



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 26, 2016 – 10:43 PM EDT

PDB ID : 5L1G
Title : AMPA subtype ionotropic glutamate receptor GluA2 in complex with GYKI-Br
Authors : Yelshanskaya, M.V.; Singh, A.K.; Sampson, J.M.; Sobolevsky, A.I.
Deposited on : 2016-07-29
Resolution : 4.51 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-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

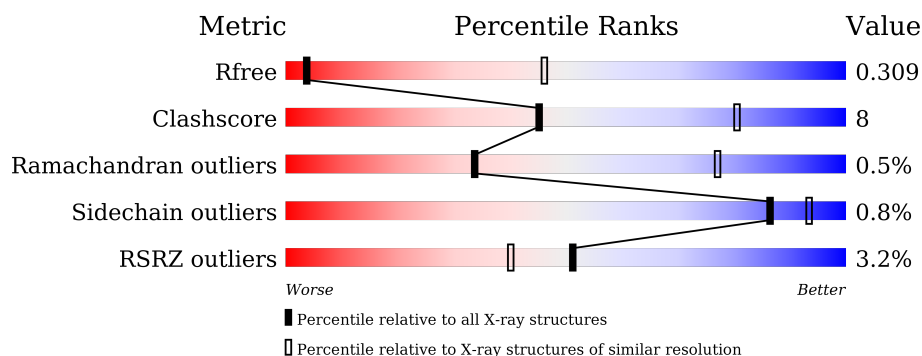
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.51 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	803	<div> <div>2%</div> <div>80%</div> <div>16%</div> <div>.</div> </div>
1	B	803	<div> <div>3%</div> <div>76%</div> <div>20%</div> <div>.</div> </div>
1	C	803	<div> <div>3%</div> <div>77%</div> <div>19%</div> <div>.</div> </div>
1	D	803	<div> <div>3%</div> <div>78%</div> <div>18%</div> <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
2	NAG	A	901	-	-	-	X
3	GYB	A	902	-	-	-	X
3	GYB	A	903	X	-	X	X
3	GYB	C	902	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 24087 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
			5987	3848	992	1118	29			
1	B	773	Total	C	N	O	S	0	0	0
			5990	3844	989	1128	29			
1	C	774	Total	C	N	O	S	0	0	0
			5952	3824	986	1114	28			
1	D	777	Total	C	N	O	S	0	0	0
			5967	3831	990	1119	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

Continued on next page...

Continued from previous page...

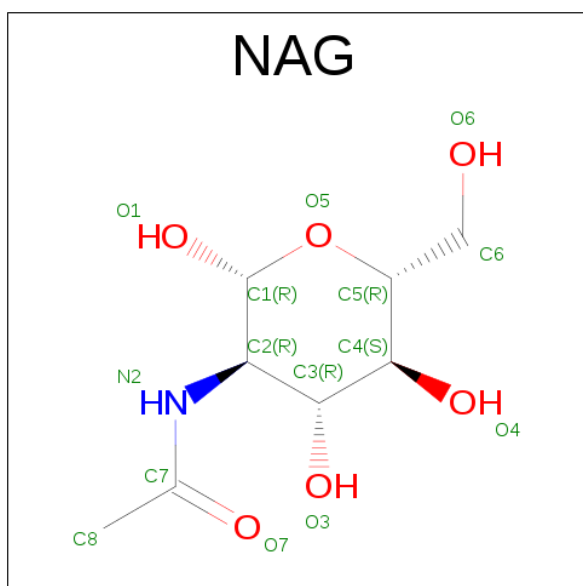
Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	LEU	deletion	UNP P19491
B	?	-	PRO	deletion	UNP P19491
B	?	-	SER	deletion	UNP P19491
B	?	-	GLY	deletion	UNP P19491
B	385	ASP	ASN	engineered mutation	UNP P19491
B	392	GLN	ASN	engineered mutation	UNP P19491
B	564	ASP	-	linker	UNP P19491
B	565	THR	-	linker	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
C	564	ASP	-	linker	UNP P19491
C	565	THR	-	linker	UNP P19491
C	566	ASP	-	linker	UNP P19491
C	589	ALA	CYS	engineered mutation	UNP P19491
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

Continued on next page...

Continued from previous page...

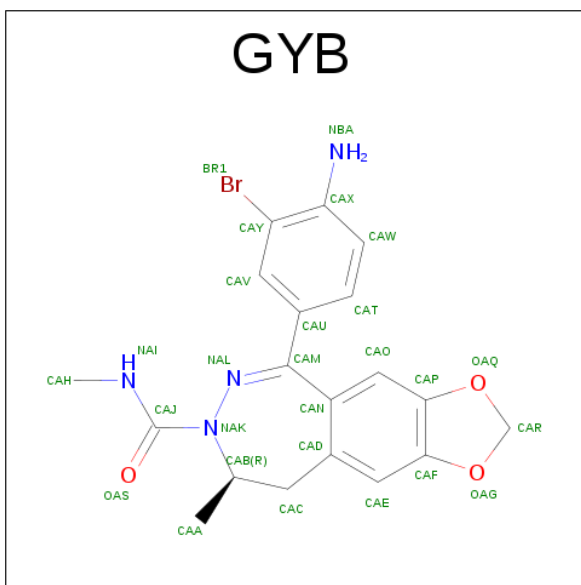
Chain	Residue	Modelled	Actual	Comment	Reference
D	564	ASP	-	linker	UNP P19491
D	565	THR	-	linker	UNP P19491
D	566	ASP	-	linker	UNP P19491
D	589	ALA	CYS	engineered mutation	UNP P19491
D	827	GLY	-	cloning artifact	UNP P19491
D	828	LEU	-	cloning artifact	UNP P19491
D	829	VAL	-	cloning artifact	UNP P19491
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
			14	8	1	5		
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 (8R)-5-(4-amino-3-bromophenyl)-N,8-dimethyl-8,9-dihydro-2H,7H-[1,3]dioxolo[4,5-h][2,3]benzodiazepine-7-carboxamide (three-letter code: GYB) (formula: $C_{19}H_{19}BrN_4O_3$).

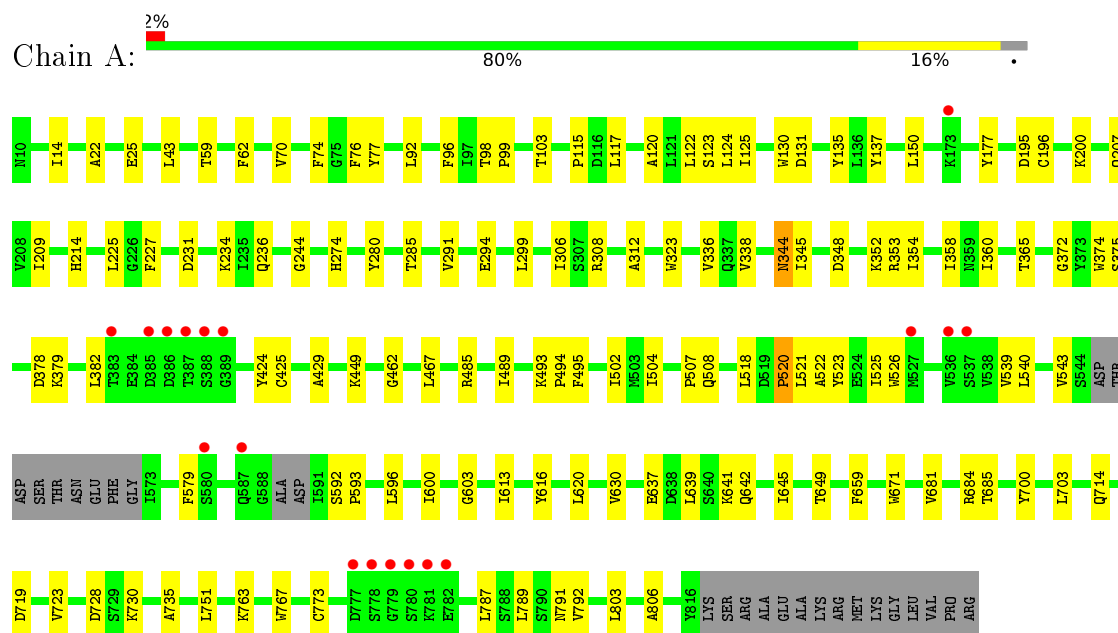


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 27	Br 1	C 19	N 4	O 3	0	0
3	A	1	Total 27	Br 1	C 19	N 4	O 3	0	0
3	B	1	Total 27	Br 1	C 19	N 4	O 3	0	0
3	C	1	Total 27	Br 1	C 19	N 4	O 3	0	0
3	D	1	Total 27	Br 1	C 19	N 4	O 3	0	0

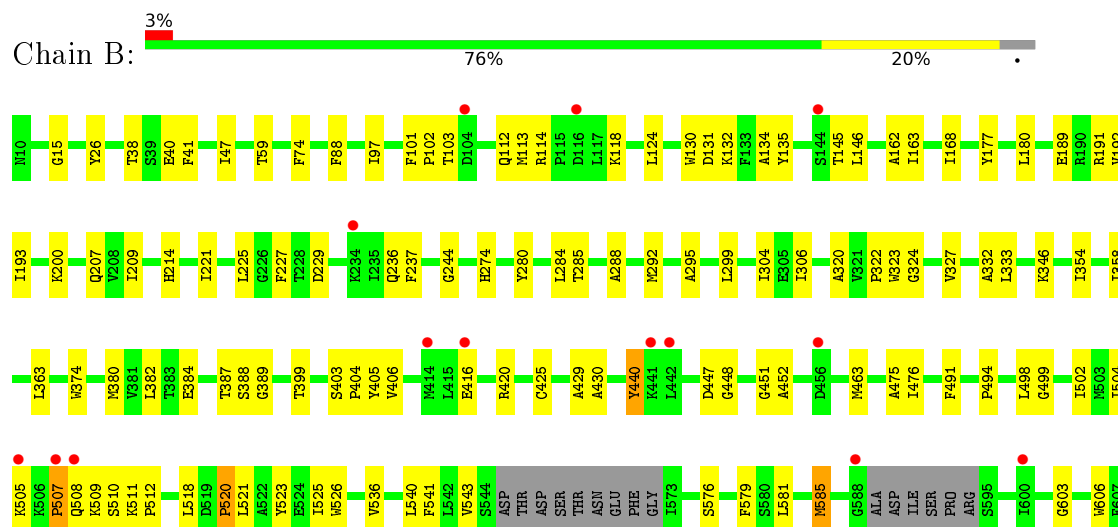
3 Residue-property plots

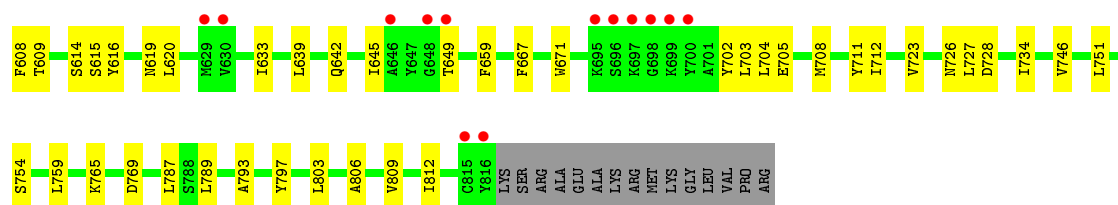
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

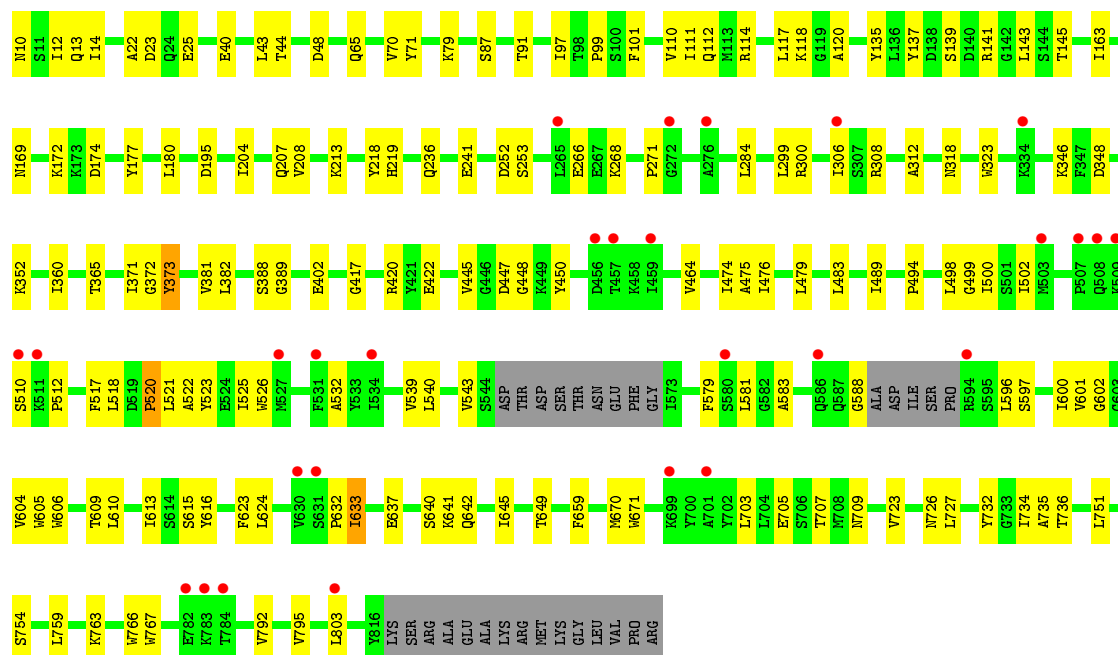
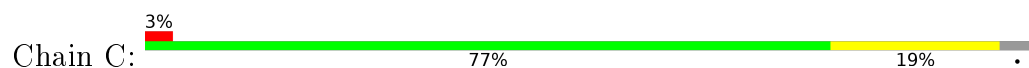


• Molecule 1: Glutamate receptor 2

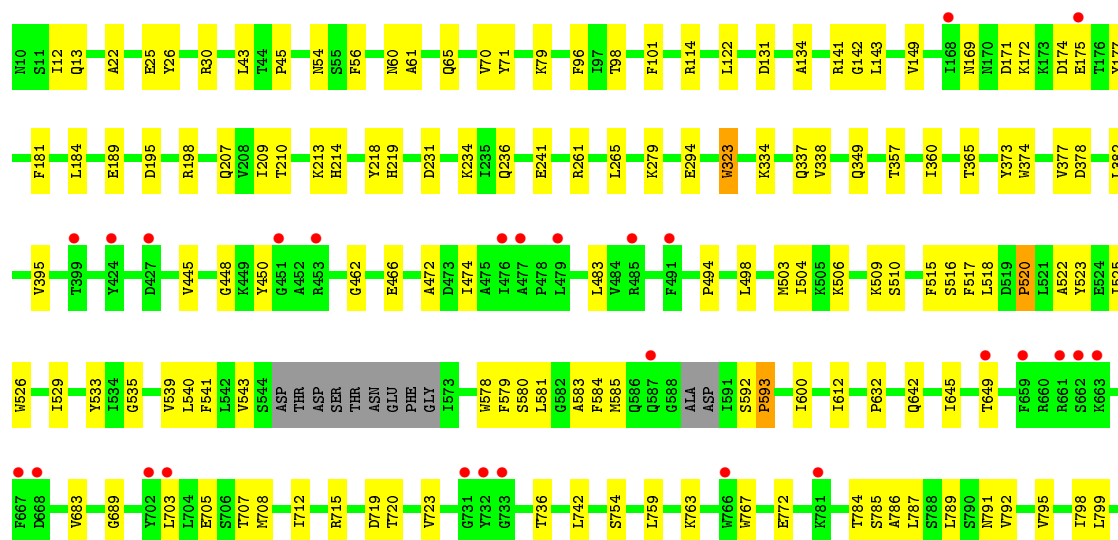
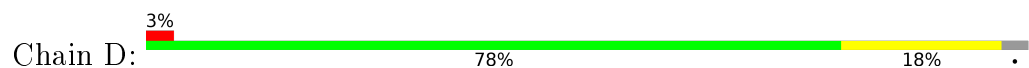




• Molecule 1: Glutamate receptor 2



• Molecule 1: Glutamate receptor 2



6802	6803	6806	6809	6812	6813	6816	LYS	SER	ARG	ALA	GLU	ALA	LYS	ARG	MET	LYS	GLY	LEU	VAL	PRO	ARG
------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	92.79Å 110.40Å 600.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.91 – 4.51 48.91 – 4.51	Depositor EDS
% Data completeness (in resolution range)	99.1 (48.91-4.51) 99.2 (48.91-4.51)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 4.45Å)	Xtriage
Refinement program	PHENIX (1.10.1 _2155: ???)	Depositor
R, R_{free}	0.257 , 0.295 0.273 , 0.309	Depositor DCC
R_{free} test set	1865 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	206.9	Xtriage
Anisotropy	0.233	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.22 , 181.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	24087	wwPDB-VP
Average B, all atoms (Å ²)	246.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.38% 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, GYB

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	0/6110	0.42	0/8271
1	B	0.26	0/6112	0.45	0/8270
1	C	0.25	0/6074	0.43	0/8225
1	D	0.25	0/6090	0.42	0/8248
All	All	0.25	0/24386	0.43	0/33014

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	5987	0	5885	83	0
1	B	5990	0	5902	108	0
1	C	5952	0	5823	124	0
1	D	5967	0	5830	100	0
2	A	14	0	13	0	0
2	B	14	0	13	0	0
2	C	14	0	13	1	0
2	D	14	0	13	1	0
3	A	54	0	0	22	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	27	0	0	3	0
3	C	27	0	0	1	0
3	D	27	0	0	3	0
All	All	24087	0	23492	371	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 8.

All (371) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:903:GYB:CAR	1:C:610:LEU:HA	1.68	1.22
3:A:903:GYB:OAQ	1:C:613:ILE:CD1	1.89	1.20
3:A:903:GYB:CAP	1:C:613:ILE:HD11	1.72	1.19
3:A:903:GYB:CAR	1:C:613:ILE:HD11	1.76	1.15
3:A:903:GYB:OAQ	1:C:613:ILE:HD11	0.92	1.09
3:A:903:GYB:OAQ	1:C:610:LEU:HD12	1.52	1.07
1:C:498:LEU:HD11	1:C:705:GLU:HB2	1.47	0.97
3:A:903:GYB:CAR	1:C:613:ILE:CD1	2.40	0.97
1:A:449:LYS:HB3	1:A:462:GLY:HA2	1.44	0.96
1:A:613:ILE:HG21	3:A:903:GYB:CAH	2.03	0.89
3:A:903:GYB:CAR	1:C:610:LEU:CA	2.54	0.83
3:A:903:GYB:CAP	1:C:613:ILE:CD1	2.50	0.83
1:D:198:ARG:HH21	1:D:279:LYS:HD3	1.45	0.80
1:C:360:ILE:HB	1:C:372:GLY:HA3	1.66	0.78
1:B:346:LYS:HG3	1:B:354:ILE:HG13	1.67	0.77
1:B:451:GLY:HA2	1:B:452:ALA:HB3	1.67	0.76
1:C:596:LEU:HD13	1:D:578:TRP:HA	1.68	0.75
1:C:521:LEU:HG	1:C:616:TYR:HD2	1.52	0.75
1:A:659:PHE:HB3	1:A:671:TRP:HB2	1.68	0.75
3:A:903:GYB:OAQ	1:C:610:LEU:CD1	2.33	0.74
1:A:649:THR:HG22	1:A:703:LEU:HB2	1.72	0.72
1:B:504:ILE:HD13	1:B:633:ILE:HD12	1.72	0.69
1:C:143:LEU:HG	1:D:143:LEU:HD11	1.75	0.69
1:B:102:PRO:HA	1:B:112:GLN:HG2	1.75	0.68
1:C:177:TYR:HB3	1:C:207:GLN:HG2	1.75	0.68
1:C:12:ILE:HG23	1:C:71:TYR:HD2	1.59	0.68
1:D:377:VAL:HG13	1:D:378:ASP:H	1.57	0.68
1:B:649:THR:HG22	1:B:703:LEU:HB2	1.76	0.67
1:C:522:ALA:H	1:D:787:LEU:HD22	1.58	0.67
1:A:70:VAL:O	1:A:308:ARG:NH1	2.28	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:649:THR:HG22	1:C:703:LEU:HB2	1.75	0.67
1:B:765:LYS:HA	1:B:769:ASP:HB2	1.77	0.67
1:C:101:PHE:HA	1:C:114:ARG:HD2	1.77	0.67
1:C:346:LYS:NZ	2:C:901:NAG:O7	2.29	0.66
1:B:494:PRO:HG3	1:C:494:PRO:HG3	1.77	0.66
3:A:903:GYB:BR1	1:B:614:SER:OG	2.66	0.66
3:A:903:GYB:CAP	1:C:610:LEU:HD12	2.25	0.66
1:C:498:LEU:HD13	1:C:707:THR:HG23	1.78	0.65
3:A:903:GYB:CAP	1:C:610:LEU:CD1	2.75	0.65
1:B:510:SER:OG	3:B:902:GYB:OAS	2.13	0.65
1:B:101:PHE:HA	1:B:114:ARG:HD2	1.78	0.64
1:A:603:GLY:HA2	1:B:585:MET:HB3	1.79	0.63
1:B:416:GLU:HA	1:B:420:ARG:HD3	1.80	0.63
1:D:71:TYR:HA	1:D:323:TRP:HH2	1.63	0.63
1:C:596:LEU:HG	1:D:809:VAL:HG11	1.81	0.62
1:C:642:GLN:HE22	1:C:645:ILE:HB	1.65	0.61
1:A:299:LEU:HD13	1:A:306:ILE:HG21	1.81	0.61
1:D:172:LYS:NZ	1:D:175:GLU:OE1	2.33	0.61
1:C:588:GLY:HA2	1:C:605:TRP:HD1	1.65	0.61
1:B:608:PHE:HD1	1:C:795:VAL:HG12	1.66	0.61
1:B:536:VAL:HG22	1:C:803:LEU:HD21	1.83	0.61
1:C:518:LEU:O	1:C:526:TRP:NE1	2.34	0.61
1:C:14:ILE:HD13	1:C:43:LEU:HD23	1.82	0.61
1:D:337:GLN:NE2	2:D:901:NAG:O7	2.34	0.60
1:C:517:PHE:CE1	1:C:795:VAL:HG22	2.38	0.59
1:A:135:TYR:CE1	1:A:137:TYR:HB3	2.38	0.59
1:B:508:GLN:N	1:B:509:LYS:HA	2.18	0.59
1:A:525:ILE:HG13	1:B:789:LEU:HD12	1.85	0.59
1:A:522:ALA:H	1:B:787:LEU:HD22	1.67	0.59
1:A:539:VAL:HG21	1:B:803:LEU:HD22	1.85	0.59
1:C:540:LEU:HA	1:C:543:VAL:HG22	1.85	0.59
1:B:498:LEU:HD12	1:B:705:GLU:HB2	1.84	0.58
1:B:447:ASP:N	1:B:448:GLY:HA2	2.18	0.58
1:C:445:VAL:HG22	1:C:448:GLY:H	1.68	0.58
1:C:640:SER:HB3	1:C:670:MET:HG2	1.84	0.58
1:B:134:ALA:HB3	1:B:192:VAL:HG22	1.86	0.58
1:C:117:LEU:HD12	1:C:120:ALA:HB3	1.86	0.58
1:C:522:ALA:HB3	1:C:525:ILE:HD13	1.85	0.58
1:C:597:SER:N	1:D:813:GLU:OE2	2.37	0.58
1:B:425:CYS:O	1:B:429:ALA:N	2.37	0.57
1:B:103:THR:HG23	1:B:112:GLN:HE21	1.69	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:476:ILE:HG22	1:B:734:ILE:HG23	1.87	0.57
1:D:498:LEU:HD12	1:D:705:GLU:HB2	1.86	0.57
1:A:124:LEU:HD13	1:A:360:ILE:HD13	1.86	0.57
3:A:903:GYB:CAR	1:C:613:ILE:HD13	2.33	0.57
1:B:168:ILE:HD11	1:B:200:LYS:HZ1	1.70	0.57
1:C:299:LEU:HD13	1:C:306:ILE:HD13	1.87	0.57
1:A:344:ASN:HD22	1:A:345:ILE:H	1.51	0.57
1:A:344:ASN:O	1:A:353:ARG:NH2	2.38	0.56
1:D:22:ALA:HB1	1:D:25:GLU:HB2	1.87	0.56
1:C:402:GLU:OE1	1:C:450:TYR:OH	2.22	0.56
1:A:806:ALA:HA	1:D:600:ILE:HD11	1.85	0.56
1:B:168:ILE:O	1:B:168:ILE:HD12	2.05	0.56
1:B:382:LEU:HD13	1:B:384:GLU:HG3	1.88	0.56
1:D:231:ASP:HB3	1:D:234:LYS:HE2	1.86	0.56
1:D:134:ALA:HB2	1:D:189:GLU:HG2	1.87	0.56
1:A:714:GLN:HA	1:A:773:CYS:HB2	1.88	0.56
1:C:13:GLN:HA	1:C:44:THR:HB	1.87	0.56
1:C:447:ASP:OD1	1:C:447:ASP:N	2.40	0.55
1:B:606:TRP:HA	1:B:609:THR:HG22	1.88	0.55
1:C:623:PHE:HZ	1:D:786:ALA:HA	1.71	0.55
1:B:615:SER:HB3	3:C:902:GYB:BR1	2.61	0.55
1:C:474:ILE:HG13	1:C:736:THR:HG22	1.87	0.55
1:D:294:GLU:HG3	1:D:338:VAL:HG11	1.87	0.55
1:A:792:VAL:HG21	1:D:525:ILE:HG12	1.89	0.55
1:C:604:VAL:HG12	1:D:799:LEU:HD12	1.88	0.55
1:D:649:THR:HG22	1:D:703:LEU:HB2	1.88	0.55
1:C:48:ASP:OD1	1:C:65:GLN:NE2	2.40	0.54
1:B:603:GLY:HA3	1:C:581:LEU:HD21	1.87	0.54
1:C:10:ASN:HB3	1:C:300:ARG:HH22	1.70	0.54
1:A:177:TYR:HD2	1:A:207:GLN:HG3	1.72	0.54
1:A:521:LEU:HD13	1:A:616:TYR:HD2	1.73	0.54
1:C:754:SER:HB2	1:C:759:LEU:HD12	1.88	0.54
1:A:209:ILE:HA	1:A:214:HIS:CD2	2.42	0.54
1:B:15:GLY:O	1:B:74:PHE:N	2.38	0.54
3:A:903:GYB:CAR	1:C:610:LEU:HD12	2.36	0.54
1:A:59:THR:HG21	1:B:59:THR:HG21	1.91	0.53
1:B:667:PHE:HE1	1:B:727:LEU:HD13	1.73	0.53
1:B:751:LEU:HB2	1:C:483:LEU:HD13	1.90	0.53
1:A:684:ARG:HG2	1:A:685:THR:HG23	1.89	0.53
1:B:227:PHE:CD1	1:B:244:GLY:HA3	2.43	0.53
1:B:633:ILE:HD13	1:B:639:LEU:HD12	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:579:PHE:HE1	1:A:592:SER:H	1.56	0.53
1:B:131:ASP:OD1	1:B:132:LYS:N	2.42	0.53
1:B:510:SER:HB3	1:B:512:PRO:HD3	1.90	0.53
1:B:754:SER:HB2	1:B:759:LEU:HD12	1.91	0.52
1:B:274:HIS:ND1	1:B:274:HIS:O	2.42	0.52
1:D:540:LEU:HA	1:D:543:VAL:HG22	1.91	0.52
1:D:213:LYS:NZ	1:D:218:TYR:OH	2.34	0.52
1:A:231:ASP:HB3	1:A:234:LYS:HE2	1.92	0.52
1:A:294:GLU:HG3	1:A:338:VAL:HG11	1.91	0.52
1:B:510:SER:HB3	1:B:511:LYS:HA	1.92	0.52
1:A:751:LEU:HB2	1:D:483:LEU:HD13	1.90	0.52
1:C:600:ILE:HA	1:D:581:LEU:HD21	1.91	0.52
1:A:344:ASN:HD22	1:A:345:ILE:N	2.07	0.52
1:D:498:LEU:HB3	1:D:707:THR:HG23	1.91	0.52
1:A:803:LEU:HD22	1:D:539:VAL:HG21	1.92	0.52
1:C:141:ARG:NH2	1:C:195:ASP:OD1	2.43	0.51
1:D:141:ARG:NH2	1:D:195:ASP:OD1	2.42	0.51
1:A:137:TYR:HA	1:A:195:ASP:HB3	1.92	0.51
1:B:620:LEU:HD21	3:B:902:GYB:BR1	2.65	0.51
1:B:659:PHE:HB3	1:B:671:TRP:HB2	1.91	0.51
1:C:521:LEU:HD23	1:D:787:LEU:HD13	1.92	0.51
1:B:708:MET:O	1:B:712:ILE:HG12	2.10	0.51
1:B:642:GLN:HE22	1:B:645:ILE:HB	1.75	0.51
1:D:12:ILE:HG23	1:D:71:TYR:HD2	1.76	0.51
1:D:715:ARG:HD3	1:D:772:GLU:HG2	1.92	0.51
1:A:494:PRO:HG3	1:D:494:PRO:HG3	1.93	0.51
1:B:388:SER:HB3	1:B:389:GLY:HA3	1.92	0.51
1:A:22:ALA:HB1	1:A:25:GLU:HB2	1.93	0.50
1:D:517:PHE:CE1	1:D:795:VAL:HG22	2.46	0.50
1:A:681:VAL:O	1:A:700:TYR:OH	2.24	0.50
1:B:163:ILE:HG21	1:B:180:LEU:HD13	1.93	0.50
1:D:174:ASP:OD1	1:D:207:GLN:NE2	2.44	0.50
1:D:509:LYS:HA	1:D:510:SER:C	2.31	0.50
1:A:520:PRO:HG3	1:A:620:LEU:HD13	1.94	0.50
3:A:903:GYB:CAR	1:C:610:LEU:CD1	2.89	0.50
1:C:97:ILE:HA	1:C:111:ILE:HB	1.94	0.50
1:C:99:PRO:HB3	1:C:284:LEU:HB2	1.93	0.50
1:A:227:PHE:CD1	1:A:244:GLY:HA3	2.48	0.49
1:B:97:ILE:HD11	1:B:333:LEU:HD22	1.95	0.49
1:D:450:TYR:HA	1:D:462:GLY:HA3	1.94	0.49
1:A:502:ILE:HD13	1:A:639:LEU:HD13	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:619:ASN:HA	1:C:624:LEU:HD13	1.94	0.49
1:D:236:GLN:NE2	1:D:365:THR:O	2.44	0.49
1:A:117:LEU:HD13	1:A:225:LEU:HD21	1.93	0.49
1:A:308:ARG:NE	1:A:312:ALA:HB2	2.27	0.49
1:A:14:ILE:HD13	1:A:43:LEU:HD23	1.95	0.49
1:B:135:TYR:CD2	1:B:146:LEU:HD13	2.48	0.49
1:B:502:ILE:HD13	1:B:639:LEU:HD13	1.94	0.49
1:B:702:TYR:CE2	1:B:704:LEU:HB3	2.47	0.49
1:C:252:ASP:OD1	1:C:253:SER:N	2.45	0.49
1:D:784:THR:HA	1:D:785:SER:HB3	1.93	0.49
1:B:508:GLN:H	1:B:509:LYS:HA	1.78	0.48
1:A:425:CYS:O	1:A:429:ALA:N	2.43	0.48
1:C:13:GLN:HG2	1:C:70:VAL:HG12	1.95	0.48
1:D:516:SER:HB2	3:D:902:GYB:CAA	2.43	0.48
1:D:474:ILE:HG13	1:D:736:THR:HG22	1.96	0.48
1:B:405:TYR:HB3	1:B:425:CYS:SG	2.54	0.48
1:D:382:LEU:H	1:D:382:LEU:HD23	1.77	0.48
1:C:579:PHE:O	1:C:583:ALA:N	2.47	0.48
1:A:493:LYS:HG3	1:A:751:LEU:HD21	1.94	0.48
1:B:38:THR:HG23	1:B:40:GLU:H	1.78	0.48
1:C:118:LYS:HG2	1:C:145:THR:HG22	1.95	0.48
1:B:225:LEU:HB2	1:B:280:TYR:CD2	2.49	0.48
1:B:499:GLY:HA3	1:B:726:ASN:HB3	1.95	0.47
1:C:213:LYS:NZ	1:C:218:TYR:OH	2.39	0.47
1:A:485:ARG:O	1:A:489:ILE:HG13	2.14	0.47
1:C:373:TYR:HB3	1:C:381:VAL:O	2.14	0.47
1:D:708:MET:O	1:D:712:ILE:HG12	2.14	0.47
1:A:177:TYR:CD2	1:A:207:GLN:HG3	2.48	0.47
1:A:150:LEU:HD22	1:B:162:ALA:HB3	1.96	0.47
1:D:209:ILE:HA	1:D:214:HIS:CD2	2.49	0.47
1:A:522:ALA:N	1:B:787:LEU:HD22	2.29	0.47
1:C:169:ASN:HD21	1:C:172:LYS:HD3	1.79	0.47
1:D:763:LYS:O	1:D:767:TRP:HB2	2.14	0.47
1:B:430:ALA:HA	1:B:440:TYR:HE1	1.79	0.47
1:B:505:LYS:HE2	1:B:507:PRO:HB3	1.96	0.47
1:C:632:PRO:HB2	1:C:633:ILE:HB	1.96	0.47
1:D:787:LEU:HD21	1:D:792:VAL:HG21	1.95	0.47
1:A:196:CYS:HB3	1:A:200:LYS:HB2	1.96	0.47
1:C:502:ILE:HB	1:C:723:VAL:HG23	1.96	0.47
1:B:193:ILE:HG12	1:B:221:ILE:HB	1.96	0.47
1:D:592:SER:N	1:D:593:PRO:HD3	2.29	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:371:ILE:HA	1:C:382:LEU:HD22	1.97	0.47
1:C:600:ILE:HD11	1:D:806:ALA:HA	1.97	0.47
1:C:177:TYR:CB	1:C:207:GLN:HG2	2.45	0.46
1:A:291:VAL:HA	1:A:336:VAL:HG11	1.97	0.46
1:A:489:ILE:HD13	1:A:735:ALA:HB1	1.98	0.46
1:B:124:LEU:HA	1:B:380:MET:HE1	1.95	0.46
1:B:540:LEU:HA	1:B:543:VAL:HG22	1.97	0.46
1:D:504:ILE:HD11	1:D:723:VAL:HG11	1.96	0.46
1:D:754:SER:HB2	1:D:759:LEU:HD12	1.98	0.46
1:A:375:SER:N	1:A:378:ASP:O	2.46	0.46
1:C:79:LYS:HD2	1:C:139:SER:O	2.16	0.46
1:D:789:LEU:HA	1:D:792:VAL:HB	1.98	0.46
1:B:463:MET:HE3	1:B:475:ALA:HB1	1.98	0.46
1:A:789:LEU:HA	1:D:525:ILE:HD11	1.96	0.46
1:A:637:GLU:O	1:A:641:LYS:N	2.49	0.46
1:A:620:LEU:HD21	3:A:902:GYB:BR1	2.71	0.46
1:A:358:ILE:HD12	1:A:374:TRP:HE1	1.79	0.46
1:B:387:THR:N	1:B:388:SER:HA	2.31	0.46
1:B:404:PRO:HG3	1:B:711:TYR:CD1	2.51	0.46
1:A:540:LEU:HA	1:A:543:VAL:HG22	1.98	0.45
1:D:181:PHE:HA	1:D:184:LEU:HB2	1.97	0.45
1:B:734:ILE:HG21	1:B:746:VAL:HG11	1.98	0.45
1:B:132:LYS:NZ	1:B:189:GLU:OE2	2.49	0.45
1:B:399:THR:HG21	1:B:406:VAL:HG21	1.97	0.45
1:A:787:LEU:O	1:D:522:ALA:HB2	2.16	0.45
1:A:236:GLN:NE2	1:A:365:THR:O	2.49	0.45
1:A:719:ASP:N	1:A:719:ASP:OD1	2.47	0.45
1:B:74:PHE:CZ	1:B:285:THR:HG23	2.51	0.45
1:B:26:TYR:HE1	1:B:47:ILE:HG12	1.81	0.45
1:C:604:VAL:HG21	1:D:802:GLY:HA3	1.99	0.45
1:C:475:ALA:HB3	1:C:735:ALA:HB3	1.97	0.45
1:A:131:ASP:N	1:A:131:ASP:OD1	2.49	0.45
1:D:357:THR:HG23	1:D:373:TYR:HB2	1.99	0.45
1:B:118:LYS:HB3	1:B:145:THR:HG22	1.98	0.45
1:B:177:TYR:HB3	1:B:207:GLN:HG2	1.98	0.45
1:B:406:VAL:HG23	1:B:425:CYS:HB2	1.99	0.45
1:B:502:ILE:HB	1:B:723:VAL:HG23	1.97	0.45
1:C:23:ASP:HB3	1:C:271:PRO:HG2	1.99	0.45
1:C:600:ILE:HG22	1:D:581:LEU:CD1	2.46	0.45
1:A:372:GLY:HA2	1:A:382:LEU:HB3	1.99	0.45
1:B:520:PRO:HG3	1:B:620:LEU:HD13	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:236:GLN:NE2	1:C:365:THR:O	2.45	0.45
1:D:131:ASP:N	1:D:131:ASP:OD1	2.47	0.45
1:D:198:ARG:NH2	1:D:279:LYS:HD3	2.22	0.45
1:C:464:VAL:HG22	1:C:479:LEU:HD21	1.98	0.45
1:D:683:VAL:HG11	1:D:689:GLY:HA2	1.98	0.45
1:A:103:THR:O	1:A:352:LYS:NZ	2.43	0.44
1:A:125:ILE:HG23	1:A:130:TRP:HB2	1.99	0.44
1:A:518:LEU:O	1:A:526:TRP:NE1	2.50	0.44
1:B:387:THR:O	1:B:387:THR:OG1	2.24	0.44
1:C:499:GLY:HA3	1:C:726:ASN:HB3	1.98	0.44
1:C:498:LEU:HD22	1:C:732:TYR:CZ	2.53	0.44
1:D:360:ILE:HD11	1:D:374:TRP:HB2	1.98	0.44
1:A:504:ILE:HD11	1:A:723:VAL:HG11	1.99	0.44
1:B:299:LEU:HD13	1:B:306:ILE:HG21	1.99	0.44
1:C:135:TYR:CE2	1:C:137:TYR:HB3	2.53	0.44
1:C:476:ILE:HG12	1:C:734:ILE:HG23	1.99	0.44
1:D:143:LEU:HD23	1:D:143:LEU:H	1.82	0.44
1:C:521:LEU:HA	1:D:787:LEU:HD13	1.99	0.44
1:A:642:GLN:HE22	1:A:645:ILE:HB	1.83	0.44
1:B:358:ILE:O	1:B:374:TRP:N	2.49	0.44
1:C:539:VAL:HG21	1:D:803:LEU:HD22	1.99	0.44
1:A:507:PRO:HA	1:A:508:GLN:CB	2.48	0.44
1:A:62:PHE:HE2	1:A:92:LEU:HD12	1.82	0.44
1:B:130:TRP:CE2	1:B:191:ARG:HD3	2.52	0.44
1:D:79:LYS:HD2	1:D:142:GLY:HA2	1.98	0.44
1:B:576:SER:HA	1:B:579:PHE:HB3	1.99	0.44
1:B:74:PHE:HA	1:B:97:ILE:O	2.18	0.44
1:A:791:ASN:OD1	3:A:902:GYB:NAI	2.50	0.43
3:A:903:GYB:OAG	1:C:606:TRP:NE1	2.51	0.43
1:B:299:LEU:HD21	1:B:332:ALA:HB2	2.00	0.43
1:C:388:SER:H	1:C:389:GLY:HA2	1.82	0.43
1:C:417:GLY:O	1:C:420:ARG:NE	2.51	0.43
1:D:122:LEU:HD21	1:D:149:VAL:HA	2.01	0.43
1:A:467:LEU:HD23	1:A:467:LEU:HA	1.88	0.43
1:B:304:ILE:HD12	1:B:304:ILE:O	2.19	0.43
1:B:793:ALA:HB1	1:B:797:TYR:CE2	2.54	0.43
1:A:600:ILE:HD11	1:B:806:ALA:HA	1.99	0.43
1:B:809:VAL:O	1:B:812:ILE:HG12	2.19	0.43
1:D:101:PHE:HA	1:D:114:ARG:HD2	2.00	0.43
1:D:169:ASN:ND2	1:D:171:ASP:OD1	2.51	0.43
1:D:518:LEU:O	1:D:526:TRP:NE1	2.51	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:163:ILE:HG21	1:C:180:LEU:HD13	2.00	0.43
1:C:22:ALA:HB1	1:C:25:GLU:HB2	2.00	0.43
1:C:500:ILE:HB	1:C:727:LEU:HB2	1.99	0.43
1:C:500:ILE:O	1:C:727:LEU:N	2.51	0.43
1:D:171:ASP:OD1	1:D:172:LYS:N	2.51	0.43
1:D:506:LYS:N	1:D:719:ASP:O	2.43	0.43
1:C:763:LYS:HD2	1:C:767:TRP:CE3	2.54	0.43
1:D:26:TYR:CE2	1:D:30:ARG:HD2	2.53	0.43
1:C:520:PRO:HB2	1:C:616:TYR:CE2	2.54	0.43
1:A:115:PRO:HA	1:A:353:ARG:HB2	2.01	0.43
1:D:517:PHE:O	1:D:520:PRO:HD2	2.18	0.43
1:C:615:SER:OG	3:D:902:GYB:NBA	2.52	0.43
1:B:608:PHE:CD1	1:C:795:VAL:HG12	2.49	0.42
1:C:87:SER:OG	1:D:54:ASN:OD1	2.36	0.42
1:D:529:ILE:HD13	1:D:612:ILE:HD12	2.01	0.42
1:B:295:ALA:HB2	1:B:333:LEU:HD23	2.02	0.42
1:C:219:HIS:HA	1:C:241:GLU:O	2.19	0.42
1:C:464:VAL:HG13	1:C:489:ILE:HG12	2.00	0.42
1:D:503:MET:HG3	1:D:720:THR:HB	2.02	0.42
1:B:320:ALA:O	1:B:322:PRO:HD3	2.19	0.42
1:B:521:LEU:HD13	1:B:616:TYR:HD1	1.84	0.42
1:D:61:ALA:O	1:D:65:GLN:HG2	2.18	0.42
1:A:120:ALA:HB2	1:A:374:TRP:NE1	2.34	0.42
1:D:466:GLU:O	1:D:472:ALA:N	2.52	0.42
1:D:580:SER:O	1:D:584:PHE:N	2.53	0.42
1:D:809:VAL:HA	1:D:812:ILE:HG12	2.02	0.42
1:A:613:ILE:CG2	3:A:903:GYB:CAH	2.87	0.42
1:B:518:LEU:HB2	1:B:526:TRP:CE2	2.54	0.42
1:C:266:GLU:HG2	1:C:268:LYS:H	1.85	0.42
1:D:261:ARG:HA	1:D:261:ARG:HD2	1.81	0.42
1:D:43:LEU:O	1:D:45:PRO:HD3	2.20	0.42
1:B:237:PHE:HB2	1:D:210:THR:HG22	2.02	0.42
1:B:403:SER:HA	1:B:404:PRO:HA	1.87	0.42
1:D:13:GLN:HG3	1:D:70:VAL:HG12	2.02	0.42
1:A:225:LEU:HB2	1:A:280:TYR:CD2	2.55	0.42
1:B:209:ILE:HG23	1:B:214:HIS:NE2	2.33	0.42
1:A:123:SER:OG	1:A:379:LYS:HD3	2.20	0.41
1:C:588:GLY:C	1:C:602:GLY:HA2	2.41	0.41
1:D:219:HIS:HA	1:D:241:GLU:O	2.20	0.41
1:A:600:ILE:HA	1:B:581:LEU:HD21	2.01	0.41
1:A:728:ASP:OD2	1:A:730:LYS:HE3	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:THR:HG23	1:B:41:PHE:H	1.84	0.41
1:C:110:VAL:HG12	1:C:112:GLN:HG3	2.02	0.41
1:C:308:ARG:HE	1:C:312:ALA:HB2	1.85	0.41
1:C:597:SER:O	1:C:601:VAL:HG23	2.20	0.41
1:D:334:LYS:NZ	1:D:349:GLN:O	2.34	0.41
1:A:424:TYR:HE2	1:A:495:PHE:HE2	1.68	0.41
1:C:637:GLU:HG2	1:C:641:LYS:HE3	2.01	0.41
1:C:659:PHE:HB3	1:C:671:TRP:HB2	2.02	0.41
1:D:395:VAL:HG21	1:D:742:LEU:HD21	2.02	0.41
3:D:902:GYB:CAT	3:D:902:GYB:CAO	2.97	0.41
1:D:795:VAL:O	1:D:798:ILE:HG22	2.20	0.41
1:B:518:LEU:O	1:B:526:TRP:NE1	2.53	0.41
1:B:525:ILE:HG12	1:C:792:VAL:HG11	2.02	0.41
1:D:579:PHE:O	1:D:583:ALA:N	2.54	0.41
1:A:763:LYS:O	1:A:767:TRP:HB2	2.20	0.41
1:B:324:GLY:O	1:B:327:VAL:HG12	2.21	0.41
1:C:204:ILE:O	1:C:208:VAL:HG23	2.20	0.41
1:C:525:ILE:HD11	1:D:789:LEU:HB3	2.03	0.41
1:C:604:VAL:HG11	1:D:802:GLY:HA3	2.02	0.41
1:B:288:ALA:O	1:B:292:MET:HG3	2.20	0.41
1:B:507:PRO:HD2	1:B:508:GLN:HA	2.02	0.41
1:D:515:PHE:HA	1:D:515:PHE:HD2	1.77	0.41
1:D:535:GLY:O	1:D:539:VAL:HG23	2.21	0.41
1:C:600:ILE:HG22	1:D:581:LEU:HD13	2.03	0.41
1:D:715:ARG:HA	1:D:715:ARG:HD3	1.91	0.41
1:B:236:GLN:HG3	1:B:363:LEU:HD11	2.03	0.41
1:C:751:LEU:HD23	1:C:751:LEU:HA	1.86	0.41
1:D:377:VAL:HG13	1:D:378:ASP:N	2.32	0.41
1:A:348:ASP:HB3	1:A:354:ILE:HG21	2.03	0.41
1:C:135:TYR:HH	1:C:145:THR:HG1	1.64	0.41
1:C:502:ILE:O	1:C:709:ASN:ND2	2.52	0.41
1:D:96:PHE:CE2	1:D:98:THR:HB	2.56	0.41
1:A:76:PHE:CE2	1:A:99:PRO:HG2	2.56	0.41
1:C:532:ALA:HB1	1:C:605:TRP:HZ3	1.86	0.41
1:D:642:GLN:HE22	1:D:645:ILE:HB	1.86	0.41
1:B:113:MET:HB3	1:B:284:LEU:HD22	2.03	0.40
1:C:174:ASP:OD1	1:C:207:GLN:NE2	2.54	0.40
1:C:318:ASN:HB2	1:D:60:ASN:HD21	1.86	0.40
3:A:903:GYB:CAP	1:C:610:LEU:HD13	2.51	0.40
1:B:728:ASP:OD1	1:B:728:ASP:N	2.54	0.40
1:C:422:GLU:HB2	1:C:766:TRP:HH2	1.87	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:445:VAL:HG13	1:D:448:GLY:HA2	2.03	0.40
1:A:122:LEU:HA	1:A:122:LEU:HD23	1.93	0.40
1:A:308:ARG:HE	1:A:312:ALA:HB2	1.85	0.40
1:B:229:ASP:OD2	1:B:280:TYR:N	2.54	0.40
1:C:91:THR:HG21	1:D:56:PHE:CE1	2.56	0.40
1:A:96:PHE:CE2	1:A:98:THR:HB	2.57	0.40
1:C:10:ASN:ND2	1:C:40:GLU:O	2.51	0.40
1:C:606:TRP:HA	1:C:609:THR:HG22	2.03	0.40
1:D:261:ARG:O	1:D:265:LEU:HG	2.22	0.40
1:A:74:PHE:CZ	1:A:285:THR:HG23	2.56	0.40
1:B:620:LEU:HD11	3:B:902:GYB:CAY	2.52	0.40
1:C:348:ASP:OD1	1:C:352:LYS:N	2.54	0.40
1:C:388:SER:N	1:C:389:GLY:HA2	2.37	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%)	715 (93%)	52 (7%)	4 (0%)	34	77
1	B	767/803 (96%)	708 (92%)	57 (7%)	2 (0%)	46	83
1	C	768/803 (96%)	715 (93%)	48 (6%)	5 (1%)	26	71
1	D	771/803 (96%)	720 (93%)	48 (6%)	3 (0%)	39	80
All	All	3077/3212 (96%)	2858 (93%)	205 (7%)	14 (0%)	34	77

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	510	SER
1	A	596	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	593	PRO
1	C	373	TYR
1	A	520	PRO
1	A	630	VAL
1	D	520	PRO
1	C	512	PRO
1	C	520	PRO
1	B	520	PRO
1	C	633	ILE
1	D	632	PRO
1	A	593	PRO
1	B	507	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%)	622 (99%)	5 (1%)	86	93
1	B	634/683 (93%)	627 (99%)	7 (1%)	80	90
1	C	619/683 (91%)	617 (100%)	2 (0%)	94	96
1	D	620/683 (91%)	613 (99%)	7 (1%)	80	90
All	All	2500/2732 (92%)	2479 (99%)	21 (1%)	86	93

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

Mol	Chain	Res	Type
1	A	77	TYR
1	A	274	HIS
1	A	323	TRP
1	A	344	ASN
1	A	523	TYR
1	B	88	PHE
1	B	323	TRP
1	B	440	TYR
1	B	491	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	523	TYR
1	B	541	PHE
1	B	585	MET
1	C	323	TRP
1	C	523	TYR
1	D	177	TYR
1	D	323	TRP
1	D	523	TYR
1	D	533	TYR
1	D	541	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	791	ASN
1	C	207	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](#)

9 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	1	14,14,15	0.75	1 (7%)	15,19,21	0.66	0
3	GYB	A	902	-	25,30,30	3.77	12 (48%)	34,44,44	3.21	14 (41%)
3	GYB	A	903	-	25,30,30	2.31	6 (24%)	34,44,44	3.75	9 (26%)
2	NAG	B	901	1	14,14,15	0.35	0	15,19,21	0.55	0
3	GYB	B	902	-	25,30,30	3.85	12 (48%)	34,44,44	3.11	14 (41%)
2	NAG	C	901	1	14,14,15	0.35	0	15,19,21	0.59	1 (6%)
3	GYB	C	902	-	25,30,30	3.63	12 (48%)	34,44,44	3.42	15 (44%)
2	NAG	D	901	1	14,14,15	0.50	0	15,19,21	0.57	0
3	GYB	D	902	-	25,30,30	3.70	12 (48%)	34,44,44	3.54	14 (41%)

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	1	-	0/6/23/26	0/1/1/1
3	GYB	A	902	-	-	0/6/32/32	0/3/4/4
3	GYB	A	903	-	1/1/4/5	0/6/32/32	0/3/4/4
2	NAG	B	901	1	-	0/6/23/26	0/1/1/1
3	GYB	B	902	-	-	0/6/32/32	0/3/4/4
2	NAG	C	901	1	-	0/6/23/26	0/1/1/1
3	GYB	C	902	-	-	0/6/32/32	0/3/4/4
2	NAG	D	901	1	-	0/6/23/26	0/1/1/1
3	GYB	D	902	-	-	0/6/32/32	0/3/4/4

All (55) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	903	GYB	CAU-CAM	-6.74	1.40	1.49
3	D	902	GYB	OAG-CAR	-5.41	1.33	1.43
3	C	902	GYB	OAG-CAR	-5.41	1.33	1.43
3	A	902	GYB	OAG-CAR	-5.41	1.33	1.43
3	C	902	GYB	OAQ-CAR	-5.40	1.33	1.43
3	D	902	GYB	OAQ-CAR	-5.37	1.33	1.43
3	A	902	GYB	OAQ-CAR	-5.33	1.33	1.43
3	B	902	GYB	OAG-CAR	-5.31	1.33	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	902	GYB	OAQ-CAR	-5.29	1.33	1.43
3	A	903	GYB	CAN-CAM	-5.08	1.41	1.49
3	D	902	GYB	OAS-CAJ	-4.23	1.14	1.23
3	B	902	GYB	OAS-CAJ	-4.21	1.14	1.23
3	A	902	GYB	OAS-CAJ	-4.18	1.14	1.23
3	C	902	GYB	OAS-CAJ	-4.15	1.15	1.23
3	A	903	GYB	CAC-CAD	-3.02	1.44	1.51
3	A	903	GYB	CAO-CAP	-2.63	1.33	1.38
3	A	903	GYB	CAE-CAF	-2.52	1.34	1.38
2	A	901	NAG	C1-C2	2.60	1.56	1.52
3	C	902	GYB	CAE-CAF	2.95	1.44	1.38
3	A	902	GYB	CAE-CAF	3.07	1.44	1.38
3	D	902	GYB	CAE-CAF	3.25	1.44	1.38
3	D	902	GYB	CAO-CAP	3.34	1.45	1.38
3	C	902	GYB	CAO-CAN	3.43	1.45	1.39
3	C	902	GYB	CAO-CAP	3.43	1.45	1.38
3	B	902	GYB	CAE-CAF	3.44	1.45	1.38
3	C	902	GYB	CAJ-NAK	3.47	1.47	1.39
3	D	902	GYB	CAJ-NAK	3.50	1.47	1.39
3	B	902	GYB	CAO-CAP	3.51	1.45	1.38
3	A	902	GYB	CAO-CAP	3.52	1.45	1.38
3	B	902	GYB	CAX-NBA	3.57	1.49	1.37
3	A	902	GYB	CAO-CAN	3.59	1.45	1.39
3	D	902	GYB	CAX-NBA	3.68	1.49	1.37
3	A	902	GYB	CAX-NBA	3.68	1.49	1.37
3	C	902	GYB	CAX-NBA	3.69	1.49	1.37
3	B	902	GYB	CAO-CAN	3.72	1.46	1.39
3	D	902	GYB	CAO-CAN	3.76	1.46	1.39
3	B	902	GYB	CAJ-NAK	3.79	1.47	1.39
3	D	902	GYB	CAE-CAD	3.83	1.46	1.39
3	C	902	GYB	CAE-CAD	3.85	1.46	1.39
3	A	902	GYB	CAE-CAD	3.91	1.46	1.39
3	A	902	GYB	CAJ-NAK	3.92	1.48	1.39
3	B	902	GYB	CAU-CAM	4.03	1.54	1.49
3	D	902	GYB	CAU-CAM	4.08	1.55	1.49
3	C	902	GYB	CAU-CAM	4.16	1.55	1.49
3	B	902	GYB	CAE-CAD	4.26	1.46	1.39
3	A	902	GYB	CAU-CAM	4.39	1.55	1.49
3	A	903	GYB	CAA-CAB	4.53	1.66	1.52
3	D	902	GYB	CAN-CAM	4.79	1.56	1.49
3	C	902	GYB	CAN-CAM	4.80	1.56	1.49
3	A	902	GYB	CAN-CAM	4.84	1.56	1.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	902	GYB	CAN-CAM	5.10	1.57	1.49
3	C	902	GYB	CAJ-NAI	11.23	1.47	1.34
3	D	902	GYB	CAJ-NAI	11.64	1.48	1.34
3	A	902	GYB	CAJ-NAI	11.99	1.48	1.34
3	B	902	GYB	CAJ-NAI	12.36	1.48	1.34

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	902	GYB	CAN-CAM-NAL	-10.39	112.83	126.13
3	B	902	GYB	CAN-CAM-NAL	-10.27	112.98	126.13
3	C	902	GYB	CAH-NAI-CAJ	-9.17	111.55	120.78
3	C	902	GYB	CAN-CAM-NAL	-9.03	114.57	126.13
3	A	902	GYB	CAN-CAM-NAL	-8.73	114.95	126.13
3	B	902	GYB	CAU-CAM-NAL	-7.14	105.54	117.79
3	D	902	GYB	CAU-CAM-NAL	-6.37	106.86	117.79
3	A	902	GYB	CAU-CAM-NAL	-6.26	107.05	117.79
3	D	902	GYB	CAH-NAI-CAJ	-6.05	114.69	120.78
3	A	903	GYB	CAT-CAU-CAM	-5.90	113.19	120.61
3	C	902	GYB	CAU-CAM-NAL	-5.88	107.69	117.79
3	D	902	GYB	CAN-CAM-CAU	-5.61	111.35	118.10
3	D	902	GYB	CAA-CAB-CAC	-5.61	105.50	111.43
3	C	902	GYB	CAN-CAM-CAU	-4.83	112.28	118.10
3	A	902	GYB	CAN-CAM-CAU	-4.68	112.47	118.10
3	A	902	GYB	CAH-NAI-CAJ	-4.52	116.23	120.78
3	B	902	GYB	OAG-CAF-CAP	-3.81	105.02	109.77
3	A	903	GYB	CAO-CAN-CAM	-3.65	114.27	118.98
3	D	902	GYB	OAG-CAF-CAP	-3.63	105.25	109.77
3	B	902	GYB	CAN-CAM-CAU	-3.51	113.87	118.10
3	C	902	GYB	OAG-CAF-CAP	-3.40	105.53	109.77
3	A	902	GYB	OAG-CAF-CAP	-3.33	105.63	109.77
3	C	902	GYB	OAS-CAJ-NAI	-3.23	117.42	123.35
3	A	902	GYB	OAS-CAJ-NAI	-3.13	117.62	123.35
3	A	902	GYB	OAQ-CAP-CAF	-2.72	106.38	109.77
3	D	902	GYB	OAS-CAJ-NAI	-2.60	118.58	123.35
3	C	902	GYB	OAQ-CAP-CAF	-2.57	106.57	109.77
3	C	902	GYB	CAO-CAN-CAM	-2.52	115.74	118.98
3	A	903	GYB	CAC-CAD-CAE	-2.40	111.52	118.06
3	D	902	GYB	OAQ-CAP-CAF	-2.35	106.84	109.77
3	A	903	GYB	CAH-NAI-CAJ	-2.33	118.43	120.78
3	B	902	GYB	CAV-CAY-CAX	-2.27	119.13	121.46
3	A	902	GYB	CAO-CAN-CAM	-2.27	116.06	118.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	902	GYB	OAQ-CAP-CAF	-2.23	107.00	109.77
3	B	902	GYB	CAA-CAB-CAC	-2.09	109.22	111.43
3	A	903	GYB	CAT-CAW-CAX	-2.08	118.75	121.35
3	B	902	GYB	CAH-NAI-CAJ	-2.05	118.72	120.78
3	B	902	GYB	CAO-CAN-CAM	-2.03	116.36	118.98
3	C	902	GYB	CAT-CAU-CAM	2.00	123.14	120.61
3	A	903	GYB	NAI-CAJ-NAK	2.01	117.68	115.75
2	C	901	NAG	C1-O5-C5	2.09	115.21	112.14
3	D	902	GYB	CAR-OAQ-CAP	2.09	108.38	105.32
3	C	902	GYB	CAR-OAQ-CAP	2.13	108.43	105.32
3	A	902	GYB	CAR-OAQ-CAP	2.29	108.66	105.32
3	C	902	GYB	CAR-OAG-CAF	2.47	108.92	105.32
3	A	902	GYB	CAR-OAG-CAF	2.58	109.09	105.32
3	D	902	GYB	CAR-OAG-CAF	2.75	109.34	105.32
3	B	902	GYB	CAR-OAG-CAF	2.86	109.50	105.32
3	C	902	GYB	OAQ-CAP-CAO	3.43	132.73	127.87
3	B	902	GYB	CAC-CAD-CAN	3.44	123.75	120.21
3	C	902	GYB	CAC-CAD-CAN	3.58	123.90	120.21
3	A	902	GYB	OAQ-CAP-CAO	3.76	133.20	127.87
3	A	902	GYB	CAC-CAD-CAN	3.78	124.10	120.21
3	B	902	GYB	OAQ-CAP-CAO	3.80	133.26	127.87
3	D	902	GYB	OAQ-CAP-CAO	3.86	133.34	127.87
3	A	903	GYB	CAV-CAU-CAM	4.21	128.20	120.38
3	D	902	GYB	CAC-CAD-CAN	4.56	124.91	120.21
3	C	902	GYB	OAG-CAF-CAE	4.75	134.61	127.87
3	A	902	GYB	OAG-CAF-CAE	4.82	134.70	127.87
3	D	902	GYB	OAG-CAF-CAE	5.22	135.28	127.87
3	B	902	GYB	OAG-CAF-CAE	5.27	135.35	127.87
3	B	902	GYB	NAI-CAJ-NAK	5.76	121.28	115.75
3	D	902	GYB	NAI-CAJ-NAK	7.32	122.77	115.75
3	C	902	GYB	NAI-CAJ-NAK	7.68	123.12	115.75
3	A	902	GYB	NAI-CAJ-NAK	8.58	123.99	115.75
3	A	903	GYB	CAC-CAD-CAN	11.01	131.54	120.21
3	A	903	GYB	CAA-CAB-CAC	15.84	128.17	111.43

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	903	GYB	CAB

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	902	GYB	2	0
3	A	903	GYB	20	0
3	B	902	GYB	3	0
2	C	901	NAG	1	0
3	C	902	GYB	1	0
2	D	901	NAG	1	0
3	D	902	GYB	3	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	777/803 (96%)	-0.13	18 (2%) 64 54	153, 228, 329, 363	0
1	B	773/803 (96%)	-0.06	27 (3%) 48 38	172, 212, 312, 365	0
1	C	774/803 (96%)	0.07	28 (3%) 46 37	146, 255, 314, 341	0
1	D	777/803 (96%)	-0.04	27 (3%) 48 38	202, 266, 336, 372	0
All	All	3101/3212 (96%)	-0.04	100 (3%) 51 40	146, 242, 325, 372	0

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	733	GLY	7.3
1	A	781	LYS	5.6
1	C	276	ALA	5.6
1	B	816	TYR	5.0
1	D	731	GLY	4.9
1	A	389	GLY	4.9
1	C	510	SER	4.6
1	D	732	TYR	4.6
1	C	511	LYS	4.3
1	B	698	GLY	4.3
1	A	782	GLU	4.3
1	D	662	SER	4.1
1	D	661	ARG	4.1
1	D	451	GLY	4.0
1	C	784	THR	4.0
1	A	778	SER	4.0
1	B	697	LYS	4.0
1	C	783	LYS	3.9
1	B	699	LYS	3.9
1	D	175	GLU	3.8
1	D	453	ARG	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	388	SER	3.8
1	C	586	GLN	3.8
1	A	385	ASP	3.7
1	B	700	TYR	3.6
1	D	587	GLN	3.5
1	D	476	ILE	3.4
1	C	782	GLU	3.2
1	A	587	GLN	3.2
1	A	527	MET	3.1
1	A	780	SER	3.1
1	A	536	VAL	3.0
1	C	456	ASP	3.0
1	A	386	ASP	2.9
1	C	272	GLY	2.9
1	D	766	TRP	2.9
1	B	649	THR	2.9
1	B	507	PRO	2.9
1	A	173	LYS	2.9
1	D	659	PHE	2.8
1	C	334	LYS	2.8
1	D	663	LYS	2.8
1	C	509	LYS	2.8
1	D	702	TYR	2.8
1	B	416	GLU	2.8
1	C	457	THR	2.8
1	C	508	GLN	2.7
1	B	815	CYS	2.7
1	D	649	THR	2.7
1	A	387	THR	2.6
1	C	527	MET	2.6
1	B	630	VAL	2.6
1	D	477	ALA	2.6
1	A	777	ASP	2.5
1	B	505	LYS	2.5
1	D	168	ILE	2.5
1	C	306	ILE	2.5
1	B	104	ASP	2.5
1	B	144	SER	2.5
1	C	580	SER	2.5
1	C	531	PHE	2.5
1	B	234	LYS	2.5
1	D	703	LEU	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	479	LEU	2.4
1	B	508	GLN	2.4
1	B	695	LYS	2.4
1	C	503	MET	2.4
1	C	265	LEU	2.4
1	C	459	ILE	2.4
1	B	456	ASP	2.4
1	C	803	LEU	2.3
1	B	648	GLY	2.3
1	A	580	SER	2.3
1	C	594	ARG	2.3
1	A	537	SER	2.2
1	C	630	VAL	2.3
1	A	779	GLY	2.2
1	D	399	THR	2.2
1	D	667	PHE	2.2
1	B	414	MET	2.2
1	D	491	PHE	2.2
1	D	781	LYS	2.2
1	A	383	THR	2.2
1	D	668	ASP	2.2
1	C	507	PRO	2.1
1	B	442	LEU	2.1
1	B	696	SER	2.1
1	C	534	ILE	2.1
1	B	588	GLY	2.1
1	B	441	LYS	2.1
1	D	424	TYR	2.1
1	B	116	ASP	2.1
1	B	600	ILE	2.1
1	C	631	SER	2.1
1	B	629	MET	2.0
1	D	485	ARG	2.0
1	C	701	ALA	2.0
1	B	646	ALA	2.0
1	C	699	LYS	2.0
1	D	427	ASP	2.0

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

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

6.3 Carbohydrates [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(\AA^2)	Q<0.9
3	GYB	A	903	27/27	0.62	0.78	7.61	58,205,248,257	27
2	NAG	A	901	14/15	0.33	1.03	4.72	344,344,346,352	0
3	GYB	A	902	27/27	0.64	0.62	2.58	259,264,270,279	0
3	GYB	C	902	27/27	0.70	0.88	2.23	252,261,270,281	0
3	GYB	B	902	27/27	0.72	0.40	1.63	253,263,269,275	0
3	GYB	D	902	27/27	0.72	0.19	-0.56	253,264,269,292	0
2	NAG	B	901	14/15	0.81	0.34	-	285,285,287,290	0
2	NAG	D	901	14/15	0.52	0.64	-	358,358,359,362	0
2	NAG	C	901	14/15	0.32	0.89	-	505,505,507,515	0

6.5 Other polymers [i](#)

There are no such residues in this entry.