Full wwPDB X-ray Structure Validation Report

Jan 31, 2016 – 10:15 PM GMT

PDB ID	:	1SGF
Title	:	CRYSTAL STRUCTURE OF 7S NGF: A COMPLEX OF NERVE GROWTH FACTOR WITH FOUR BINDING PROTEINS (SERINE PROTEINASES)
Authors	:	Bax, B.D.V.; Blundell, T.L.; Murray-Rust, J.; Mcdonald, N.Q.
Deposited on	:	1997-08-08
Resolution	:	3.15 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

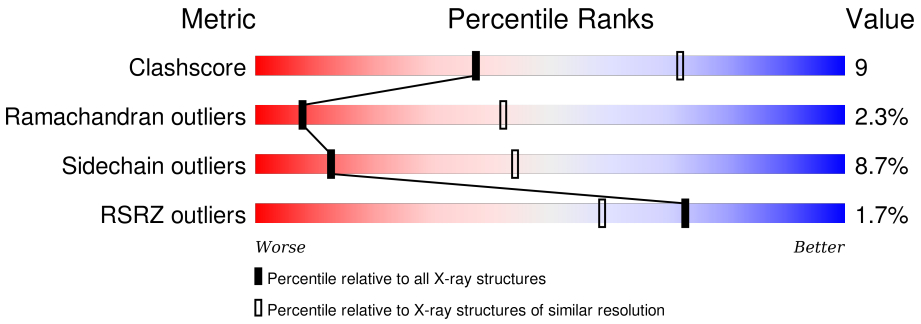
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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

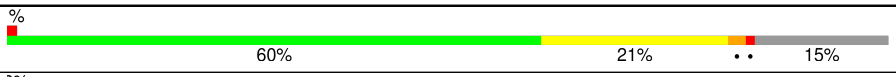
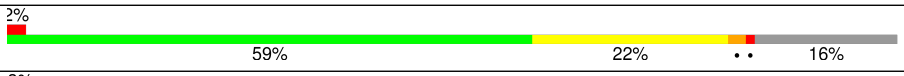
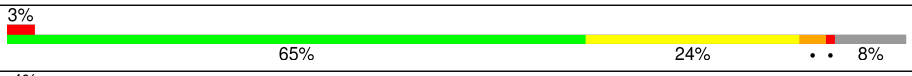
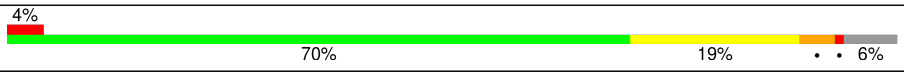
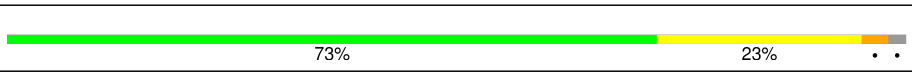
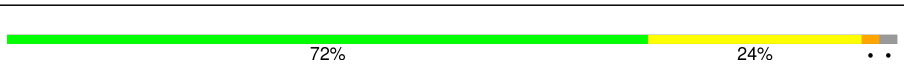
The reported resolution of this entry is 3.15 Å.

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))
Clashscore	102246	1249 (3.20-3.12)
Ramachandran outliers	100387	1222 (3.20-3.12)
Sidechain outliers	100360	1221 (3.20-3.12)
RSRZ outliers	91569	1117 (3.20-3.12)

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 <=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	240	
1	X	240	
2	B	118	
2	Y	118	
3	G	237	
3	Z	237	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8549 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 NERVE GROWTH FACTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	203	Total	C	N	O	S	0	0	0
			1574	991	262	306	15			
1	X	202	Total	C	N	O	S	0	0	0
			1559	980	260	304	15			

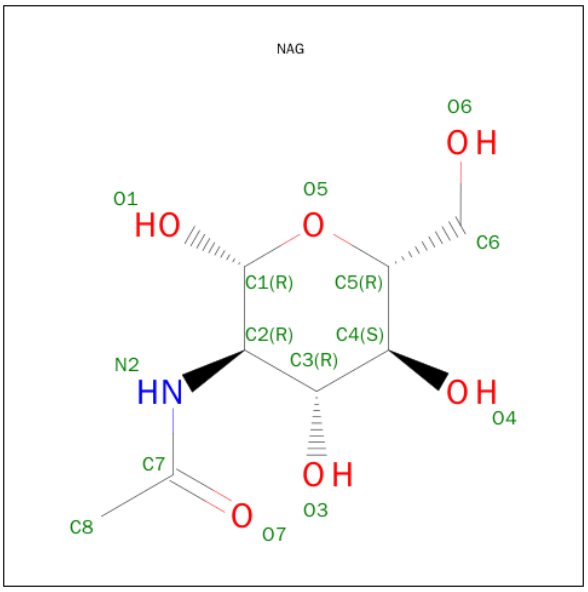
- Molecule 2 is a protein called NERVE GROWTH FACTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	109	Total	C	N	O	S	0	0	0
			858	535	152	165	6			
2	Y	111	Total	C	N	O	S	0	0	0
			871	543	154	167	7			

- Molecule 3 is a protein called NERVE GROWTH FACTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	232	Total	C	N	O	S	0	0	0
			1799	1148	294	341	16			
3	Z	232	Total	C	N	O	S	0	0	0
			1802	1150	294	341	17			

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 14 8 1 5	0	0
4	X	1	Total C N O 14 8 1 5	0	0

- Molecule 5 is a polymer of unknown type called SUGAR (N-ACETYL-D-GLUCOSAMINE).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	G	2	Total C N O 28 16 2 10	0	0

- Molecule 6 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	Z	2	Total C N O 28 16 2 10	0	0

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

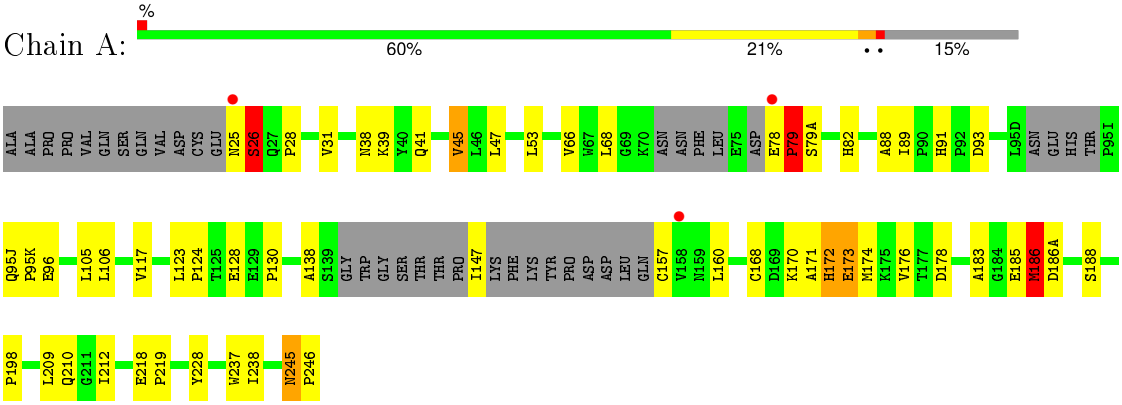
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	X	1	Total Zn 1 1	0	0
7	A	1	Total Zn 1 1	0	0

3 Residue-property plots (i)

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.

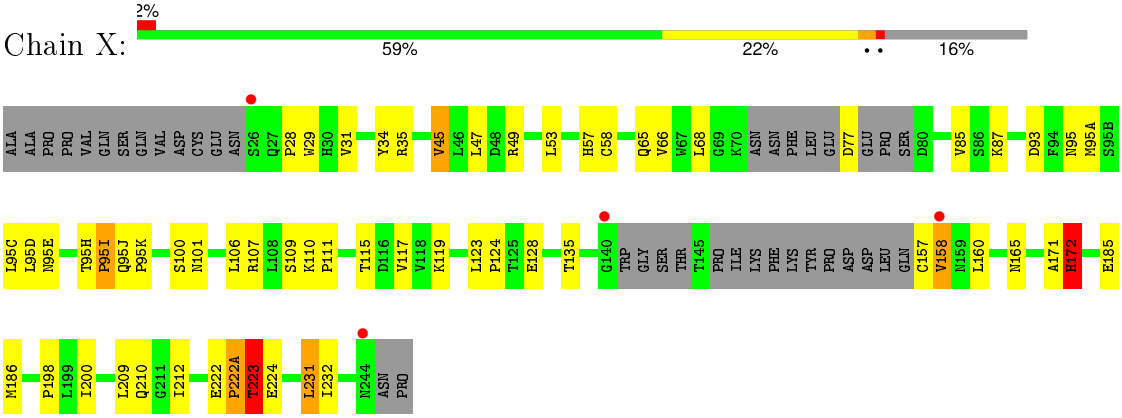
- Molecule 1: NERVE GROWTH FACTOR

Chain A:



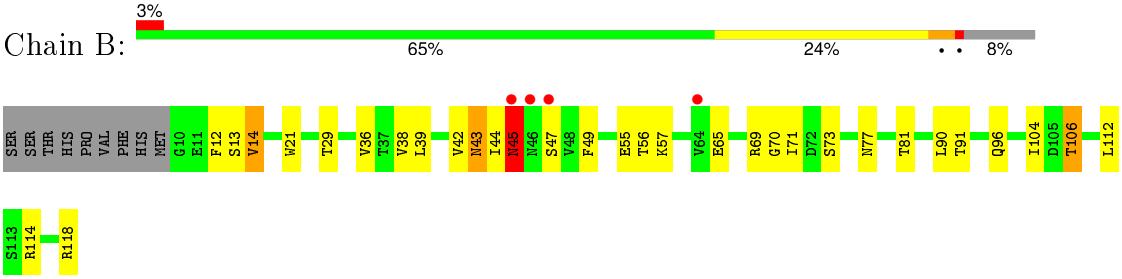
- Molecule 1: NERVE GROWTH FACTOR

Chain X:



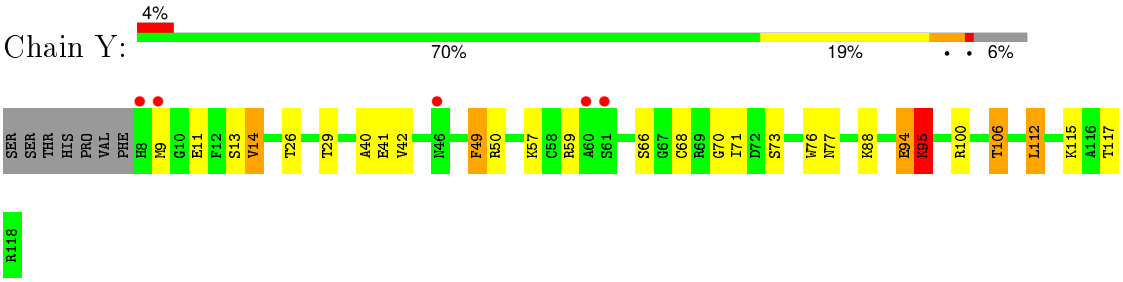
- Molecule 2: NERVE GROWTH FACTOR

Chain B:



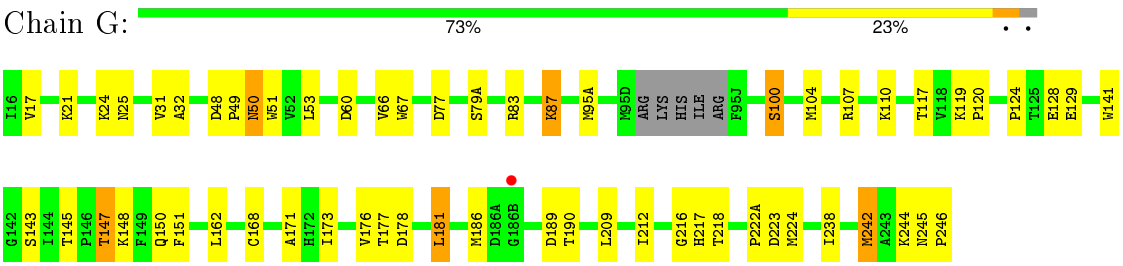
- Molecule 2: NERVE GROWTH FACTOR

Chain Y:



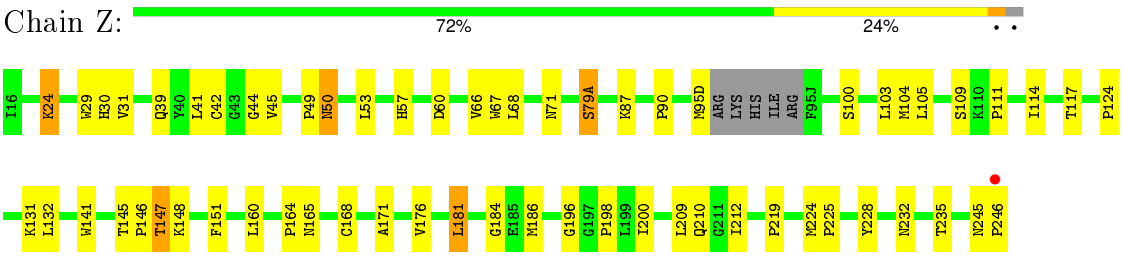
- Molecule 3: NERVE GROWTH FACTOR

Chain G:



- Molecule 3: NERVE GROWTH FACTOR

Chain Z:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	95.68Å 96.59Å 147.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 3.15 19.87 – 3.10	Depositor EDS
% Data completeness (in resolution range)	97.0 (8.00-3.15) 95.7 (19.87-3.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.68 (at 3.09Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.246 , 0.282 0.233 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	75.8	Xtriage
Anisotropy	0.575	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.24 , 49.6	EDS
Estimated twinning fraction	0.011 for k,h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 24184 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	8549	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.39% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, NAG, NDG

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	0.41	0/1611	0.83	5/2187 (0.2%)
1	X	0.40	0/1595	0.78	0/2168
2	B	0.43	0/874	0.76	0/1182
2	Y	0.43	0/887	0.77	0/1199
3	G	0.41	0/1848	0.76	0/2511
3	Z	0.40	0/1851	0.75	1/2514 (0.0%)
All	All	0.41	0/8666	0.78	6/11761 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	26	SER	N-CA-C	6.90	129.63	111.00
1	A	79	PRO	N-CA-C	6.12	128.02	112.10
1	A	79(A)	SER	N-CA-C	-5.63	95.79	111.00
1	A	186	MET	N-CA-C	5.29	125.27	111.00
1	A	186(A)	ASP	N-CA-C	5.22	125.10	111.00
3	Z	103	LEU	CA-CB-CG	5.16	127.16	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	1574	0	1502	25	0
1	X	1559	0	1483	34	0
2	B	858	0	834	23	0
2	Y	871	0	845	14	0
3	G	1799	0	1737	37	0
3	Z	1802	0	1743	36	0
4	A	14	0	13	0	0
4	X	14	0	13	0	0
5	G	28	0	25	0	0
6	Z	28	0	25	1	0
7	A	1	0	0	0	0
7	X	1	0	0	0	0
All	All	8549	0	8220	156	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 9.

All (156) 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:Z:57:HIS:HB2	3:Z:95(D):MET:HG3	1.47	0.96
1:A:245:ASN:N	1:A:246:PRO:HD3	1.93	0.83
1:X:185:GLU:O	1:X:186:MET:HG2	1.82	0.80
3:G:124:PRO:HG3	3:G:209:LEU:O	1.85	0.76
3:Z:31:VAL:HG13	3:Z:66:VAL:HG13	1.70	0.73
1:X:35:ARG:NH1	1:X:58:CYS:HA	2.04	0.71
1:A:124:PRO:HG3	1:A:209:LEU:O	1.92	0.69
6:Z:531:NDG:H6C2	6:Z:532:NAG:O7	1.93	0.68
3:Z:45:VAL:HG12	3:Z:198:PRO:HG3	1.76	0.67
2:Y:94:GLU:O	2:Y:95:LYS:HB3	1.94	0.66
3:G:147:THR:HG23	3:G:148:LYS:H	1.61	0.64
3:Z:57:HIS:CB	3:Z:95(D):MET:HG3	2.24	0.63
1:X:35:ARG:HH11	1:X:58:CYS:HA	1.64	0.63
1:X:222(A):PRO:O	1:X:223:THR:HG23	1.99	0.62
3:G:53:LEU:HG	3:G:212:ILE:HD11	1.81	0.62
2:B:42:VAL:HG22	2:B:90:LEU:HD12	1.81	0.61
3:Z:57:HIS:HB2	3:Z:95(D):MET:CG	2.27	0.59
1:A:245:ASN:H	1:A:246:PRO:HD3	1.65	0.59
1:A:185:GLU:O	1:A:186:MET:HG2	2.02	0.59
3:Z:79(A):SER:HB3	3:Z:117:THR:HG21	1.85	0.58
3:G:50:ASN:HD22	3:G:50:ASN:N	2.01	0.58
1:A:105:LEU:HD11	1:A:238:ILE:HG23	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:87:LYS:HB2	1:X:107:ARG:HB3	1.86	0.58
2:B:38:VAL:HA	2:B:91:THR:HG22	1.85	0.57
3:G:25:ASN:OD1	3:G:117:THR:HG22	2.04	0.57
3:Z:31:VAL:CG1	3:Z:66:VAL:HG13	2.33	0.57
3:G:50:ASN:HD22	3:G:50:ASN:H	1.52	0.57
2:B:36:VAL:HG22	2:B:91:THR:HB	1.86	0.57
3:Z:245:ASN:N	3:Z:246:PRO:HD3	2.19	0.56
3:Z:171:ALA:HB1	3:Z:224:MET:SD	2.46	0.56
2:B:39:LEU:HD23	2:B:90:LEU:HD13	1.87	0.56
1:X:85:VAL:HG11	1:X:106:LEU:HG	1.87	0.56
1:X:57:HIS:HA	1:X:95(D):LEU:HD21	1.89	0.54
1:A:245:ASN:N	1:A:246:PRO:CD	2.67	0.54
2:B:106:THR:HG21	2:Y:106:THR:HG21	1.90	0.53
3:G:162:LEU:HD11	3:G:181:LEU:HG	1.88	0.53
2:Y:66:SER:HB2	2:Y:73:SER:HB3	1.91	0.53
2:B:42:VAL:HG12	2:B:43:ASN:N	2.23	0.53
3:G:177:THR:OG1	3:G:178:ASP:N	2.42	0.52
1:A:47:LEU:HD11	1:A:53:LEU:HD22	1.91	0.52
2:B:42:VAL:CG1	2:B:43:ASN:N	2.71	0.52
2:B:114:ARG:HH21	3:G:218:THR:HG21	1.74	0.52
3:G:83:ARG:HD2	3:G:110:LYS:HG3	1.91	0.52
1:X:222:GLU:O	1:X:224:GLU:HB2	2.10	0.52
2:B:112:LEU:O	2:Y:11:GLU:HA	2.10	0.51
1:X:128:GLU:O	1:X:232:ILE:HD11	2.11	0.51
1:A:82:HIS:HB3	2:Y:9:MET:HE2	1.93	0.51
3:G:107:ARG:HH12	3:G:245:ASN:HB2	1.75	0.51
1:X:158:VAL:HG12	1:X:160:LEU:HG	1.93	0.51
3:G:53:LEU:HD12	3:G:104:MET:O	2.11	0.50
3:G:32:ALA:HB2	3:G:141:TRP:CZ3	2.47	0.50
3:Z:29:TRP:O	3:Z:45:VAL:HA	2.11	0.50
3:Z:186:MET:CE	3:Z:225:PRO:HG3	2.41	0.50
2:Y:40:ALA:O	2:Y:50:ARG:HG3	2.13	0.49
1:X:47:LEU:HD11	1:X:53:LEU:HD22	1.93	0.49
3:G:245:ASN:N	3:G:246:PRO:HD3	2.27	0.49
1:A:78:GLU:N	1:A:79:PRO:HD3	2.27	0.49
3:Z:29:TRP:NE1	3:Z:200:ILE:HD11	2.28	0.49
1:X:100:SER:O	1:X:101:ASN:HB2	2.12	0.49
1:X:31:VAL:HG21	1:X:66:VAL:HG13	1.95	0.48
2:B:70:GLY:HA3	2:Y:112:LEU:HD21	1.94	0.48
1:X:160:LEU:HD23	1:X:185:GLU:HB3	1.95	0.48
3:Z:31:VAL:HG22	3:Z:68:LEU:HD23	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:100:SER:OG	3:G:177:THR:HG21	2.14	0.48
2:B:118:ARG:HH21	3:G:217:HIS:N	2.12	0.48
3:Z:44:GLY:HA2	3:Z:196:GLY:O	2.14	0.48
3:G:48:ASP:HB3	3:G:51:TRP:HB2	1.94	0.48
1:A:171:ALA:O	1:A:173:GLU:N	2.47	0.48
2:B:21:TRP:CD2	1:X:222(A):PRO:HG3	2.49	0.48
2:B:118:ARG:NH2	3:G:217:HIS:H	2.12	0.48
1:A:31:VAL:HG21	1:A:66:VAL:HG13	1.96	0.48
3:Z:50:ASN:N	3:Z:50:ASN:HD22	2.11	0.47
1:X:124:PRO:HG3	1:X:209:LEU:O	2.15	0.47
2:B:118:ARG:CZ	3:G:216:GLY:HA3	2.45	0.47
1:A:147:ILE:HG23	1:A:219:PRO:HG3	1.95	0.47
3:G:143:SER:HA	3:G:150:GLN:O	2.15	0.47
3:Z:147:THR:HG23	3:Z:148:LYS:H	1.80	0.47
1:A:183:ALA:HB3	1:A:228:TYR:CE1	2.50	0.46
3:Z:90:PRO:HG3	3:Z:104:MET:SD	2.55	0.46
3:Z:151:PHE:N	3:Z:151:PHE:CD1	2.84	0.46
1:X:95(C):LEU:HD23	1:X:95(C):LEU:HA	1.63	0.46
1:X:222:GLU:HA	1:X:222(A):PRO:HD3	1.66	0.46
3:G:17:VAL:HG22	3:G:189:ASP:O	2.16	0.46
1:A:45:VAL:HG22	1:A:198:PRO:HG3	1.97	0.45
2:B:118:ARG:NH1	3:G:190:THR:O	2.49	0.45
3:Z:151:PHE:HD1	3:Z:151:PHE:N	2.14	0.45
3:Z:53:LEU:HG	3:Z:212:ILE:CD1	2.47	0.45
3:G:171:ALA:HB1	3:G:224:MET:HE1	1.99	0.45
1:X:157:CYS:O	1:X:158:VAL:HG23	2.17	0.45
3:Z:29:TRP:HE1	3:Z:200:ILE:HD11	1.80	0.45
1:X:95(A):MET:O	1:X:95(D):LEU:HB2	2.16	0.45
1:X:171:ALA:O	1:X:172:HIS:C	2.55	0.45
2:B:112:LEU:HD21	2:Y:70:GLY:HA3	1.98	0.45
3:G:222(A):PRO:O	3:G:223:ASP:HB2	2.17	0.45
3:Z:24:LYS:O	3:Z:71:ASN:ND2	2.50	0.44
3:G:151:PHE:CD1	3:G:151:PHE:N	2.86	0.44
1:A:95(J):GLN:HA	1:A:95(K):PRO:HD3	1.75	0.44
2:Y:49:PHE:CD1	2:Y:49:PHE:C	2.91	0.44
2:B:12:PHE:HZ	2:Y:76:TRP:CZ3	2.35	0.44
3:Z:87:LYS:HD3	3:Z:246:PRO:OXT	2.17	0.44
3:G:238:ILE:O	3:G:242:MET:HB2	2.18	0.44
1:X:77:ASP:OD2	3:Z:219:PRO:HD2	2.18	0.43
3:Z:145:THR:HA	3:Z:146:PRO:HD3	1.81	0.43
3:Z:50:ASN:ND2	3:Z:111:PRO:HG3	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:ALA:O	1:A:157:CYS:HA	2.18	0.43
3:Z:124:PRO:HG3	3:Z:209:LEU:O	2.18	0.43
1:X:34:TYR:HB3	1:X:65:GLN:HB3	2.00	0.43
3:G:31:VAL:HG13	3:G:66:VAL:HG13	2.00	0.43
3:Z:160:LEU:HD22	3:Z:184:GLY:HA2	1.99	0.43
1:X:209:LEU:HG	1:X:231:LEU:HD23	2.00	0.43
3:G:145:THR:HG21	3:G:150:GLN:NE2	2.34	0.43
2:Y:115:LYS:HD3	2:Y:117:THR:OG1	2.19	0.43
1:X:95(J):GLN:HA	1:X:95(K):PRO:HD3	1.66	0.43
3:Z:168:CYS:HB3	3:Z:176:VAL:HG21	2.01	0.43
1:A:168:CYS:HB3	1:A:176:VAL:HG21	2.00	0.43
2:Y:14:VAL:HG13	2:Y:68:CYS:HB3	2.00	0.43
3:Z:105:LEU:HD23	3:Z:105:LEU:HA	1.86	0.43
1:A:218:GLU:HA	1:A:219:PRO:C	2.39	0.43
2:B:90:LEU:HD23	2:B:90:LEU:HA	1.90	0.43
2:Y:9:MET:N	2:Y:9:MET:SD	2.92	0.42
3:Z:41:LEU:O	3:Z:42:CYS:SG	2.77	0.42
1:X:49:ARG:HH21	1:X:111:PRO:HB2	1.83	0.42
3:G:128:GLU:HG3	3:G:129:GLU:H	1.84	0.42
1:A:185:GLU:C	1:A:186:MET:HG2	2.40	0.42
1:X:31:VAL:CG2	1:X:66:VAL:HG13	2.50	0.42
3:G:173:ILE:HG22	3:G:173:ILE:O	2.20	0.42
1:A:138:ALA:HB2	1:A:160:LEU:HD11	2.00	0.42
2:B:14:VAL:HG22	2:B:69:ARG:O	2.18	0.42
1:X:28:PRO:HB2	1:X:119:LYS:HB2	2.01	0.42
3:G:119:LYS:HA	3:G:120:PRO:HD3	1.81	0.42
3:G:171:ALA:HB1	3:G:224:MET:CE	2.49	0.42
3:Z:181:LEU:HA	3:Z:181:LEU:HD12	1.94	0.42
3:G:168:CYS:HB3	3:G:176:VAL:HG21	2.00	0.42
1:A:26:SER:O	1:A:28:PRO:HD3	2.20	0.42
2:B:44:ILE:CG2	2:B:45:ASN:N	2.83	0.42
3:G:87:LYS:HZ2	3:G:87:LYS:HB2	1.83	0.42
1:X:95:ASN:O	1:X:95(C):LEU:HB2	2.19	0.42
3:Z:30:HIS:HD2	3:Z:141:TRP:CZ3	2.38	0.42
3:Z:228:TYR:N	3:Z:228:TYR:CD1	2.86	0.41
1:X:115:THR:C	1:X:117:VAL:H	2.23	0.41
1:A:130:PRO:HG3	1:A:210:GLN:OE1	2.20	0.41
1:A:31:VAL:CG2	1:A:66:VAL:HG13	2.51	0.41
2:B:71:ILE:HD13	2:Y:71:ILE:HD13	2.01	0.41
3:G:181:LEU:HD12	3:G:181:LEU:HA	1.95	0.41
3:G:244:LYS:O	3:G:245:ASN:C	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Z:132:LEU:HD13	3:Z:164:PRO:HG3	2.02	0.41
3:G:50:ASN:N	3:G:50:ASN:ND2	2.67	0.41
1:X:29:TRP:NE1	1:X:200:ILE:HD11	2.36	0.41
1:X:165:ASN:N	1:X:165:ASN:HD22	2.19	0.40
1:A:91:HIS:HD2	1:A:237:TRP:CE2	2.39	0.40
1:X:45:VAL:HG22	1:X:198:PRO:HG3	2.02	0.40
2:B:56:THR:HB	2:B:106:THR:O	2.22	0.40
1:X:95(H):THR:HA	1:X:95(I):PRO:HD3	1.92	0.40
2:B:55:GLU:HG2	2:B:104:ILE:HG23	2.02	0.40
3:Z:53:LEU:HG	3:Z:212:ILE:HD11	2.03	0.40
1:A:88:ALA:C	1:A:89:ILE:HG13	2.41	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	193/240 (80%)	169 (88%)	19 (10%)	5 (3%)	7 38
1	X	194/240 (81%)	169 (87%)	19 (10%)	6 (3%)	5 32
2	B	107/118 (91%)	98 (92%)	5 (5%)	4 (4%)	4 27
2	Y	109/118 (92%)	102 (94%)	5 (5%)	2 (2%)	11 49
3	G	228/237 (96%)	205 (90%)	20 (9%)	3 (1%)	15 57
3	Z	228/237 (96%)	204 (90%)	20 (9%)	4 (2%)	11 49
All	All	1059/1190 (89%)	947 (89%)	88 (8%)	24 (2%)	8 42

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	26	SER

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Mol	Chain	Res	Type
1	A	172	HIS
3	G	24	LYS
3	G	100	SER
1	X	172	HIS
1	X	222(A)	PRO
1	X	223	THR
2	B	45	ASN
2	B	65	GLU
1	X	95(E)	ASN
2	Y	94	GLU
2	Y	95	LYS
3	Z	100	SER
2	B	43	ASN
1	X	95(I)	PRO
1	X	158	VAL
3	Z	109	SER
3	G	147	THR
1	A	79	PRO
1	A	93	ASP
2	B	73	SER
3	Z	24	LYS
1	A	245	ASN
3	Z	114	ILE

5.3.2 Protein sidechains (i)

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	178/213 (84%)	159 (89%)	19 (11%)	8 32
1	X	175/213 (82%)	163 (93%)	12 (7%)	19 57
2	B	96/105 (91%)	85 (88%)	11 (12%)	7 29
2	Y	97/105 (92%)	82 (84%)	15 (16%)	3 15
3	G	199/205 (97%)	187 (94%)	12 (6%)	24 63
3	Z	200/205 (98%)	187 (94%)	13 (6%)	21 60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	945/1046 (90%)	863 (91%)	82 (9%)	13 44

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	ASN
1	A	38	ASN
1	A	39	LYS
1	A	41	GLN
1	A	45	VAL
1	A	68	LEU
1	A	96	GLU
1	A	106	LEU
1	A	117	VAL
1	A	123	LEU
1	A	128	GLU
1	A	170	LYS
1	A	172	HIS
1	A	173	GLU
1	A	174	MET
1	A	178	ASP
1	A	186	MET
1	A	188	SER
1	A	212	ILE
2	B	13	SER
2	B	14	VAL
2	B	29	THR
2	B	45	ASN
2	B	47	SER
2	B	49	PHE
2	B	57	LYS
2	B	77	ASN
2	B	81	THR
2	B	96	GLN
2	B	106	THR
3	G	21	LYS
3	G	49	PRO
3	G	50	ASN
3	G	60	ASP
3	G	67	TRP
3	G	77	ASP
3	G	79(A)	SER

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Mol	Chain	Res	Type
3	G	87	LYS
3	G	95(A)	MET
3	G	181	LEU
3	G	186	MET
3	G	242	MET
1	X	45	VAL
1	X	68	LEU
1	X	93	ASP
1	X	109	SER
1	X	110	LYS
1	X	123	LEU
1	X	135	THR
1	X	172	HIS
1	X	210	GLN
1	X	212	ILE
1	X	223	THR
1	X	231	LEU
2	Y	13	SER
2	Y	14	VAL
2	Y	26	THR
2	Y	29	THR
2	Y	41	GLU
2	Y	42	VAL
2	Y	49	PHE
2	Y	57	LYS
2	Y	59	ARG
2	Y	77	ASN
2	Y	88	LYS
2	Y	95	LYS
2	Y	100	ARG
2	Y	106	THR
2	Y	112	LEU
3	Z	39	GLN
3	Z	49	PRO
3	Z	50	ASN
3	Z	60	ASP
3	Z	67	TRP
3	Z	79(A)	SER
3	Z	131	LYS
3	Z	147	THR
3	Z	165	ASN
3	Z	181	LEU

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Mol	Chain	Res	Type
3	Z	210	GLN
3	Z	232	ASN
3	Z	235	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	ASN
1	A	91	HIS
1	A	101	ASN
2	B	62	ASN
2	B	77	ASN
3	G	50	ASN
3	G	101	ASN
3	G	232	ASN
1	X	30	HIS
1	X	50	ASN
1	X	165	ASN
2	Y	77	ASN
3	Z	25	ASN
3	Z	30	HIS
3	Z	71	ASN
3	Z	101	ASN
3	Z	165	ASN
3	Z	210	GLN

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

4 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	$\#\|Z\| > 2$
5	NAG	G	247	3,5	14,14,15	0.40	0	15,19,21	0.82	1 (6%)
5	NAG	G	248	5	14,14,15	0.65	0	15,19,21	0.79	0
6	NDG	Z	531	3,6	14,14,15	1.34	2 (14%)	15,19,21	1.73	3 (20%)
6	NAG	Z	532	6	14,14,15	1.06	1 (7%)	15,19,21	1.62	4 (26%)

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
5	NAG	G	247	3,5	-	0/6/23/26	0/1/1/1
5	NAG	G	248	5	-	0/6/23/26	0/1/1/1
6	NDG	Z	531	3,6	-	0/6/23/26	0/1/1/1
6	NAG	Z	532	6	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	Z	531	NDG	O4-C4	2.21	1.48	1.43
6	Z	532	NAG	C1-C2	2.94	1.56	1.52
6	Z	531	NDG	C1-C2	3.75	1.57	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	Z	532	NAG	C4-C3-C2	-3.23	106.20	111.23
6	Z	531	NDG	C8-C7-N2	-2.85	110.65	116.11
5	G	247	NAG	C2-N2-C7	-2.46	119.88	123.04
6	Z	532	NAG	C8-C7-N2	-2.25	111.80	116.11
6	Z	532	NAG	C1-O5-C5	2.32	115.19	112.25
6	Z	531	NDG	C2-N2-C7	2.75	126.57	123.04
6	Z	532	NAG	C2-N2-C7	3.56	127.62	123.04
6	Z	531	NDG	C1-O-C5	3.61	116.83	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	Z	531	NDG	1	0
6	Z	532	NAG	1	0

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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	11	1	14,14,15	0.45	0	15,19,21	0.79	0
4	NAG	X	511	1	14,14,15	0.47	0	15,19,21	0.58	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	11	1	-	0/6/23/26	0/1/1/1
4	NAG	X	511	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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, 95^{th} 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	203/240 (84%)	-0.42	3 (1%)	76	62	2, 32, 79, 113	0
1	X	202/240 (84%)	-0.23	4 (1%)	68	52	12, 48, 84, 101	0
2	B	109/118 (92%)	-0.22	4 (3%)	45	28	2, 35, 91, 118	0
2	Y	111/118 (94%)	-0.23	5 (4%)	37	21	2, 39, 96, 151	0
3	G	232/237 (97%)	-0.39	1 (0%)	93	90	2, 35, 77, 103	0
3	Z	232/237 (97%)	-0.51	1 (0%)	93	90	2, 31, 74, 109	0
All	All	1089/1190 (91%)	-0.35	18 (1%)	73	59	2, 37, 82, 151	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	46	ASN	5.1
2	B	45	ASN	5.0
2	Y	61	SER	4.1
2	Y	46	ASN	3.3
1	A	158	VAL	3.2
1	A	25	ASN	3.2
2	Y	8	HIS	2.9
2	Y	9	MET	2.7
1	X	244	ASN	2.7
1	X	140	GLY	2.6
2	Y	60	ALA	2.5
2	B	47	SER	2.5
3	Z	246	PRO	2.5
2	B	64	VAL	2.3
1	X	26	SER	2.2
3	G	186(B)	GLY	2.1
1	A	78	GLU	2.1
1	X	158	VAL	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, 95^{th} 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
6	NAG	Z	532	14/15	0.79	0.23	-0.83	81,81,81,81	0
6	NDG	Z	531	14/15	0.86	0.29	-	87,87,87,87	0
5	NAG	G	248	14/15	0.83	0.31	-	86,86,86,86	0
5	NAG	G	247	14/15	0.91	0.19	-	75,75,75,75	0

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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
7	ZN	X	501	1/1	0.99	0.08	-1.90	2,2,2,2	0
7	ZN	A	1	1/1	0.96	0.05	-2.98	2,2,2,2	0
4	NAG	A	11	14/15	0.82	0.22	-	79,79,79,79	0
4	NAG	X	511	14/15	0.88	0.26	-	84,84,84,84	0

6.5 Other polymers (i)

There are no such residues in this entry.