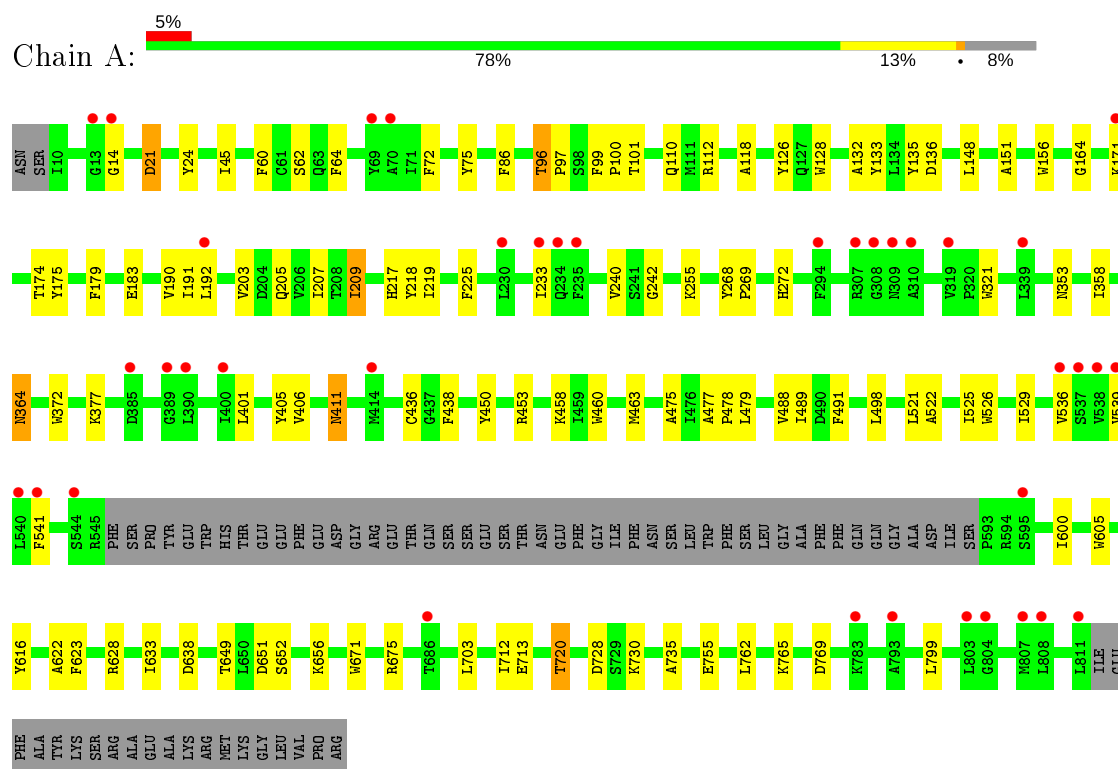


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	C	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

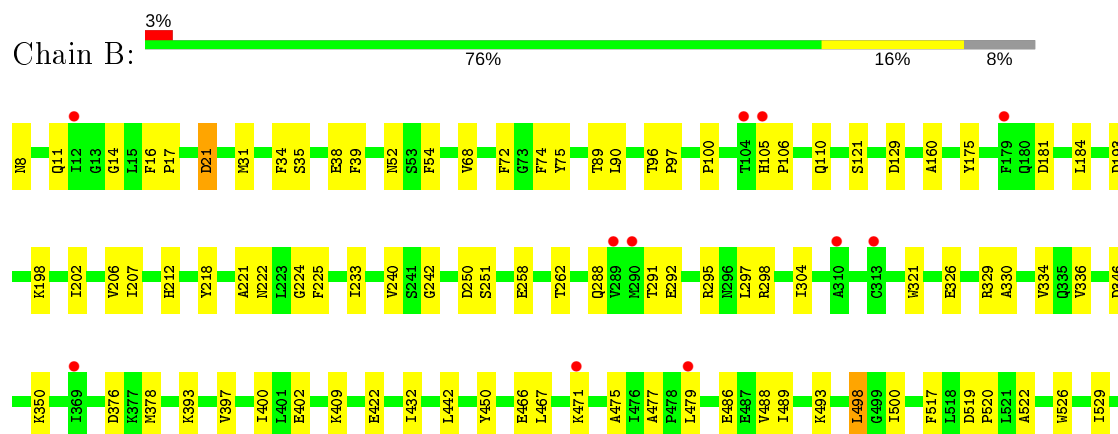
3 Residue-property plots [i](#)

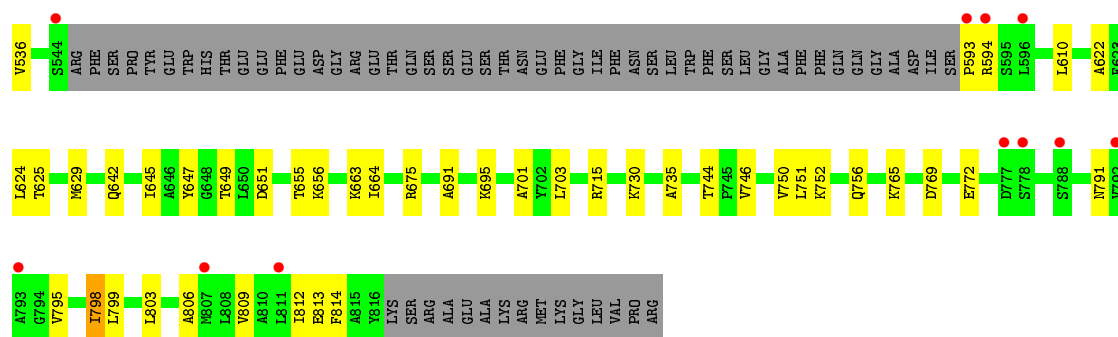
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Glutamate receptor 2

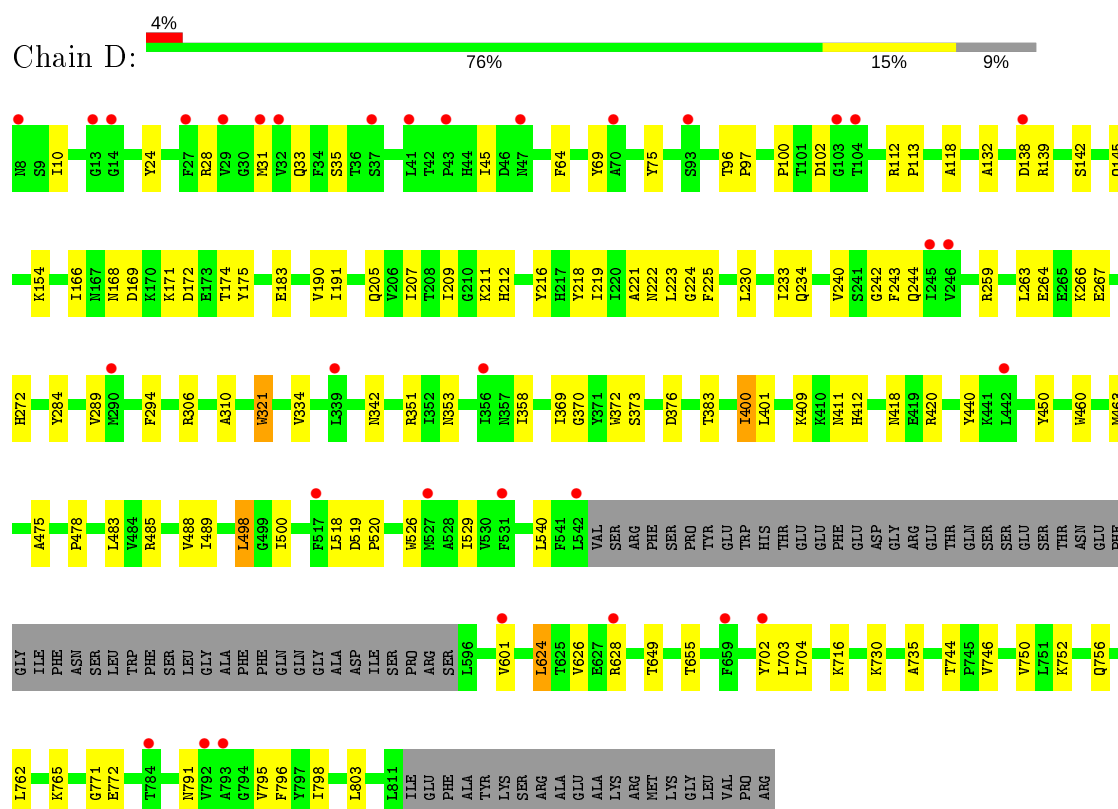


- Molecule 1: Glutamate receptor 2

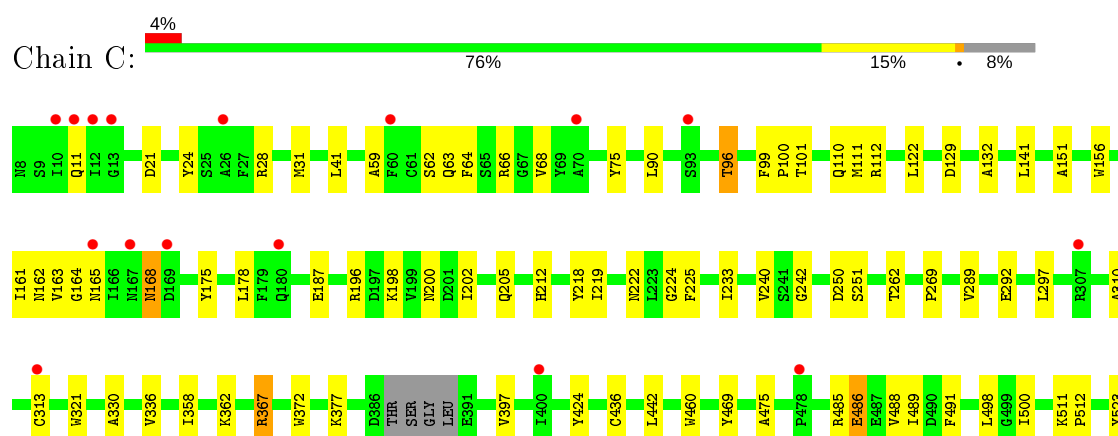


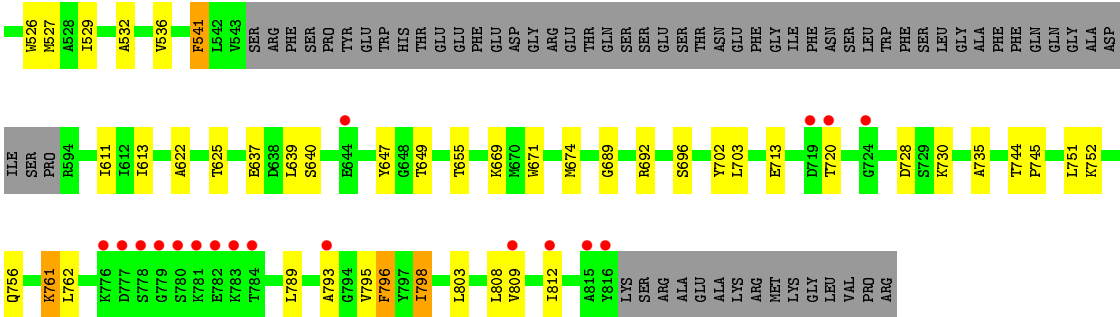


• Molecule 1: Glutamate receptor 2



• 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, α , β , γ	107.81Å 149.13Å 352.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.00 – 3.24 49.00 – 3.24	Depositor EDS
% Data completeness (in resolution range)	72.2 (49.00-3.24) 72.2 (49.00-3.24)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.68 (at 3.25Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.250 , 0.288 0.250 , 0.288	Depositor DCC
R_{free} test set	3377 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	107.7	Xtriage
Anisotropy	0.150	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.20 , 79.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	22388	wwPDB-VP
Average B, all atoms (Å ²)	181.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.80% 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: NAG, MES

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	0.25	0/5614	0.46	0/7661
1	B	0.25	0/5773	0.45	0/7854
1	C	0.26	0/5703	0.46	0/7759
1	D	0.26	0/5664	0.48	0/7721
All	All	0.26	0/22754	0.46	0/30995

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	5496	0	5031	67	0
1	B	5653	0	5313	91	0
1	C	5587	0	5248	83	0
1	D	5548	0	5169	78	0
2	A	14	0	13	1	0
2	B	14	0	12	0	0
2	C	14	0	13	0	0
2	D	14	0	13	1	0
3	A	12	0	13	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	12	0	13	0	0
3	C	12	0	13	0	0
3	D	12	0	13	1	0
All	All	22388	0	20864	291	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 (291) 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:626:VAL:HG13	1:D:628:ARG:H	1.39	0.88
1:C:175:TYR:HD2	1:C:205:GLN:HG3	1.44	0.81
1:C:475:ALA:HB3	1:C:735:ALA:HB3	1.63	0.79
1:B:664:ILE:HG12	1:C:761:LYS:HE2	1.64	0.78
1:B:475:ALA:HB3	1:B:735:ALA:HB3	1.65	0.78
1:D:132:ALA:HB3	1:D:190:VAL:HG12	1.67	0.76
1:C:100:PRO:HA	1:C:110:GLN:HG2	1.66	0.76
1:A:628:ARG:HE	1:D:626:VAL:HG11	1.52	0.74
1:A:21:ASP:N	1:A:21:ASP:OD1	2.21	0.73
1:D:488:VAL:HG23	1:D:489:ILE:HG23	1.70	0.73
1:A:488:VAL:HG23	1:A:489:ILE:HG23	1.71	0.72
1:A:649:THR:HG22	1:A:703:LEU:HB2	1.70	0.72
1:D:373:SER:HB3	1:D:376:ASP:HB2	1.74	0.70
1:B:649:THR:HG22	1:B:703:LEU:HB2	1.73	0.69
1:A:364:ASN:N	1:A:364:ASN:OD1	2.23	0.69
1:D:353:ASN:ND2	2:D:1001:NAG:O7	2.25	0.69
1:A:100:PRO:HA	1:A:110:GLN:HG2	1.75	0.69
1:B:175:TYR:OH	1:B:198:LYS:NZ	2.28	0.67
1:B:488:VAL:HG23	1:B:489:ILE:HG23	1.75	0.67
1:A:218:TYR:HB2	1:A:240:VAL:HG22	1.77	0.66
1:B:663:LYS:HE3	1:C:761:LYS:HD2	1.79	0.65
1:C:500:ILE:HD13	1:C:655:THR:HG23	1.79	0.65
1:A:136:ASP:HA	1:A:164:GLY:HA3	1.78	0.64
1:C:488:VAL:HG23	1:C:489:ILE:HG23	1.78	0.64
1:A:600:ILE:HD11	1:B:806:ALA:HA	1.80	0.62
1:A:358:ILE:HD11	1:A:372:TRP:HB2	1.81	0.62
1:D:518:LEU:HG	1:D:795:VAL:HG22	1.82	0.62
1:A:100:PRO:HD3	1:A:112:ARG:HD2	1.82	0.61
1:A:622:ALA:HA	1:B:625:THR:HG22	1.80	0.61
1:B:500:ILE:HD13	1:B:655:THR:HG23	1.82	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:475:ALA:HB3	1:D:735:ALA:HB3	1.81	0.61
1:B:409:LYS:HE3	1:B:422:GLU:HB3	1.82	0.61
1:C:11:GLN:HG2	1:C:68:VAL:HG12	1.83	0.61
1:B:175:TYR:HE2	1:B:202:ILE:HG12	1.64	0.61
1:A:539:VAL:HG21	1:B:803:LEU:HD22	1.82	0.60
1:A:353:ASN:ND2	2:A:1001:NAG:O7	2.34	0.59
1:D:358:ILE:HD11	1:D:372:TRP:HB2	1.84	0.59
1:D:75:TYR:CE2	1:D:96:THR:HG21	2.38	0.59
1:B:663:LYS:H	1:C:761:LYS:NZ	2.00	0.59
1:B:517:PHE:HB2	1:B:791:ASN:HB3	1.85	0.58
1:D:649:THR:HG22	1:D:703:LEU:HB2	1.86	0.58
1:D:75:TYR:HE2	1:D:96:THR:HG21	1.67	0.58
1:B:207:ILE:HA	1:B:212:HIS:ND1	2.18	0.58
1:C:99:PHE:HA	1:C:112:ARG:HD2	1.85	0.58
1:C:225:PHE:CD1	1:C:242:GLY:HA3	2.39	0.57
1:D:409:LYS:O	1:D:412:HIS:ND1	2.36	0.57
1:B:326:GLU:OE1	1:B:329:ARG:NH2	2.37	0.57
1:D:289:VAL:HG13	1:D:334:VAL:HG11	1.86	0.57
1:A:191:ILE:HG12	1:A:219:ILE:HB	1.86	0.57
1:B:536:VAL:HG22	1:C:803:LEU:HD11	1.87	0.56
1:A:536:VAL:HG22	1:B:803:LEU:HD21	1.86	0.56
1:D:450:TYR:HE1	1:D:478:PRO:HG2	1.70	0.56
1:B:663:LYS:HB2	1:C:761:LYS:HD3	1.87	0.56
1:C:793:ALA:HA	1:C:796:PHE:HB3	1.88	0.56
1:B:647:TYR:HB3	1:B:701:ALA:HB3	1.87	0.56
1:C:649:THR:HG22	1:C:703:LEU:HB2	1.88	0.55
1:D:795:VAL:HG11	1:C:611:ILE:HG21	1.87	0.55
1:D:624:LEU:HB3	1:C:622:ALA:HB2	1.89	0.55
1:A:755:GLU:OE2	1:D:483:LEU:N	2.33	0.55
1:B:222:ASN:ND2	1:B:224:GLY:O	2.41	0.54
1:B:498:LEU:HD22	1:B:730:LYS:HG3	1.90	0.54
1:D:752:LYS:O	1:D:756:GLN:HG2	2.06	0.54
1:B:250:ASP:OD1	1:B:251:SER:N	2.40	0.54
1:C:162:ASN:ND2	1:C:165:ASN:OD1	2.40	0.54
1:D:191:ILE:HG12	1:D:219:ILE:HB	1.89	0.54
1:C:460:TRP:HB2	1:C:469:TYR:HE2	1.73	0.53
1:D:500:ILE:HD13	1:D:655:THR:HG23	1.89	0.53
1:B:610:LEU:HD21	1:C:613:ILE:HG21	1.91	0.53
1:C:358:ILE:HD11	1:C:372:TRP:HB2	1.91	0.53
1:C:362:LYS:HG3	1:C:367:ARG:NH2	2.23	0.53
1:A:401:LEU:HD23	1:A:406:VAL:HG12	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:222:ASN:ND2	1:D:224:GLY:O	2.41	0.52
1:B:795:VAL:HA	1:B:798:ILE:HG22	1.91	0.52
1:B:11:GLN:HG2	1:B:68:VAL:HG12	1.91	0.52
1:B:402:GLU:OE1	1:B:450:TYR:OH	2.26	0.52
1:C:809:VAL:HA	1:C:812:ILE:HG12	1.92	0.52
1:D:218:TYR:HB2	1:D:240:VAL:HG22	1.90	0.52
1:A:728:ASP:OD2	1:A:730:LYS:HE3	2.10	0.52
1:C:196:ARG:O	1:C:200:ASN:ND2	2.34	0.52
1:A:62:SER:O	1:A:64:PHE:N	2.36	0.52
1:D:69:TYR:HA	1:D:321:TRP:HH2	1.74	0.52
1:A:24:TYR:HE1	1:A:45:ILE:HG12	1.74	0.51
1:A:450:TYR:O	1:A:463:MET:N	2.36	0.51
1:A:99:PHE:HA	1:A:112:ARG:HD2	1.92	0.51
1:B:663:LYS:H	1:C:761:LYS:HZ2	1.58	0.51
1:C:795:VAL:O	1:C:798:ILE:HG22	2.10	0.51
1:A:62:SER:C	1:A:64:PHE:H	2.13	0.51
1:B:31:MET:O	1:B:35:SER:HB3	2.11	0.51
1:C:222:ASN:ND2	1:C:224:GLY:O	2.42	0.51
1:B:400:ILE:HG21	1:B:450:TYR:CE1	2.45	0.51
1:B:21:ASP:N	1:B:21:ASP:OD1	2.43	0.51
1:C:168:ASN:ND2	1:C:168:ASN:O	2.35	0.51
1:C:24:TYR:CE2	1:C:28:ARG:HD2	2.45	0.51
1:B:39:PHE:HB3	1:B:298:ARG:HH11	1.76	0.51
1:B:75:TYR:HE1	1:B:96:THR:HG21	1.74	0.51
1:A:372:TRP:HA	1:A:377:LYS:O	2.11	0.51
1:A:60:PHE:CE2	1:A:86:PHE:HB3	2.46	0.51
1:B:291:THR:HG22	1:B:295:ARG:HH12	1.76	0.51
1:C:75:TYR:HE2	1:C:96:THR:HG21	1.76	0.51
1:B:129:ASP:N	1:B:129:ASP:OD1	2.44	0.50
1:D:519:ASP:N	1:D:520:PRO:HD2	2.26	0.50
1:D:771:GLY:O	1:C:669:LYS:NZ	2.44	0.50
1:C:175:TYR:CD2	1:C:205:GLN:HG3	2.35	0.50
1:C:489:ILE:HD12	1:C:735:ALA:HB1	1.92	0.50
1:D:796:PHE:CZ	1:C:532:ALA:HB2	2.46	0.50
1:A:475:ALA:HB3	1:A:735:ALA:HB3	1.94	0.50
1:B:218:TYR:HB2	1:B:240:VAL:HG22	1.93	0.50
1:C:292:GLU:HG3	1:C:336:VAL:HG11	1.93	0.50
1:D:102:ASP:OD2	1:D:142:SER:HB2	2.11	0.49
1:A:651:ASP:OD1	1:A:652:SER:N	2.43	0.49
1:B:400:ILE:HG12	1:B:450:TYR:HE1	1.76	0.49
1:D:69:TYR:HA	1:D:321:TRP:CH2	2.47	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:412:HIS:HB2	1:D:420:ARG:HB3	1.93	0.49
1:B:34:PHE:CE2	1:B:288:GLN:HB2	2.48	0.49
1:B:517:PHE:CB	1:B:791:ASN:HB3	2.43	0.49
1:A:148:LEU:HD13	1:B:160:ALA:HB3	1.94	0.49
1:D:145:GLN:HE21	1:C:141:LEU:HD21	1.77	0.49
1:C:250:ASP:OD1	1:C:251:SER:N	2.46	0.49
1:D:450:TYR:CZ	3:D:1002:MES:H51	2.47	0.49
1:B:297:LEU:HD21	1:B:330:ALA:HB2	1.94	0.48
1:C:297:LEU:HD21	1:C:330:ALA:HB2	1.95	0.48
1:C:671:TRP:HE3	1:C:674:MET:HE3	1.77	0.48
1:A:101:THR:H	1:A:110:GLN:HE21	1.60	0.48
1:B:493:LYS:NZ	1:C:486:GLU:OE2	2.43	0.48
1:B:526:TRP:O	1:B:529:ILE:HG22	2.13	0.48
1:D:223:LEU:O	1:D:244:GLN:HA	2.13	0.48
1:D:540:LEU:HD21	1:D:601:VAL:HG11	1.96	0.48
1:A:171:LYS:O	1:A:175:TYR:HB3	2.13	0.48
1:C:101:THR:H	1:C:110:GLN:HE21	1.61	0.48
1:C:637:GLU:O	1:C:640:SER:OG	2.20	0.48
1:B:75:TYR:CE1	1:B:96:THR:HG21	2.49	0.48
1:C:526:TRP:O	1:C:529:ILE:HG22	2.13	0.47
1:A:521:LEU:HD13	1:A:616:TYR:HD1	1.79	0.47
1:B:14:GLY:HA2	1:B:72:PHE:O	2.13	0.47
1:A:633:ILE:HB	1:A:638:ASP:CB	2.44	0.47
1:B:297:LEU:HD13	1:B:304:ILE:HG21	1.96	0.47
1:C:161:ILE:HG21	1:C:178:LEU:HD11	1.97	0.47
1:A:628:ARG:HB3	1:D:626:VAL:HG21	1.97	0.47
1:A:713:GLU:HG2	1:A:720:THR:O	2.14	0.47
1:B:752:LYS:O	1:B:756:GLN:HG3	2.15	0.47
1:D:460:TRP:HE1	1:D:488:VAL:HG11	1.80	0.47
1:C:424:TYR:CE1	1:C:762:LEU:HB3	2.50	0.47
1:C:31:MET:HE1	1:C:41:LEU:HB2	1.97	0.46
1:C:511:LYS:HA	1:C:512:PRO:HD3	1.68	0.46
1:D:702:TYR:CE2	1:D:704:LEU:HB3	2.49	0.46
1:B:519:ASP:N	1:B:520:PRO:HD2	2.31	0.46
1:D:100:PRO:HD3	1:D:112:ARG:HD2	1.97	0.46
1:A:712:ILE:HG22	1:A:720:THR:HG21	1.97	0.46
1:D:342:ASN:O	1:D:351:ARG:NH2	2.47	0.46
1:A:453:ARG:HD2	1:A:460:TRP:CZ2	2.50	0.46
1:C:523:TYR:O	1:C:527:MET:HG2	2.16	0.46
1:B:105:HIS:HA	1:B:106:PRO:HD3	1.77	0.46
1:B:765:LYS:HA	1:B:769:ASP:HB2	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:75:TYR:CE2	1:C:96:THR:HG21	2.50	0.46
1:B:181:ASP:O	1:B:184:LEU:HB3	2.16	0.46
1:C:21:ASP:HB2	1:C:269:PRO:HB2	1.98	0.46
1:B:52:ASN:OD1	1:B:54:PHE:HB3	2.16	0.46
1:B:121:SER:HB3	1:B:378:MET:HE2	1.98	0.45
1:A:536:VAL:HG21	1:A:605:TRP:CE3	2.52	0.45
1:B:292:GLU:HG3	1:B:336:VAL:HG11	1.99	0.45
1:C:64:PHE:CZ	1:C:310:ALA:HB1	2.51	0.45
1:A:268:TYR:HA	1:A:269:PRO:HD2	1.81	0.45
1:B:663:LYS:HB2	1:C:761:LYS:CD	2.46	0.45
1:C:397:VAL:HB	1:C:442:LEU:HD23	1.99	0.45
1:D:460:TRP:NE1	1:D:488:VAL:HG11	2.30	0.45
1:B:486:GLU:HG3	1:C:751:LEU:HD11	1.98	0.45
1:D:230:LEU:O	1:D:234:GLN:HB2	2.16	0.45
1:C:436:CYS:SG	1:C:745:PRO:HB2	2.57	0.45
1:D:225:PHE:CD1	1:D:242:GLY:HA3	2.52	0.45
1:D:221:ALA:HA	1:D:243:PHE:HD2	1.81	0.45
1:D:369:ILE:HG13	1:D:370:GLY:H	1.82	0.45
1:D:526:TRP:O	1:D:529:ILE:HG22	2.16	0.45
1:C:129:ASP:OD1	1:C:129:ASP:N	2.43	0.44
1:C:218:TYR:HB2	1:C:240:VAL:HG22	1.98	0.44
1:A:205:GLN:O	1:A:209:ILE:HG23	2.16	0.44
1:D:418:ASN:ND2	1:D:440:TYR:O	2.50	0.44
1:A:151:ALA:HA	1:A:156:TRP:HB2	1.99	0.44
1:D:498:LEU:HD22	1:D:730:LYS:HG3	2.00	0.44
1:B:493:LYS:HG3	1:B:751:LEU:HD21	1.98	0.44
1:D:264:GLU:HG2	1:D:266:LYS:H	1.83	0.44
1:B:642:GLN:OE1	1:B:645:ILE:N	2.40	0.44
1:D:450:TYR:CE1	1:D:478:PRO:HG2	2.52	0.44
1:D:112:ARG:HA	1:D:113:PRO:HD3	1.81	0.44
1:A:411:ASN:N	1:A:411:ASN:OD1	2.51	0.44
1:B:489:ILE:HD12	1:B:735:ALA:HB1	2.00	0.44
1:B:715:ARG:HH11	1:B:772:GLU:HG3	1.83	0.44
1:D:33:GLN:HG2	1:D:284:TYR:OH	2.18	0.44
1:A:233:ILE:HD12	1:A:240:VAL:HG21	1.99	0.44
1:B:400:ILE:HG12	1:B:450:TYR:CE1	2.52	0.43
1:B:651:ASP:O	1:B:656:LYS:HD3	2.18	0.43
1:C:752:LYS:O	1:C:756:GLN:HG3	2.18	0.43
1:D:172:ASP:HA	1:D:175:TYR:CE2	2.53	0.43
1:A:628:ARG:NE	1:D:626:VAL:HG11	2.28	0.43
1:C:90:LEU:HD11	1:C:313:CYS:HB2	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:169:ASP:C	1:D:171:LYS:H	2.22	0.43
1:B:376:ASP:C	1:B:378:MET:H	2.22	0.43
1:D:207:ILE:HA	1:D:212:HIS:ND1	2.33	0.43
1:A:24:TYR:CE1	1:A:45:ILE:HG12	2.52	0.43
1:A:765:LYS:HA	1:A:769:ASP:HB2	2.00	0.43
1:C:744:THR:N	1:C:745:PRO:HD2	2.34	0.43
1:D:485:ARG:O	1:D:489:ILE:HG12	2.19	0.43
1:A:99:PHE:HA	1:A:100:PRO:HD3	1.80	0.43
1:B:346:ASP:OD1	1:B:350:LYS:N	2.52	0.43
1:D:118:ALA:HA	1:D:372:TRP:CD1	2.53	0.43
1:A:14:GLY:HA2	1:A:72:PHE:O	2.19	0.43
1:C:692:ARG:O	1:C:696:SER:OG	2.28	0.43
1:D:96:THR:HA	1:D:97:PRO:HD3	1.77	0.43
1:B:100:PRO:HA	1:B:110:GLN:HG2	2.00	0.43
1:C:100:PRO:HD3	1:C:112:ARG:HD2	2.00	0.43
1:D:791:ASN:O	1:D:795:VAL:HG23	2.19	0.43
1:C:485:ARG:O	1:C:489:ILE:HG12	2.19	0.43
1:B:8:ASN:HB2	1:B:39:PHE:HA	2.01	0.42
1:D:10:ILE:HG21	1:D:294:PHE:CE2	2.53	0.42
1:C:151:ALA:HA	1:C:156:TRP:HB2	2.00	0.42
1:C:59:ALA:O	1:C:63:GLN:HG2	2.18	0.42
1:D:259:ARG:O	1:D:263:LEU:HG	2.18	0.42
1:D:306:ARG:HH21	1:D:310:ALA:HB2	1.85	0.42
1:B:642:GLN:NE2	1:B:645:ILE:HB	2.34	0.42
1:B:691:ALA:O	1:B:695:LYS:HG2	2.19	0.42
1:C:541:PHE:HA	1:C:541:PHE:HD1	1.73	0.42
1:A:128:TRP:HZ2	1:A:217:HIS:CD2	2.37	0.42
1:D:31:MET:O	1:D:35:SER:HB3	2.20	0.42
1:A:203:VAL:O	1:A:207:ILE:HG13	2.19	0.42
1:B:233:ILE:HD13	1:B:240:VAL:HG21	2.00	0.42
1:C:132:ALA:HB2	1:C:187:GLU:OE2	2.19	0.42
1:D:369:ILE:HG13	1:D:370:GLY:N	2.34	0.42
1:D:64:PHE:CE2	1:D:310:ALA:HB1	2.54	0.42
1:C:111:MET:HE1	1:C:289:VAL:HG21	2.01	0.42
1:D:221:ALA:HA	1:D:243:PHE:CD2	2.55	0.42
1:B:74:PHE:CE2	1:B:97:PRO:HG2	2.55	0.42
1:C:377:LYS:HA	1:C:377:LYS:HD3	1.75	0.42
1:D:489:ILE:HD12	1:D:735:ALA:HB1	2.02	0.42
1:A:132:ALA:HB3	1:A:190:VAL:HG12	2.01	0.42
1:A:225:PHE:CD1	1:A:242:GLY:HA3	2.55	0.42
1:A:526:TRP:O	1:A:529:ILE:HG22	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:689:GLY:HA3	1:C:702:TYR:CE1	2.55	0.42
1:A:405:TYR:CE1	1:A:478:PRO:HB3	2.55	0.41
1:A:118:ALA:HA	1:A:372:TRP:CD1	2.55	0.41
1:D:209:ILE:HG13	1:D:211:LYS:HG2	2.03	0.41
1:A:477:ALA:O	1:A:479:LEU:N	2.53	0.41
1:A:651:ASP:O	1:A:656:LYS:HD3	2.20	0.41
1:B:193:ASP:HB2	1:B:221:ALA:HB3	2.02	0.41
1:B:225:PHE:CD1	1:B:242:GLY:HA3	2.55	0.41
1:A:133:TYR:CE2	1:A:135:TYR:HB3	2.55	0.41
1:B:746:VAL:O	1:B:750:VAL:HG23	2.21	0.41
1:B:96:THR:HA	1:B:97:PRO:HD3	1.77	0.41
1:C:163:VAL:HG21	1:C:202:ILE:HD11	2.03	0.41
1:C:713:GLU:HG3	1:C:720:THR:O	2.20	0.41
1:D:762:LEU:O	1:D:765:LYS:HB3	2.20	0.41
1:A:126:TYR:HB3	1:A:128:TRP:NE1	2.35	0.41
1:D:746:VAL:O	1:D:750:VAL:HG23	2.21	0.41
1:D:803:LEU:HD21	1:C:536:VAL:HG12	2.03	0.41
1:B:16:PHE:HA	1:B:17:PRO:HD3	1.95	0.41
1:B:467:LEU:HA	1:B:467:LEU:HD23	1.85	0.41
1:B:522:ALA:H	1:C:789:LEU:CD1	2.34	0.41
1:C:164:GLY:HA2	1:C:198:LYS:HE2	2.02	0.41
1:D:400:ILE:HG21	1:D:450:TYR:CE1	2.56	0.41
1:D:716:LYS:HG3	1:D:772:GLU:OE2	2.20	0.41
1:A:192:LEU:HD21	1:A:218:TYR:HD2	1.85	0.41
1:B:730:LYS:HE2	1:B:730:LYS:HB3	1.91	0.41
1:B:89:THR:HG22	1:B:90:LEU:HD23	2.02	0.41
1:C:639:LEU:HD21	1:C:647:TYR:CB	2.51	0.41
1:C:728:ASP:OD2	1:C:730:LYS:HE2	2.21	0.41
1:D:24:TYR:HE1	1:D:45:ILE:HG13	1.85	0.41
1:A:671:TRP:CE2	1:A:675:ARG:HD3	2.56	0.41
1:A:96:THR:HA	1:A:97:PRO:HD3	1.84	0.41
1:B:809:VAL:O	1:B:812:ILE:HG13	2.20	0.41
1:B:258:GLU:O	1:B:262:THR:OG1	2.38	0.41
1:B:477:ALA:O	1:B:479:LEU:N	2.54	0.41
1:D:175:TYR:CD2	1:D:205:GLN:HG2	2.56	0.41
1:A:175:TYR:O	1:A:179:PHE:HD2	2.04	0.41
1:A:522:ALA:HB3	1:A:525:ILE:HG12	2.01	0.41
1:B:397:VAL:HB	1:B:442:LEU:HD23	2.03	0.41
1:A:762:LEU:O	1:A:765:LYS:HB3	2.21	0.40
1:B:330:ALA:O	1:B:334:VAL:HG23	2.21	0.40
1:A:255:LYS:HD2	1:A:255:LYS:HA	1.76	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:436:CYS:HB2	1:A:438:PHE:CE1	2.57	0.40
1:B:175:TYR:CE2	1:B:202:ILE:HG12	2.52	0.40
1:B:466:GLU:O	1:B:471:LYS:N	2.50	0.40
1:B:593:PRO:HB2	1:B:594:ARG:H	1.71	0.40
1:C:297:LEU:HD23	1:C:297:LEU:HA	1.89	0.40
1:D:216:TYR:HD1	1:D:216:TYR:N	2.20	0.40
1:B:202:ILE:O	1:B:206:VAL:HG23	2.22	0.40
1:C:122:LEU:HD23	1:C:219:ILE:HD13	2.03	0.40
1:B:751:LEU:HD11	1:C:486:GLU:HG3	2.03	0.40
1:C:62:SER:O	1:C:66:ARG:HG3	2.21	0.40
1:B:393:LYS:HD2	1:B:393:LYS:HA	1.92	0.40
1:B:622:ALA:HA	1:C:625:THR:HG22	2.03	0.40
1:C:808:LEU:O	1:C:812:ILE:HG23	2.21	0.40
1:D:28:ARG:NH2	1:D:267:GLU:OE2	2.54	0.40
1:D:450:TYR:O	1:D:463:MET:N	2.50	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	751/824 (91%)	728 (97%)	23 (3%)	0	100	100
1	B	757/824 (92%)	741 (98%)	16 (2%)	0	100	100
1	C	749/824 (91%)	728 (97%)	21 (3%)	0	100	100
1	D	747/824 (91%)	727 (97%)	20 (3%)	0	100	100
All	All	3004/3296 (91%)	2924 (97%)	80 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	521/701 (74%)	504 (97%)	17 (3%)	38	68
1	B	556/701 (79%)	543 (98%)	13 (2%)	50	76
1	C	545/701 (78%)	531 (97%)	14 (3%)	46	74
1	D	546/701 (78%)	528 (97%)	18 (3%)	38	68
All	All	2168/2804 (77%)	2106 (97%)	62 (3%)	42	71

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	ASP
1	A	75	TYR
1	A	96	THR
1	A	174	THR
1	A	183	GLU
1	A	209	ILE
1	A	272	HIS
1	A	321	TRP
1	A	364	ASN
1	A	411	ASN
1	A	458	LYS
1	A	491	PHE
1	A	498	LEU
1	A	541	PHE
1	A	623	PHE
1	A	720	THR
1	A	799	LEU
1	B	21	ASP
1	B	38	GLU
1	B	321	TRP
1	B	432	ILE
1	B	498	LEU
1	B	624	LEU
1	B	629	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	675	ARG
1	B	744	THR
1	B	798	ILE
1	B	799	LEU
1	B	813	GLU
1	B	814	PHE
1	D	138	ASP
1	D	139	ARG
1	D	154	LYS
1	D	166	ILE
1	D	168	ASN
1	D	174	THR
1	D	183	GLU
1	D	233	ILE
1	D	272	HIS
1	D	321	TRP
1	D	383	THR
1	D	400	ILE
1	D	401	LEU
1	D	411	ASN
1	D	498	LEU
1	D	624	LEU
1	D	744	THR
1	D	798	ILE
1	C	96	THR
1	C	168	ASN
1	C	212	HIS
1	C	233	ILE
1	C	262	THR
1	C	321	TRP
1	C	367	ARG
1	C	486	GLU
1	C	491	PHE
1	C	498	LEU
1	C	541	PHE
1	C	761	LYS
1	C	796	PHE
1	C	798	ILE

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

Mol	Chain	Res	Type
1	A	168	ASN
1	C	162	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	C	1001	1	14,14,15	0.29	0	17,19,21	1.16	2 (11%)
3	MES	B	1002	-	12,12,12	1.94	4 (33%)	14,16,16	7.48	5 (35%)
3	MES	D	1002	-	12,12,12	1.81	3 (25%)	14,16,16	1.22	1 (7%)
3	MES	C	1002	-	12,12,12	1.85	3 (25%)	14,16,16	1.14	3 (21%)
2	NAG	D	1001	1	14,14,15	2.04	5 (35%)	17,19,21	4.06	11 (64%)
2	NAG	B	1001	1	14,14,15	2.36	7 (50%)	17,19,21	4.59	9 (52%)
3	MES	A	1002	-	12,12,12	1.76	3 (25%)	14,16,16	1.20	3 (21%)
2	NAG	A	1001	1	14,14,15	1.44	3 (21%)	17,19,21	2.38	8 (47%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.
'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1001	1	-	4/6/23/26	0/1/1/1
3	MES	B	1002	-	-	0/6/14/14	0/1/1/1
3	MES	D	1002	-	-	0/6/14/14	0/1/1/1
3	MES	C	1002	-	-	3/6/14/14	0/1/1/1
2	NAG	D	1001	1	-	3/6/23/26	0/1/1/1
2	NAG	B	1001	1	-	2/6/23/26	0/1/1/1
3	MES	A	1002	-	-	3/6/14/14	0/1/1/1
2	NAG	A	1001	1	-	4/6/23/26	0/1/1/1

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1002	MES	C8-S	4.43	1.83	1.77
2	B	1001	NAG	C1-C2	4.41	1.58	1.52
3	D	1002	MES	C8-S	4.37	1.83	1.77
3	C	1002	MES	C8-S	4.36	1.83	1.77
3	A	1002	MES	C8-S	4.09	1.83	1.77
2	D	1001	NAG	C1-C2	4.08	1.58	1.52
2	B	1001	NAG	O5-C1	3.88	1.49	1.43
2	D	1001	NAG	O5-C1	3.31	1.49	1.43
3	B	1002	MES	O1S-S	3.25	1.54	1.45
3	B	1002	MES	O2S-S	3.13	1.54	1.45
3	C	1002	MES	O2S-S	3.05	1.54	1.45
3	C	1002	MES	O1S-S	2.90	1.53	1.45
3	A	1002	MES	O2S-S	2.88	1.53	1.45
3	D	1002	MES	O1S-S	2.87	1.53	1.45
3	A	1002	MES	O1S-S	2.87	1.53	1.45
3	D	1002	MES	O2S-S	2.80	1.53	1.45
2	B	1001	NAG	O7-C7	2.79	1.29	1.23
2	B	1001	NAG	C4-C5	2.40	1.58	1.53
2	B	1001	NAG	C4-C3	2.34	1.58	1.52
2	A	1001	NAG	C1-C2	2.25	1.55	1.52
2	A	1001	NAG	O7-C7	2.24	1.28	1.23
2	D	1001	NAG	C4-C3	2.20	1.57	1.52
2	A	1001	NAG	O5-C5	2.20	1.47	1.43
2	D	1001	NAG	O5-C5	2.08	1.47	1.43
2	B	1001	NAG	C3-C2	2.04	1.56	1.52
2	B	1001	NAG	C2-N2	2.04	1.49	1.46
2	D	1001	NAG	C8-C7	2.02	1.54	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1002	MES	O3S-S	2.00	1.54	1.47

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1002	MES	O2S-S-C8	-17.59	85.73	106.92
3	B	1002	MES	O1S-S-C8	-17.43	85.92	106.92
3	B	1002	MES	O3S-S-C8	-11.88	86.55	105.77
2	D	1001	NAG	C2-N2-C7	-11.18	106.98	122.90
2	B	1001	NAG	C1-O5-C5	-10.43	98.06	112.19
2	B	1001	NAG	C2-N2-C7	-8.01	111.50	122.90
2	B	1001	NAG	C1-C2-N2	7.94	124.05	110.49
2	B	1001	NAG	O5-C5-C6	6.05	116.69	107.20
2	D	1001	NAG	O3-C3-C2	-5.40	98.29	109.47
2	A	1001	NAG	C1-O5-C5	5.33	119.41	112.19
2	B	1001	NAG	O3-C3-C2	-5.22	98.66	109.47
2	B	1001	NAG	O5-C1-C2	-4.68	103.90	111.29
2	D	1001	NAG	O5-C1-C2	-4.48	104.22	111.29
2	D	1001	NAG	C1-C2-N2	4.26	117.76	110.49
2	D	1001	NAG	O5-C5-C6	4.11	113.65	107.20
2	D	1001	NAG	C1-O5-C5	-3.88	106.93	112.19
2	A	1001	NAG	O5-C5-C6	3.81	113.17	107.20
2	A	1001	NAG	C1-C2-N2	3.74	116.88	110.49
2	D	1001	NAG	C8-C7-N2	3.51	122.05	116.10
3	B	1002	MES	O3S-S-O1S	3.51	119.85	111.27
2	D	1001	NAG	O4-C4-C5	-3.39	100.88	109.30
2	A	1001	NAG	C4-C3-C2	-3.36	106.10	111.02
3	D	1002	MES	O3S-S-C8	3.34	111.17	105.77
2	B	1001	NAG	C6-C5-C4	3.26	120.63	113.00
2	B	1001	NAG	O6-C6-C5	-3.24	100.17	111.29
2	D	1001	NAG	O7-C7-N2	-3.20	116.06	121.95
3	B	1002	MES	O3S-S-O2S	3.11	118.86	111.27
2	D	1001	NAG	C3-C4-C5	2.91	115.44	110.24
2	A	1001	NAG	C2-N2-C7	-2.87	118.81	122.90
2	D	1001	NAG	O3-C3-C4	2.83	116.90	110.35
2	C	1001	NAG	O5-C5-C6	2.55	111.19	107.20
2	C	1001	NAG	C4-C3-C2	-2.44	107.44	111.02
3	A	1002	MES	O3S-S-C8	2.27	109.45	105.77
2	A	1001	NAG	O4-C4-C3	2.19	115.42	110.35
2	A	1001	NAG	C3-C4-C5	-2.17	106.37	110.24
3	C	1002	MES	O2S-S-C8	2.16	109.52	106.92
2	B	1001	NAG	C4-C3-C2	2.13	114.14	111.02

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1002	MES	O1S-S-C8	2.12	109.47	106.92
3	C	1002	MES	O3S-S-C8	2.08	109.14	105.77
3	C	1002	MES	O1S-S-C8	2.02	109.34	106.92
2	A	1001	NAG	O4-C4-C5	2.01	114.29	109.30
3	A	1002	MES	O2S-S-C8	2.01	109.33	106.92

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1002	MES	C7-C8-S-O1S
3	C	1002	MES	C7-C8-S-O3S
2	A	1001	NAG	O5-C5-C6-O6
2	A	1001	NAG	C4-C5-C6-O6
2	B	1001	NAG	O5-C5-C6-O6
2	B	1001	NAG	C4-C5-C6-O6
2	C	1001	NAG	C4-C5-C6-O6
2	D	1001	NAG	C8-C7-N2-C2
2	C	1001	NAG	O5-C5-C6-O6
2	D	1001	NAG	O7-C7-N2-C2
2	D	1001	NAG	C4-C5-C6-O6
3	A	1002	MES	C7-C8-S-O3S
2	C	1001	NAG	C8-C7-N2-C2
2	C	1001	NAG	O7-C7-N2-C2
3	C	1002	MES	C7-C8-S-O2S
3	A	1002	MES	C7-C8-S-O1S
2	A	1001	NAG	C3-C2-N2-C7
3	A	1002	MES	C7-C8-S-O2S
2	A	1001	NAG	C1-C2-N2-C7

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1002	MES	1	0
2	D	1001	NAG	1	0
2	A	1001	NAG	1	0

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, 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	755/824 (91%)	0.09	38 (5%)	28	18	110, 176, 267, 324	0
1	B	761/824 (92%)	0.03	22 (2%)	51	40	103, 176, 267, 348	0
1	C	755/824 (91%)	0.04	34 (4%)	33	23	106, 175, 269, 334	0
1	D	751/824 (91%)	0.06	33 (4%)	34	24	105, 175, 261, 305	0
All	All	3022/3296 (91%)	0.06	127 (4%)	36	25	103, 176, 266, 348	0

All (127) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	385	ASP	7.7
1	A	811	LEU	6.8
1	A	540	LEU	6.5
1	B	777	ASP	5.8
1	B	792	VAL	5.5
1	C	784	THR	5.1
1	A	307	ARG	5.0
1	C	11	GLN	5.0
1	C	167	ASN	4.9
1	D	792	VAL	4.6
1	C	816	TYR	4.5
1	C	815	ALA	4.5
1	D	527	MET	4.5
1	A	595	SER	4.3
1	A	308	GLY	4.3
1	A	234	GLN	4.2
1	B	596	LEU	4.2
1	A	537	SER	4.2
1	B	793	ALA	4.1
1	D	601	VAL	4.0
1	A	390	LEU	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	783	LYS	3.8
1	D	246	VAL	3.8
1	B	544	SER	3.8
1	A	544	SER	3.7
1	A	233	ILE	3.6
1	A	541	PHE	3.6
1	A	539	VAL	3.6
1	D	517	PHE	3.5
1	C	812	ILE	3.5
1	C	307	ARG	3.5
1	B	369	ILE	3.4
1	A	14	GLY	3.4
1	A	793	ALA	3.4
1	B	788	SER	3.3
1	C	778	SER	3.3
1	D	356	ILE	3.3
1	D	70	ALA	3.3
1	A	808	LEU	3.3
1	A	235	PHE	3.3
1	A	69	TYR	3.2
1	D	290	MET	3.1
1	D	542	LEU	3.1
1	D	14	GLY	3.0
1	D	339	LEU	3.0
1	A	807	MET	3.0
1	C	779	GLY	3.0
1	C	313	CYS	3.0
1	D	43	PRO	3.0
1	A	803	LEU	2.9
1	A	192	LEU	2.9
1	D	442	LEU	2.8
1	B	807	MET	2.8
1	A	230	LEU	2.8
1	D	8	ASN	2.8
1	A	538	VAL	2.7
1	C	165	ASN	2.7
1	C	793	ALA	2.7
1	D	702	TYR	2.7
1	A	804	GLY	2.7
1	C	13	GLY	2.7
1	B	594	ARG	2.6
1	B	12	ILE	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	478	PRO	2.6
1	D	784	THR	2.6
1	D	531	PHE	2.6
1	A	310	ALA	2.6
1	C	93	SER	2.6
1	D	93	SER	2.6
1	D	32	VAL	2.6
1	B	104	THR	2.6
1	A	686	THR	2.5
1	D	37	SER	2.5
1	A	309	ASN	2.5
1	C	781	LYS	2.5
1	D	31	MET	2.5
1	A	400	ILE	2.5
1	A	319	VAL	2.5
1	A	389	GLY	2.5
1	C	719	ASP	2.5
1	D	27	PHE	2.5
1	B	310	ALA	2.4
1	D	245	ILE	2.4
1	D	29	VAL	2.4
1	B	778	SER	2.4
1	D	628	ARG	2.4
1	B	179	PHE	2.4
1	D	103	GLY	2.4
1	D	104	THR	2.4
1	B	811	LEU	2.4
1	C	12	ILE	2.4
1	A	536	VAL	2.3
1	C	724	GLY	2.3
1	C	644	GLU	2.3
1	C	809	VAL	2.3
1	D	41	LEU	2.3
1	C	777	ASP	2.3
1	C	720	THR	2.3
1	C	780	SER	2.3
1	C	60	PHE	2.3
1	A	13	GLY	2.3
1	D	13	GLY	2.3
1	B	471	LYS	2.3
1	A	783	LYS	2.3
1	C	400	ILE	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	793	ALA	2.3
1	C	26	ALA	2.2
1	B	479	LEU	2.2
1	B	593	PRO	2.2
1	C	180	GLN	2.2
1	A	171	LYS	2.2
1	B	105	HIS	2.1
1	B	313	CYS	2.1
1	C	70	ALA	2.1
1	D	47	ASN	2.1
1	C	10	ILE	2.1
1	A	70	ALA	2.1
1	D	138	ASP	2.1
1	D	659	PHE	2.1
1	C	776	LYS	2.1
1	B	289	VAL	2.1
1	B	290	MET	2.1
1	A	339	LEU	2.0
1	A	414	MET	2.0
1	C	782	GLU	2.0
1	A	294	PHE	2.0
1	C	169	ASP	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 monosaccharides 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. 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	B-factors(\AA^2)	Q<0.9
2	NAG	B	1001	14/15	0.75	0.32	175,275,394,397	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NAG	D	1001	14/15	0.84	0.19	166,292,335,356	0
3	MES	C	1002	12/12	0.93	0.22	116,147,179,195	0
2	NAG	A	1001	14/15	0.94	0.25	104,192,258,311	0
3	MES	A	1002	12/12	0.95	0.32	93,148,187,245	0
2	NAG	C	1001	14/15	0.95	0.18	117,155,252,264	0
3	MES	D	1002	12/12	0.96	0.17	90,126,163,182	0
3	MES	B	1002	12/12	0.97	0.24	108,144,223,237	0

6.5 Other polymers [i](#)

There are no such residues in this entry.