



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:47 AM GMT

PDB ID : 3G0G
Title : Crystal structure of dipeptidyl peptidase IV in complex with a pyrimidinone inhibitor 3
Authors : Zhang, Z.; Wallace, M.B.; Feng, J.; Stafford, J.A.; Kaldor, S.W.; Shi, L.; Skene, R.J.; Aertgeerts, K.; Lee, B.; Jennings, A.; Xu, R.; Kassel, D.; Webb, D.R.; Gwaltney, S.L.
Deposited on : 2009-01-27
Resolution : 2.45 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
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) : trunk26865

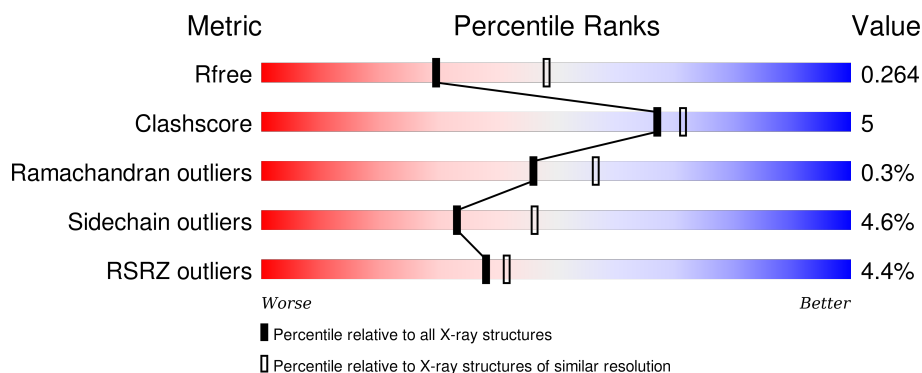
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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	4776 (2.50-2.42)
Clashscore	102246	1030 (2.48-2.44)
Ramachandran outliers	100387	1024 (2.48-2.44)
Sidechain outliers	100360	1024 (2.48-2.44)
RSRZ outliers	91569	4787 (2.50-2.42)

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	740	<div> <div>3%</div> <div> <div></div> <div>81%</div> <div>16%</div> <div>..</div> </div> </div>
1	B	740	<div> <div>%</div> <div> <div></div> <div>85%</div> <div>13%</div> <div>..</div> </div> </div>
1	C	740	<div> <div>5%</div> <div> <div></div> <div>84%</div> <div>13%</div> <div>..</div> </div> </div>
1	D	740	<div> <div>8%</div> <div> <div></div> <div>80%</div> <div>12%</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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	A	808	-	-	-	X
3	NAG	B	808	-	-	-	X
3	NAG	C	808	-	-	-	X
3	NAG	D	803	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 24783 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 Dipeptidyl peptidase 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	724	Total	C	N	O	S	0	2	0
			5933	3811	975	1121	26			
1	B	730	Total	C	N	O	S	0	2	0
			5990	3844	991	1129	26			
1	C	724	Total	C	N	O	S	0	1	0
			5929	3809	974	1120	26			
1	D	690	Total	C	N	O	S	0	1	0
			5649	3631	926	1066	26			

There are 48 discrepancies between the modelled and reference sequences:

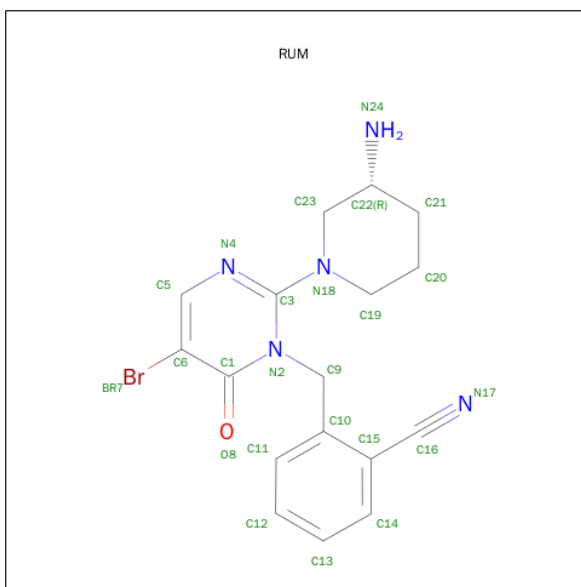
Chain	Residue	Modelled	Actual	Comment	Reference
A	27	ALA	-	EXPRESSION TAG	UNP P27487
A	28	ASP	-	EXPRESSION TAG	UNP P27487
A	29	PRO	-	EXPRESSION TAG	UNP P27487
A	30	GLY	-	EXPRESSION TAG	UNP P27487
A	31	GLY	-	EXPRESSION TAG	UNP P27487
A	32	SER	-	EXPRESSION TAG	UNP P27487
A	33	HIS	-	EXPRESSION TAG	UNP P27487
A	34	HIS	-	EXPRESSION TAG	UNP P27487
A	35	HIS	-	EXPRESSION TAG	UNP P27487
A	36	HIS	-	EXPRESSION TAG	UNP P27487
A	37	HIS	-	EXPRESSION TAG	UNP P27487
A	38	HIS	-	EXPRESSION TAG	UNP P27487
B	27	ALA	-	EXPRESSION TAG	UNP P27487
B	28	ASP	-	EXPRESSION TAG	UNP P27487
B	29	PRO	-	EXPRESSION TAG	UNP P27487
B	30	GLY	-	EXPRESSION TAG	UNP P27487
B	31	GLY	-	EXPRESSION TAG	UNP P27487
B	32	SER	-	EXPRESSION TAG	UNP P27487
B	33	HIS	-	EXPRESSION TAG	UNP P27487
B	34	HIS	-	EXPRESSION TAG	UNP P27487
B	35	HIS	-	EXPRESSION TAG	UNP P27487

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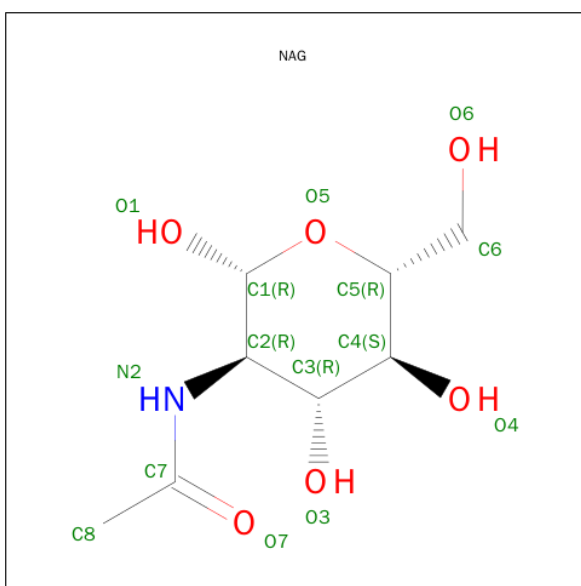
Chain	Residue	Modelled	Actual	Comment	Reference
B	36	HIS	-	EXPRESSION TAG	UNP P27487
B	37	HIS	-	EXPRESSION TAG	UNP P27487
B	38	HIS	-	EXPRESSION TAG	UNP P27487
C	27	ALA	-	EXPRESSION TAG	UNP P27487
C	28	ASP	-	EXPRESSION TAG	UNP P27487
C	29	PRO	-	EXPRESSION TAG	UNP P27487
C	30	GLY	-	EXPRESSION TAG	UNP P27487
C	31	GLY	-	EXPRESSION TAG	UNP P27487
C	32	SER	-	EXPRESSION TAG	UNP P27487
C	33	HIS	-	EXPRESSION TAG	UNP P27487
C	34	HIS	-	EXPRESSION TAG	UNP P27487
C	35	HIS	-	EXPRESSION TAG	UNP P27487
C	36	HIS	-	EXPRESSION TAG	UNP P27487
C	37	HIS	-	EXPRESSION TAG	UNP P27487
C	38	HIS	-	EXPRESSION TAG	UNP P27487
D	27	ALA	-	EXPRESSION TAG	UNP P27487
D	28	ASP	-	EXPRESSION TAG	UNP P27487
D	29	PRO	-	EXPRESSION TAG	UNP P27487
D	30	GLY	-	EXPRESSION TAG	UNP P27487
D	31	GLY	-	EXPRESSION TAG	UNP P27487
D	32	SER	-	EXPRESSION TAG	UNP P27487
D	33	HIS	-	EXPRESSION TAG	UNP P27487
D	34	HIS	-	EXPRESSION TAG	UNP P27487
D	35	HIS	-	EXPRESSION TAG	UNP P27487
D	36	HIS	-	EXPRESSION TAG	UNP P27487
D	37	HIS	-	EXPRESSION TAG	UNP P27487
D	38	HIS	-	EXPRESSION TAG	UNP P27487

- Molecule 2 is 2-({2-[(3R)-3-AMINOPIPERIDIN-1-YL]-5-BROMO-6-OXOPYRIMIDIN-1(6H)-YL}METHYL)BENZONITRILE (three-letter code: RUM) (formula: C₁₇H₁₈BrN₅O).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	Br	C	N	O	0	0
			24	1	17	5	1		
2	B	1	Total	Br	C	N	O	0	0
			24	1	17	5	1		
2	C	1	Total	Br	C	N	O	0	0
			24	1	17	5	1		
2	D	1	Total	Br	C	N	O	0	0
			24	1	17	5	1		

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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	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	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	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		
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 a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	2	Total	C	N	O	0	0
			28	16	2	10		
4	A	2	Total	C	N	O	0	0
			28	16	2	10		
4	B	2	Total	C	N	O	0	0
			28	16	2	10		
4	B	2	Total	C	N	O	0	0
			28	16	2	10		

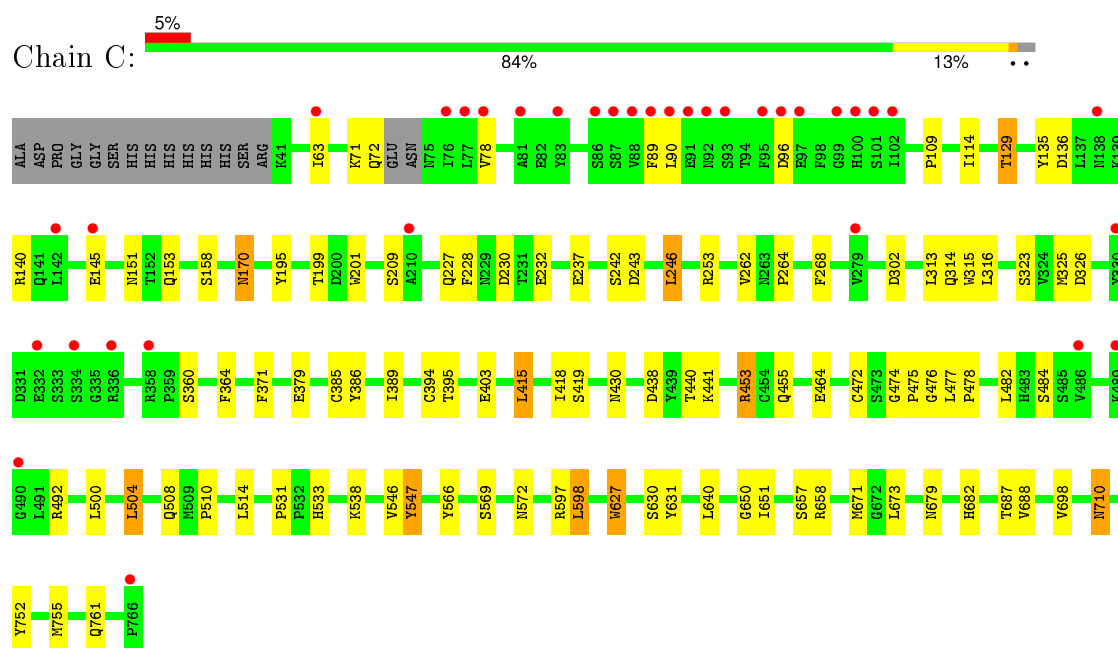
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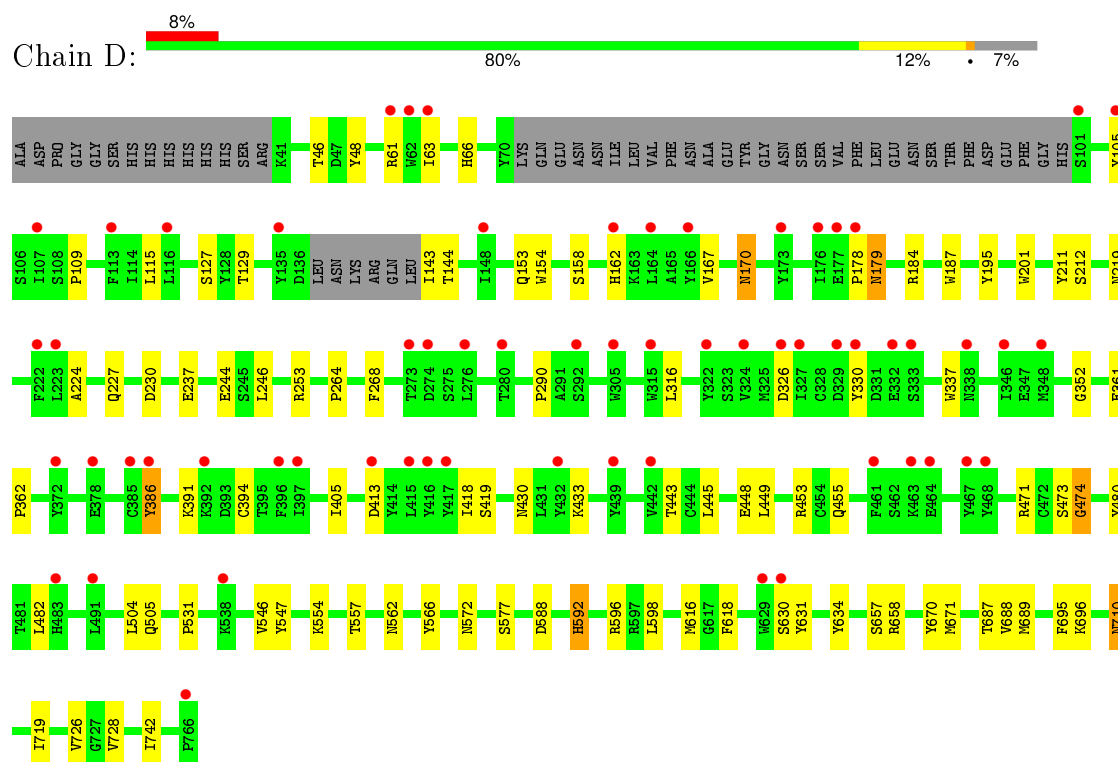
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	2	Total	C	N	O	0	0
			28	16	2	10		
4	C	2	Total	C	N	O	0	0
			28	16	2	10		
4	D	2	Total	C	N	O	0	0
			28	16	2	10		
4	D	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	39	Total	O	0	0
			39	39		
5	B	699	Total	O	0	0
			699	699		



- Molecule 1: Dipeptidyl peptidase 4



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	122.91Å 122.92Å 145.09Å 90.00° 114.77° 90.00°	Depositor
Resolution (Å)	50.00 – 2.45 48.52 – 2.45	Depositor EDS
% Data completeness (in resolution range)	95.4 (50.00-2.45) 95.4 (48.52-2.45)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.46 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.210 , 0.265 0.209 , 0.264	Depositor DCC
R_{free} test set	6854 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	47.2	Xtriage
Anisotropy	0.177	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 46.4	EDS
Estimated twinning fraction	0.012 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 136813 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	24783	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.68% 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, 0.375 respectively for untwinned datasets, and 0.333, 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, RUM

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	0.49	0/6108	0.61	0/8307
1	B	0.47	0/6169	0.61	0/8389
1	C	0.46	0/6100	0.61	1/8296 (0.0%)
1	D	0.43	0/5813	0.57	0/7908
All	All	0.46	0/24190	0.60	1/32900 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	415	LEU	CA-CB-CG	5.32	127.54	115.30

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	5933	0	5648	71	0
1	B	5990	0	5692	56	0
1	C	5929	0	5646	48	0
1	D	5649	0	5381	47	0
2	A	24	0	18	3	0
2	B	24	0	18	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	24	0	18	3	0
2	D	24	0	18	1	0
3	A	56	0	52	0	0
3	B	56	0	52	0	0
3	C	56	0	52	0	0
3	D	56	0	52	0	0
4	A	56	0	50	0	0
4	B	56	0	50	0	0
4	C	56	0	50	0	0
4	D	56	0	50	0	0
5	A	39	0	0	0	0
5	B	699	0	0	5	0
All	All	24783	0	22847	224	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 5.

All (224) 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:A:253:ARG:HH21	1:B:253:ARG:HH21	0.99	0.98
1:C:153:GLN:HE22	1:C:170:ASN:H	1.20	0.87
1:A:253:ARG:HH21	1:B:253:ARG:NH2	1.78	0.81
1:A:153:GLN:HE22	1:A:170:ASN:H	1.30	0.79
1:C:640:LEU:HD11	1:C:650:GLY:HA3	1.65	0.79
1:B:153:GLN:HE22	1:B:170:ASN:H	1.35	0.74
1:B:696:LYS:HG3	1:B:728:VAL:HG22	1.70	0.74
1:B:237:GLU:HG2	1:B:253:ARG:HG2	1.72	0.71
1:A:658:ARG:HB2	1:A:687:THR:HG22	1.73	0.71
1:C:71:LYS:HG2	1:C:72:GLN:H	1.57	0.70
1:A:531:PRO:HB3	1:A:572:ASN:HD22	1.56	0.70
1:B:498:SER:O	1:B:502:LYS:HG2	1.92	0.69
1:D:184:ARG:HH21	1:D:187:TRP:HA	1.57	0.69
1:D:179:ASN:HD22	1:D:179:ASN:H	1.39	0.69
1:A:253:ARG:NH2	1:B:253:ARG:HH21	1.82	0.68
1:A:516:PHE:CD1	1:A:523:LYS:HG2	2.29	0.68
1:B:70:TYR:HB3	1:B:79:PHE:CE1	2.30	0.67
1:D:658:ARG:HB2	1:D:687:THR:HG22	1.76	0.67
1:D:657:SER:HA	1:D:688:VAL:HG13	1.77	0.67
1:B:35:HIS:CD2	1:B:37:HIS:H	2.15	0.65
1:D:726:VAL:HG23	1:D:728:VAL:HG23	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:224:ALA:HB1	1:B:268:PHE:CZ	2.33	0.64
1:B:640:LEU:HD11	1:B:650:GLY:HA3	1.79	0.63
1:D:109:PRO:HG2	1:D:158:SER:O	1.98	0.63
1:C:136:ASP:O	1:C:140:ARG:HA	1.98	0.63
1:D:433:LYS:HE2	1:D:445:LEU:HD21	1.81	0.63
1:B:343:ARG:HD2	1:B:389:ILE:HG12	1.81	0.63
1:A:351:THR:OG1	1:A:592:HIS:HD2	1.81	0.62
1:A:640:LEU:HD11	1:A:650:GLY:HA3	1.81	0.62
1:C:78:VAL:HG23	1:C:89:PHE:HB2	1.83	0.61
1:B:78:VAL:HG23	1:B:89:PHE:HB2	1.82	0.61
1:A:336:ARG:HH12	1:A:338:ASN:HD21	1.47	0.61
1:B:35:HIS:HD2	1:B:37:HIS:H	1.47	0.60
1:D:237:GLU:HG2	1:D:253:ARG:HG2	1.82	0.60
1:C:640:LEU:HD11	1:C:650:GLY:CA	2.32	0.59
2:A:800:RUM:H9	2:A:800:RUM:H19	1.84	0.59
1:D:696:LYS:HG3	1:D:728:VAL:HG22	1.85	0.58
1:B:46:THR:O	1:B:50:LYS:HB2	2.03	0.58
1:B:129:THR:HG23	1:B:151:ASN:HA	1.86	0.57
1:A:472:CYS:O	1:A:478:PRO:HA	2.05	0.57
1:B:242:SER:HB3	1:B:246:LEU:HD12	1.86	0.56
1:C:598:LEU:HG	1:C:631:TYR:OH	2.05	0.56
1:A:242:SER:HB3	1:A:246:LEU:HD12	1.87	0.56
2:A:800:RUM:C9	2:A:800:RUM:H19	2.36	0.55
1:D:195:TYR:O	1:D:227:GLN:HA	2.07	0.55
1:A:627:TRP:HB2	1:A:651:ILE:HB	1.88	0.55
1:D:473:SER:O	1:D:474:GLY:O	2.25	0.55
1:C:302:ASP:HB3	1:C:314:GLN:HB2	1.89	0.54
1:C:114:ILE:HG23	1:C:135:TYR:HB3	1.88	0.54
1:C:510:PRO:HD3	1:C:569:SER:HB2	1.88	0.54
1:A:193:ILE:HG22	1:A:194:ILE:HG12	1.90	0.54
1:A:170:ASN:N	1:A:170:ASN:HD22	2.05	0.54
1:C:657:SER:HA	1:C:688:VAL:HG13	1.89	0.53
1:B:70:TYR:HB3	1:B:79:PHE:HE1	1.72	0.53
1:D:531:PRO:HB3	1:D:572:ASN:HD22	1.74	0.53
1:C:640:LEU:HB3	1:C:698:VAL:HG21	1.91	0.53
1:C:627:TRP:HB2	1:C:651:ILE:HB	1.90	0.53
1:A:129:THR:HG23	1:A:151:ASN:HA	1.91	0.52
1:D:588:ASP:O	1:D:592:HIS:HB2	2.09	0.52
1:D:224:ALA:HB1	1:D:268:PHE:CZ	2.45	0.52
1:C:129:THR:HG23	1:C:151:ASN:HA	1.91	0.52
1:C:364:PHE:HE2	1:C:389:ILE:HD11	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:290:PRO:HG3	1:D:326:ASP:OD1	2.09	0.52
1:B:471:ARG:HG3	1:B:480:TYR:CE1	2.44	0.52
1:D:695:PHE:HB3	1:D:728:VAL:HG11	1.92	0.52
1:B:382:ARG:NH2	5:B:1023:HOH:O	2.41	0.52
1:B:105:TYR:HB2	1:B:114:ILE:HD11	1.92	0.52
1:D:48:TYR:CE1	1:D:562:ASN:HA	2.45	0.51
1:A:135:TYR:HD1	1:A:142:LEU:HD13	1.76	0.51
1:D:455:GLN:HE21	1:D:557:THR:HG21	1.76	0.51
1:A:105:TYR:HB2	1:A:114:ILE:HD11	1.93	0.51
1:A:334:SER:HB2	1:A:336:ARG:HE	1.75	0.51
1:C:658:ARG:HB2	1:C:687:THR:HG22	1.91	0.51
1:A:702:LEU:HD12	1:A:703:ILE:N	2.26	0.50
1:B:170:ASN:N	1:B:170:ASN:HD22	2.09	0.50
1:B:403:GLU:OE1	5:B:940:HOH:O	2.19	0.50
1:C:508:GLN:OE1	1:C:533:HIS:NE2	2.41	0.50
1:B:80:ASN:HD22	1:B:83:TYR:H	1.58	0.50
1:A:277:SER:HB3	1:A:280:THR:HG22	1.94	0.49
1:B:49:LEU:HD22	1:B:749:GLN:HA	1.94	0.49
1:B:534:PHE:CE2	1:B:536:LYS:HG2	2.46	0.49
1:D:554:LYS:HB3	1:D:577:SER:HB3	1.94	0.49
1:B:751:ILE:O	1:B:755:MET:HG3	2.12	0.49
1:C:325:MET:HE3	1:C:371:PHE:CZ	2.47	0.49
1:C:195:TYR:O	1:C:227:GLN:HA	2.12	0.49
1:C:153:GLN:NE2	1:C:170:ASN:H	1.99	0.49
1:A:598:LEU:HD22	1:A:671:MET:HG2	1.95	0.49
1:B:183:TYR:CD2	1:B:276:LEU:HD23	2.48	0.49
1:A:630:SER:OG	1:A:740:HIS:NE2	2.40	0.49
1:A:44:THR:O	1:A:47:ASP:HB2	2.13	0.48
1:B:703:ILE:HG21	1:B:751:ILE:HD12	1.94	0.48
1:B:153:GLN:NE2	1:B:167:VAL:HG12	2.28	0.48
1:B:219:ASN:HB2	5:B:998:HOH:O	2.13	0.48
1:D:154:TRP:CE2	1:D:212:SER:HB3	2.48	0.48
1:C:597:ARG:NH1	1:C:679:ASN:OD1	2.46	0.48
1:B:159:PRO:HD3	1:B:216:TRP:CB	2.44	0.48
1:D:710:ASN:C	1:D:710:ASN:HD22	2.16	0.48
1:A:114:ILE:HG23	1:A:135:TYR:HB3	1.95	0.48
1:A:696:LYS:HG3	1:A:728:VAL:HG22	1.96	0.48
1:A:242:SER:OG	1:A:243:ASP:N	2.47	0.47
1:C:546:VAL:HG12	1:C:627:TRP:O	2.14	0.47
1:A:455:GLN:HE21	1:A:557:THR:HG21	1.79	0.47
1:B:329:ASP:OD2	1:B:343:ARG:NH1	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:230:ASP:OD1	1:C:264:PRO:HB3	2.13	0.47
1:C:598:LEU:HB2	1:C:671:MET:SD	2.54	0.47
1:A:159:PRO:HD3	1:A:216:TRP:HB3	1.97	0.47
1:D:630:SER:HB2	2:D:800:RUM:BR7	2.69	0.47
1:A:382:ARG:H	1:A:403:GLU:HG2	1.79	0.47
1:A:95:PHE:HB3	1:A:98:PHE:HB2	1.96	0.47
1:C:438:ASP:OD2	1:C:440:THR:HB	2.15	0.47
1:B:544:LEU:HD23	1:B:626:ILE:HD12	1.96	0.46
1:D:105:TYR:HA	1:D:115:LEU:O	2.15	0.46
1:C:455:GLN:HE21	1:C:475:PRO:HG3	1.80	0.46
1:C:453:ARG:NH2	1:C:477:LEU:O	2.48	0.46
1:A:325:MET:HE3	1:A:327:ILE:HD11	1.98	0.46
1:D:598:LEU:HD22	1:D:671:MET:HG2	1.97	0.46
1:A:702:LEU:C	1:A:702:LEU:HD12	2.36	0.46
1:D:471:ARG:HD3	1:D:480:TYR:CE1	2.50	0.46
1:C:403:GLU:O	1:C:419:SER:HB2	2.16	0.46
1:D:127:SER:HB3	1:D:211:TYR:CD2	2.49	0.46
1:A:336:ARG:NH1	1:A:338:ASN:HD21	2.12	0.46
1:B:41:LYS:NZ	1:B:506:ASN:HB3	2.31	0.46
1:B:224:ALA:HB1	1:B:268:PHE:HZ	1.77	0.46
1:B:385:CYS:HB3	1:B:387:PHE:CE1	2.51	0.46
1:D:230:ASP:OD1	1:D:264:PRO:HB3	2.16	0.46
2:A:800:RUM:H9	2:A:800:RUM:C19	2.46	0.45
5:B:1063:HOH:O	1:C:129:THR:HG22	2.16	0.45
1:A:158:SER:HA	1:A:216:TRP:CD1	2.52	0.45
1:D:143:ILE:CG2	1:D:144:THR:N	2.79	0.45
1:A:114:ILE:CG2	1:A:135:TYR:HB3	2.46	0.45
1:C:418:ILE:HA	1:C:430:ASN:O	2.15	0.45
1:C:315:TRP:O	1:C:323:SER:HB2	2.16	0.45
1:C:232:GLU:HB2	1:C:262:VAL:HG11	1.99	0.45
1:B:534:PHE:HE2	1:B:536:LYS:HG2	1.81	0.45
1:D:596:ARG:N	1:D:670:TYR:O	2.46	0.45
1:A:689:MET:HE3	1:B:244:GLU:HG3	1.98	0.45
1:C:386:TYR:O	1:C:394:CYS:HB2	2.17	0.45
1:A:701:LEU:HD13	1:A:731:GLN:HB2	1.99	0.45
1:A:405:ILE:HG12	1:A:419:SER:HA	1.99	0.45
1:B:237:GLU:HA	1:B:252:VAL:O	2.17	0.44
1:C:752:TYR:CE2	1:C:755:MET:HE3	2.52	0.44
1:C:598:LEU:O	1:C:682:HIS:NE2	2.45	0.44
1:D:418:ILE:HA	1:D:430:ASN:O	2.17	0.44
1:D:657:SER:HB2	1:D:689:MET:SD	2.57	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:1124:HOH:O	1:D:562:ASN:HB2	2.17	0.44
1:A:736:THR:O	1:A:737:ASP:HB2	2.18	0.44
1:D:657:SER:HA	1:D:688:VAL:CG1	2.48	0.44
1:B:370:SER:HB3	1:B:386:TYR:HE2	1.82	0.44
1:C:237:GLU:HG2	1:C:253:ARG:HG2	1.99	0.44
1:D:405:ILE:HG12	1:D:419:SER:HA	1.99	0.44
2:C:800:RUM:C9	2:C:800:RUM:H19	2.47	0.43
1:B:155:VAL:HG12	1:B:166:TYR:HB3	1.98	0.43
1:A:403:GLU:OE2	1:A:585:TYR:HA	2.18	0.43
1:A:680:LEU:HD11	1:A:684:ARG:CZ	2.48	0.43
1:C:472:CYS:O	1:C:478:PRO:HA	2.18	0.43
1:D:386:TYR:O	1:D:394:CYS:HB2	2.17	0.43
1:C:170:ASN:N	1:C:170:ASN:HD22	2.16	0.43
1:A:364:PHE:HE2	1:A:389:ILE:HD11	1.83	0.43
1:C:242:SER:HB3	1:C:246:LEU:HD12	2.00	0.43
1:C:547:TYR:CD1	1:C:547:TYR:C	2.91	0.43
1:B:747:ALA:O	1:B:751:ILE:HG22	2.19	0.43
1:A:626:ILE:HG23	1:A:636:THR:HG23	2.00	0.43
1:A:302:ASP:HB3	1:A:314:GLN:HB2	2.00	0.43
1:A:433:LYS:HE2	1:A:445:LEU:HD21	2.01	0.43
1:D:179:ASN:N	1:D:179:ASN:HD22	2.12	0.42
1:A:626:ILE:O	1:A:650:GLY:HA2	2.19	0.42
1:B:41:LYS:HZ3	1:B:506:ASN:HB3	1.84	0.42
1:D:330:TYR:HB2	1:D:337:TRP:CZ2	2.54	0.42
1:C:474:GLY:HA2	1:C:476:GLY:O	2.19	0.42
1:A:402:TRP:CD2	1:A:421:GLU:HB2	2.53	0.42
1:C:109:PRO:HG2	1:C:158:SER:O	2.19	0.42
1:A:129:THR:HG21	1:A:151:ASN:HD22	1.84	0.42
1:D:224:ALA:HB1	1:D:268:PHE:HZ	1.82	0.42
1:B:518:ILE:CG2	1:B:521:GLU:HA	2.49	0.42
1:C:630:SER:HB2	2:C:800:RUM:BR7	2.75	0.42
1:B:117:GLU:HB2	1:B:132:TYR:CE2	2.54	0.42
1:A:306:ALA:HB3	1:A:310:ARG:HG2	2.00	0.42
1:A:726:VAL:HG23	1:A:728:VAL:HG23	2.01	0.42
1:A:61:ARG:HH22	1:A:107:ILE:H	1.66	0.42
1:A:80:ASN:HD22	1:A:82:GLU:H	1.66	0.42
1:B:80:ASN:HD21	1:B:82:GLU:HB2	1.85	0.42
2:B:800:RUM:H9	2:B:800:RUM:H19	2.02	0.42
1:A:389:ILE:HD13	1:A:389:ILE:HA	1.89	0.42
1:B:55:LEU:HD23	1:B:500:LEU:CD2	2.50	0.42
1:A:751:ILE:O	1:A:755:MET:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:361:GLU:HA	1:D:362:PRO:HD3	1.87	0.42
1:B:765:LEU:HA	1:B:766:PRO:HD3	1.87	0.42
1:A:158:SER:OG	1:A:163:LYS:HB2	2.20	0.42
1:B:596:ARG:HA	1:B:670:TYR:O	2.19	0.42
1:C:531:PRO:HB3	1:C:572:ASN:HD22	1.85	0.41
1:A:325:MET:CE	1:A:327:ILE:HD11	2.50	0.41
1:A:482:LEU:HA	1:A:482:LEU:HD22	1.91	0.41
1:A:316:LEU:HD22	1:A:320:GLN:HA	2.02	0.41
1:C:201:TRP:CZ2	1:C:710:ASN:HA	2.56	0.41
1:A:153:GLN:NE2	1:A:167:VAL:HG12	2.35	0.41
1:D:352:GLY:HA3	1:D:592:HIS:CD2	2.56	0.41
1:A:159:PRO:HD3	1:A:216:TRP:CB	2.51	0.41
1:C:268:PHE:CD2	1:C:313:LEU:HD21	2.55	0.41
1:D:631:TYR:O	1:D:634:TYR:HB3	2.20	0.41
1:A:703:ILE:HG12	1:A:733:MET:HB3	2.03	0.41
1:D:471:ARG:HD3	1:D:480:TYR:HE1	1.86	0.41
1:B:175:LYS:CG	1:B:182:SER:HB3	2.51	0.41
1:B:640:LEU:HB3	1:B:698:VAL:HG21	2.03	0.41
1:A:640:LEU:HD11	1:A:650:GLY:CA	2.49	0.41
1:B:82:GLU:HG2	1:B:467:TYR:OH	2.20	0.41
2:C:800:RUM:H9	2:C:800:RUM:H19	2.03	0.41
1:C:199:THR:HA	1:C:228:PHE:CE2	2.55	0.41
1:D:616:MET:HB3	1:D:618:PHE:CE1	2.56	0.41
1:B:677:GLU:H	1:B:677:GLU:CD	2.23	0.41
1:A:312:SER:HA	1:A:326:ASP:O	2.20	0.41
1:C:500:LEU:HG	1:C:504:LEU:HD22	2.03	0.41
1:D:657:SER:HB3	1:D:719:ILE:HG13	2.03	0.41
1:A:109:PRO:HG2	1:A:158:SER:O	2.21	0.41
1:A:708:ASP:HA	1:A:739:ASP:HA	2.03	0.41
1:A:62:TRP:CG	1:A:462:SER:HA	2.55	0.41
1:A:199:THR:HA	1:A:228:PHE:CE2	2.55	0.41
1:A:63:ILE:HD11	1:A:69:LEU:HD12	2.02	0.41
1:A:90:LEU:HD11	1:A:137:LEU:HD21	2.02	0.41
1:D:201:TRP:CZ2	1:D:710:ASN:HA	2.56	0.40
1:D:153:GLN:HE21	1:D:167:VAL:HG12	1.86	0.40
1:D:153:GLN:HE22	1:D:170:ASN:H	1.68	0.40
1:B:504:LEU:HA	1:B:504:LEU:HD12	1.91	0.40
1:A:154:TRP:CE2	1:A:212:SER:HB3	2.57	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	721/740 (97%)	680 (94%)	40 (6%)	1 (0%)	56	71
1	B	727/740 (98%)	689 (95%)	37 (5%)	1 (0%)	56	71
1	C	720/740 (97%)	679 (94%)	41 (6%)	0	100	100
1	D	684/740 (92%)	641 (94%)	37 (5%)	6 (1%)	21	25
All	All	2852/2960 (96%)	2689 (94%)	155 (5%)	8 (0%)	46	57

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	474	GLY
1	D	244	GLU
1	D	449	LEU
1	B	244	GLU
1	A	334	SER
1	D	178	PRO
1	D	742	ILE
1	D	63	ILE

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	650/662 (98%)	618 (95%)	32 (5%)	31	43
1	B	656/662 (99%)	626 (95%)	30 (5%)	33	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	649/662 (98%)	617 (95%)	32 (5%)	31	43
1	D	618/662 (93%)	594 (96%)	24 (4%)	39	54
All	All	2573/2648 (97%)	2455 (95%)	118 (5%)	33	46

All (118) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	THR
1	A	66	HIS
1	A	77	LEU
1	A	80	ASN
1	A	91	GLU
1	A	92	ASN
1	A	129	THR
1	A	170	ASN
1	A	179	ASN
1	A	182	SER
1	A	209	SER
1	A	243	ASP
1	A	246	LEU
1	A	256	TYR
1	A	276	LEU
1	A	316	LEU
1	A	354	VAL
1	A	385	CYS
1	A	413	ASP
1	A	436	LEU
1	A	440	THR
1	A	448	GLU
1	A	453	ARG
1	A	464	GLU
1	A	472	CYS
1	A	482	LEU
1	A	514	LEU
1	A	547	TYR
1	A	566	TYR
1	A	598	LEU
1	A	710	ASN
1	A	745	SER
1	B	54	ARG
1	B	59	SER

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Mol	Chain	Res	Type
1	B	170	ASN
1	B	179	ASN
1	B	230	ASP
1	B	246	LEU
1	B	283	THR
1	B	295	ILE
1	B	316	LEU
1	B	354	VAL
1	B	360	SER
1	B	385	CYS
1	B	392	LYS
1	B	440	THR
1	B	441	LYS
1	B	453	ARG
1	B	464	GLU
1	B	477	LEU
1	B	489	LYS
1	B	492	ARG
1	B	504	LEU
1	B	505	GLN
1	B	506	ASN
1	B	538	LYS
1	B	547	TYR
1	B	622	LYS
1	B	630	SER
1	B	658	ARG
1	B	710	ASN
1	B	764	SER
1	C	63	ILE
1	C	90	LEU
1	C	96	ASP
1	C	129	THR
1	C	145	GLU
1	C	170	ASN
1	C	209	SER
1	C	243	ASP
1	C	246	LEU
1	C	316	LEU
1	C	326	ASP
1	C	360	SER
1	C	379	GLU
1	C	385	CYS

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Mol	Chain	Res	Type
1	C	395	THR
1	C	415	LEU
1	C	441	LYS
1	C	453	ARG
1	C	464	GLU
1	C	482	LEU
1	C	484	SER
1	C	492	ARG
1	C	504	LEU
1	C	514	LEU
1	C	538	LYS
1	C	547	TYR
1	C	566	TYR
1	C	598	LEU
1	C	627	TRP
1	C	673	LEU
1	C	710	ASN
1	C	761	GLN
1	D	46	THR
1	D	61	ARG
1	D	66	HIS
1	D	129	THR
1	D	162	HIS
1	D	170	ASN
1	D	179	ASN
1	D	219	ASN
1	D	246	LEU
1	D	316	LEU
1	D	386	TYR
1	D	391	LYS
1	D	413	ASP
1	D	443	THR
1	D	448	GLU
1	D	453	ARG
1	D	482	LEU
1	D	504	LEU
1	D	505	GLN
1	D	546	VAL
1	D	547	TYR
1	D	566	TYR
1	D	592	HIS
1	D	710	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	80	ASN
1	A	151	ASN
1	A	153	GLN
1	A	170	ASN
1	A	179	ASN
1	A	338	ASN
1	A	344	GLN
1	A	455	GLN
1	A	572	ASN
1	A	592	HIS
1	A	697	GLN
1	A	710	ASN
1	B	35	HIS
1	B	72	GLN
1	B	80	ASN
1	B	123	GLN
1	B	141	GLN
1	B	153	GLN
1	B	170	ASN
1	B	179	ASN
1	B	338	ASN
1	B	344	GLN
1	B	388	GLN
1	B	455	GLN
1	B	505	GLN
1	B	506	ASN
1	B	710	ASN
1	C	80	ASN
1	C	103	ASN
1	C	123	GLN
1	C	141	GLN
1	C	151	ASN
1	C	153	GLN
1	C	169	ASN
1	C	170	ASN
1	C	344	GLN
1	C	455	GLN
1	C	572	ASN
1	C	685	ASN
1	C	710	ASN

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Mol	Chain	Res	Type
1	C	761	GLN
1	D	66	HIS
1	D	123	GLN
1	D	153	GLN
1	D	169	ASN
1	D	170	ASN
1	D	179	ASN
1	D	344	GLN
1	D	435	GLN
1	D	455	GLN
1	D	505	GLN
1	D	572	ASN
1	D	592	HIS
1	D	710	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

16 carbohydrates 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	$\# Z > 2$
4	NAG	A	804	1,4	14,14,15	0.61	0	15,19,21	1.09	1 (6%)
4	NAG	A	805	4	14,14,15	0.51	0	15,19,21	1.13	2 (13%)
4	NAG	A	806	1,4	14,14,15	0.57	0	15,19,21	1.17	1 (6%)
4	NAG	A	807	4	14,14,15	0.56	0	15,19,21	0.75	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	B	804	1,4	14,14,15	0.60	0	15,19,21	0.84	0
4	NAG	B	805	4	14,14,15	0.60	0	15,19,21	1.33	2 (13%)
4	NAG	B	806	1,4	14,14,15	0.49	0	15,19,21	1.02	0
4	NAG	B	807	4	14,14,15	0.55	0	15,19,21	1.17	2 (13%)
4	NAG	C	804	1,4	14,14,15	0.60	0	15,19,21	1.30	1 (6%)
4	NAG	C	805	4	14,14,15	0.53	0	15,19,21	1.01	1 (6%)
4	NAG	C	806	1,4	14,14,15	0.66	0	15,19,21	1.32	1 (6%)
4	NAG	C	807	4	14,14,15	0.52	0	15,19,21	1.49	3 (20%)
4	NAG	D	804	1,4	14,14,15	0.51	0	15,19,21	0.85	1 (6%)
4	NAG	D	805	4	14,14,15	0.41	0	15,19,21	1.41	4 (26%)
4	NAG	D	806	1,4	14,14,15	0.52	0	15,19,21	1.28	1 (6%)
4	NAG	D	807	4	14,14,15	0.50	0	15,19,21	0.63	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
4	NAG	A	804	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	805	4	-	0/6/23/26	0/1/1/1
4	NAG	A	806	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	807	4	-	0/6/23/26	0/1/1/1
4	NAG	B	804	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	805	4	-	0/6/23/26	0/1/1/1
4	NAG	B	806	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	807	4	-	0/6/23/26	0/1/1/1
4	NAG	C	804	1,4	-	0/6/23/26	0/1/1/1
4	NAG	C	805	4	-	0/6/23/26	0/1/1/1
4	NAG	C	806	1,4	-	0/6/23/26	0/1/1/1
4	NAG	C	807	4	-	0/6/23/26	0/1/1/1
4	NAG	D	804	1,4	-	0/6/23/26	0/1/1/1
4	NAG	D	805	4	-	0/6/23/26	0/1/1/1
4	NAG	D	806	1,4	-	0/6/23/26	0/1/1/1
4	NAG	D	807	4	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	805	NAG	C4-C3-C2	-2.75	106.96	111.23
4	A	805	NAG	C2-N2-C7	-2.45	119.89	123.04
4	D	805	NAG	C2-N2-C7	-2.38	119.99	123.04
4	B	805	NAG	C1-O5-C5	-2.15	109.52	112.25
4	D	805	NAG	C3-C4-C5	-2.04	106.64	110.20
4	D	805	NAG	C1-O5-C5	2.04	114.83	112.25
4	C	807	NAG	C4-C3-C2	2.18	114.61	111.23
4	B	807	NAG	O5-C5-C6	2.20	112.11	107.35
4	B	807	NAG	C4-C3-C2	2.36	114.90	111.23
4	C	807	NAG	C1-O5-C5	2.50	115.43	112.25
4	D	804	NAG	C1-O5-C5	2.52	115.45	112.25
4	C	807	NAG	C2-N2-C7	2.62	126.40	123.04
4	C	805	NAG	C4-C3-C2	2.69	115.41	111.23
4	C	804	NAG	C4-C3-C2	2.84	115.64	111.23
4	A	804	NAG	C4-C3-C2	2.91	115.76	111.23
4	A	805	NAG	C1-O5-C5	2.94	115.98	112.25
4	B	805	NAG	C4-C3-C2	3.46	116.60	111.23
4	A	806	NAG	C1-O5-C5	3.57	116.78	112.25
4	C	806	NAG	C4-C3-C2	3.97	117.40	111.23
4	D	806	NAG	C1-O5-C5	4.21	117.59	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.6 Ligand geometry ⓘ

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	RUM	A	800	-	24,26,26	3.06	4 (16%)	23,36,36	1.88	7 (30%)
3	NAG	A	801	1	14,14,15	0.54	0	15,19,21	1.03	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	A	802	1	14,14,15	0.57	0	15,19,21	1.39	2 (13%)
3	NAG	A	803	1	14,14,15	0.60	0	15,19,21	1.02	1 (6%)
3	NAG	A	808	1	14,14,15	0.49	0	15,19,21	1.88	2 (13%)
2	RUM	B	800	-	24,26,26	3.00	4 (16%)	23,36,36	2.01	5 (21%)
3	NAG	B	801	1	14,14,15	0.60	0	15,19,21	1.07	1 (6%)
3	NAG	B	802	1	14,14,15	0.52	0	15,19,21	1.34	1 (6%)
3	NAG	B	803	1	14,14,15	0.60	0	15,19,21	0.88	0
3	NAG	B	808	1	14,14,15	0.51	0	15,19,21	1.44	1 (6%)
2	RUM	C	800	-	24,26,26	3.02	5 (20%)	23,36,36	1.77	6 (26%)
3	NAG	C	801	1	14,14,15	0.61	0	15,19,21	1.08	2 (13%)
3	NAG	C	802	1	14,14,15	0.54	0	15,19,21	1.06	1 (6%)
3	NAG	C	803	1	14,14,15	0.54	0	15,19,21	1.00	1 (6%)
3	NAG	C	808	1	14,14,15	0.70	0	15,19,21	1.33	1 (6%)
2	RUM	D	800	-	24,26,26	3.03	4 (16%)	23,36,36	1.60	2 (8%)
3	NAG	D	801	-	14,14,15	0.51	0	15,19,21	0.96	0
3	NAG	D	802	1	14,14,15	0.55	0	15,19,21	1.49	1 (6%)
3	NAG	D	803	1	14,14,15	0.45	0	15,19,21	0.72	0
3	NAG	D	808	1	14,14,15	0.62	0	15,19,21	0.93	1 (6%)

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	RUM	A	800	-	-	0/10/20/20	0/3/3/3
3	NAG	A	801	1	-	0/6/23/26	0/1/1/1
3	NAG	A	802	1	-	0/6/23/26	0/1/1/1
3	NAG	A	803	1	-	0/6/23/26	0/1/1/1
3	NAG	A	808	1	-	0/6/23/26	0/1/1/1
2	RUM	B	800	-	-	0/10/20/20	0/3/3/3
3	NAG	B	801	1	-	0/6/23/26	0/1/1/1
3	NAG	B	802	1	-	1/6/23/26	0/1/1/1
3	NAG	B	803	1	-	0/6/23/26	0/1/1/1
3	NAG	B	808	1	-	0/6/23/26	0/1/1/1
2	RUM	C	800	-	-	0/10/20/20	0/3/3/3
3	NAG	C	801	1	-	0/6/23/26	0/1/1/1
3	NAG	C	802	1	-	0/6/23/26	0/1/1/1
3	NAG	C	803	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	C	808	1	-	0/6/23/26	0/1/1/1
2	RUM	D	800	-	-	0/10/20/20	0/3/3/3
3	NAG	D	801	-	-	0/6/23/26	0/1/1/1
3	NAG	D	802	1	-	0/6/23/26	0/1/1/1
3	NAG	D	803	1	-	0/6/23/26	0/1/1/1
3	NAG	D	808	1	-	0/6/23/26	0/1/1/1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	800	RUM	C15-C16	-10.63	1.28	1.44
2	D	800	RUM	C15-C16	-10.46	1.28	1.44
2	A	800	RUM	C15-C16	-9.86	1.29	1.44
2	B	800	RUM	C15-C16	-9.58	1.30	1.44
2	C	800	RUM	C3-N4	2.03	1.37	1.33
2	C	800	RUM	C1-N2	2.08	1.41	1.38
2	D	800	RUM	C1-N2	2.25	1.41	1.38
2	B	800	RUM	C1-N2	2.40	1.41	1.38
2	A	800	RUM	C1-N2	2.58	1.42	1.38
2	C	800	RUM	C1-C6	6.35	1.46	1.38
2	D	800	RUM	C15-C10	6.96	1.49	1.40
2	C	800	RUM	C15-C10	6.98	1.50	1.40
2	D	800	RUM	C1-C6	7.10	1.47	1.38
2	B	800	RUM	C15-C10	7.21	1.50	1.40
2	A	800	RUM	C15-C10	7.35	1.50	1.40
2	A	800	RUM	C1-C6	7.41	1.48	1.38
2	B	800	RUM	C1-C6	7.54	1.48	1.38

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	800	RUM	C15-C16-N17	-3.84	171.16	177.82
2	A	800	RUM	C20-C21-C22	-3.31	107.41	111.97
3	A	808	NAG	C2-N2-C7	-2.83	119.40	123.04
2	C	800	RUM	C6-C5-N4	-2.58	119.66	123.23
2	A	800	RUM	BR7-C6-C1	-2.48	117.31	121.48
2	C	800	RUM	C20-C21-C22	-2.32	108.77	111.97
2	C	800	RUM	BR7-C6-C1	-2.27	117.66	121.48
2	B	800	RUM	C14-C15-C10	-2.23	117.70	120.64
2	A	800	RUM	C6-C5-N4	-2.06	120.38	123.23
2	D	800	RUM	C20-C21-C22	-2.03	109.17	111.97
3	C	801	NAG	O5-C5-C6	2.05	111.79	107.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	800	RUM	BR7-C6-C5	2.13	123.22	118.67
3	A	801	NAG	C1-O5-C5	2.21	115.06	112.25
3	C	802	NAG	C1-O5-C5	2.28	115.14	112.25
2	A	800	RUM	BR7-C6-C5	2.37	123.72	118.67
2	A	800	RUM	C9-C10-C15	2.43	123.48	120.26
2	B	800	RUM	C9-C10-C15	2.45	123.51	120.26
3	A	802	NAG	O5-C5-C6	2.46	112.68	107.35
3	D	808	NAG	C1-O5-C5	2.51	115.43	112.25
3	B	801	NAG	C1-O5-C5	2.62	115.57	112.25
2	C	800	RUM	C10-C15-C16	2.63	122.37	120.10
2	A	800	RUM	C10-C15-C16	2.89	122.60	120.10
3	C	801	NAG	C4-C3-C2	2.94	115.81	111.23
3	A	803	NAG	C4-C3-C2	3.00	115.89	111.23
3	C	803	NAG	C1-O5-C5	3.24	116.36	112.25
3	B	802	NAG	C1-O5-C5	3.42	116.59	112.25
3	A	802	NAG	C1-O5-C5	3.91	117.20	112.25
3	C	808	NAG	C4-C3-C2	3.97	117.40	111.23
2	B	800	RUM	C10-C15-C16	4.71	124.17	120.10
3	B	808	NAG	C1-O5-C5	4.96	118.55	112.25
3	D	802	NAG	C1-O5-C5	5.09	118.71	112.25
2	D	800	RUM	C19-N18-C23	5.26	124.34	113.30
2	A	800	RUM	C19-N18-C23	5.29	124.41	113.30
2	B	800	RUM	C19-N18-C23	5.38	124.59	113.30
2	C	800	RUM	C19-N18-C23	5.63	125.11	113.30
3	A	808	NAG	C1-O5-C5	5.86	119.69	112.25

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	802	NAG	O7-C7-N2-C2

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	800	RUM	3	0
2	B	800	RUM	1	0
2	C	800	RUM	3	0
2	D	800	RUM	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	724/740 (97%)	0.07	20 (2%) 56 60	20, 44, 71, 104	1 (0%)
1	B	730/740 (98%)	0.02	8 (1%) 82 84	21, 45, 68, 103	1 (0%)
1	C	724/740 (97%)	0.23	35 (4%) 34 37	18, 49, 75, 99	1 (0%)
1	D	690/740 (93%)	0.52	62 (8%) 12 12	26, 55, 79, 87	0
All	All	2868/2960 (96%)	0.20	125 (4%) 38 41	18, 47, 76, 104	3 (0%)

All (125) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	464	GLU	6.4
1	D	222	PHE	6.0
1	D	392	LYS	5.7
1	C	89	PHE	5.0
1	C	90	LEU	4.9
1	C	88	VAL	4.9
1	C	486	VAL	4.7
1	D	416	TYR	4.7
1	B	88	VAL	4.4
1	D	327	ILE	4.3
1	D	276	LEU	4.2
1	D	385	CYS	4.1
1	D	468	TYR	4.1
1	D	178	PRO	4.0
1	D	105	TYR	4.0
1	D	330	TYR	4.0
1	A	86	SER	3.9
1	C	93	SER	3.8
1	D	148	ILE	3.6
1	D	372	TYR	3.6
1	D	62	TRP	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	463	LYS	3.5
1	B	96	ASP	3.5
1	C	87	SER	3.5
1	C	83	TYR	3.5
1	D	467	TYR	3.4
1	C	78	VAL	3.4
1	A	98	PHE	3.4
1	D	333	SER	3.4
1	A	97	GLU	3.4
1	D	61	ARG	3.4
1	D	348	MET	3.3
1	C	77	LEU	3.3
1	C	99	GLY	3.3
1	C	336	ARG	3.2
1	C	96	ASP	3.2
1	D	415	LEU	3.1
1	A	92	ASN	3.1
1	A	88	VAL	3.1
1	C	766	PRO	3.1
1	C	86	SER	3.1
1	A	137	LEU	3.0
1	D	417	TYR	3.0
1	A	93	SER	3.0
1	C	330	TYR	3.0
1	D	461	PHE	2.9
1	D	164	LEU	2.9
1	C	100	HIS	2.8
1	D	396	PHE	2.8
1	D	162	HIS	2.8
1	D	305	TRP	2.8
1	C	81	ALA	2.8
1	C	95	PHE	2.8
1	D	397	ILE	2.7
1	D	338	ASN	2.7
1	D	538	LYS	2.7
1	A	95	PHE	2.7
1	A	99	GLY	2.7
1	D	329	ASP	2.7
1	D	326	ASP	2.6
1	D	332	GLU	2.6
1	D	439	TYR	2.6
1	D	766	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	90	LEU	2.6
1	D	176	ILE	2.6
1	A	72	GLN	2.6
1	D	432	TYR	2.6
1	D	629	TRP	2.6
1	C	332	GLU	2.6
1	D	292	SER	2.5
1	C	102	ILE	2.5
1	C	279	VAL	2.5
1	C	91	GLU	2.5
1	C	97	GLU	2.5
1	B	766	PRO	2.5
1	D	346	ILE	2.5
1	A	141	GLN	2.5
1	D	442	VAL	2.4
1	C	142	LEU	2.4
1	D	223	LEU	2.4
1	D	173	TYR	2.4
1	C	210	ALA	2.4
1	C	63	ILE	2.4
1	D	135	TYR	2.4
1	C	334	SER	2.4
1	A	148	ILE	2.4
1	D	413	ASP	2.4
1	C	145	GLU	2.4
1	D	483	HIS	2.4
1	A	75	ASN	2.3
1	D	113	PHE	2.3
1	C	92	ASN	2.3
1	D	386	TYR	2.3
1	D	315	TRP	2.3
1	A	392	LYS	2.3
1	C	101	SER	2.2
1	C	76	ILE	2.2
1	C	138	ASN	2.2
1	C	490	GLY	2.2
1	B	72	GLN	2.2
1	A	87	SER	2.2
1	D	274	ASP	2.2
1	D	322	TYR	2.2
1	A	91	GLU	2.2
1	B	77	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	166	TYR	2.1
1	D	378	GLU	2.1
1	B	139	LYS	2.1
1	A	138	ASN	2.1
1	D	116	LEU	2.1
1	D	280	THR	2.1
1	C	489	LYS	2.1
1	D	630	SER	2.1
1	B	681	ASP	2.1
1	D	63	ILE	2.1
1	D	107	ILE	2.1
1	A	69	LEU	2.1
1	D	324	VAL	2.1
1	C	358[A]	ARG	2.1
1	D	273	THR	2.1
1	D	177	GLU	2.0
1	B	78	VAL	2.0
1	A	71	LYS	2.0
1	D	101	SER	2.0
1	D	491	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

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
4	NAG	B	804	14/15	0.92	0.20	1.48	54,57,61,64	0
4	NAG	A	804	14/15	0.93	0.14	1.24	52,55,58,59	0
4	NAG	C	804	14/15	0.91	0.15	0.15	59,63,66,67	0
4	NAG	D	804	14/15	0.93	0.14	-1.00	56,57,58,59	0
4	NAG	D	805	14/15	0.73	0.21	-	60,61,63,63	0
4	NAG	C	807	14/15	0.69	0.31	-	73,75,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	NAG	B	805	14/15	0.75	0.33	-	66,68,68,69	0
4	NAG	B	807	14/15	0.73	0.35	-	71,72,74,74	0
4	NAG	B	806	14/15	0.88	0.12	-	61,64,65,68	0
4	NAG	A	806	14/15	0.84	0.15	-	66,67,69,71	0
4	NAG	D	806	14/15	0.76	0.18	-	91,92,92,93	0
4	NAG	C	805	14/15	0.82	0.31	-	70,71,73,73	0
4	NAG	A	805	14/15	0.88	0.17	-	60,61,62,62	0
4	NAG	C	806	14/15	0.63	0.23	-	68,70,71,73	0
4	NAG	D	807	14/15	0.77	0.36	-	94,94,95,95	0
4	NAG	A	807	14/15	0.82	0.22	-	73,74,75,75	0

6.4 Ligands

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	NAG	B	808	14/15	0.82	0.30	6.85	57,60,61,62	0
3	NAG	D	803	14/15	0.35	0.59	6.77	89,90,92,92	0
3	NAG	C	808	14/15	0.88	0.28	3.25	64,68,69,69	0
3	NAG	A	808	14/15	0.89	0.24	3.12	58,62,66,66	0
3	NAG	D	808	14/15	0.80	0.26	2.00	66,68,69,69	0
2	RUM	A	800	24/24	0.92	0.20	1.10	38,39,41,42	1
3	NAG	A	801	14/15	0.79	0.25	0.03	71,73,74,74	0
2	RUM	C	800	24/24	0.93	0.17	-0.09	36,40,42,46	1
3	NAG	C	801	14/15	0.69	0.29	-0.16	98,98,99,99	0
2	RUM	B	800	24/24	0.94	0.21	-0.27	41,45,46,49	1
3	NAG	B	801	14/15	0.71	0.14	-0.73	81,82,83,83	0
2	RUM	D	800	24/24	0.92	0.18	-0.96	42,46,47,50	1
3	NAG	C	803	14/15	0.88	0.15	-	66,68,68,68	0
3	NAG	A	802	14/15	0.81	0.31	-	65,65,66,67	0
3	NAG	D	801	14/15	0.64	0.42	-	92,93,93,93	0
3	NAG	B	802	14/15	0.85	0.18	-	59,62,63,64	0
3	NAG	D	802	14/15	0.68	0.21	-	72,73,73,73	0
3	NAG	C	802	14/15	0.87	0.27	-	62,63,65,65	0
3	NAG	A	803	14/15	0.78	0.29	-	63,65,67,67	0
3	NAG	B	803	14/15	0.83	0.21	-	54,57,59,60	0

6.5 Other polymers [i](#)

There are no such residues in this entry.