Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:30 PM GMT

PDB ID	:	4ILD
Title	:	Crystal structure of truncated Bovine viral diarrhea virus 1 E2 envelope protein
Authors	:	Modis, Y.; Li, Y.; Wang, J.
Deposited on	:	2012-12-30
Resolution	:	3.27 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:

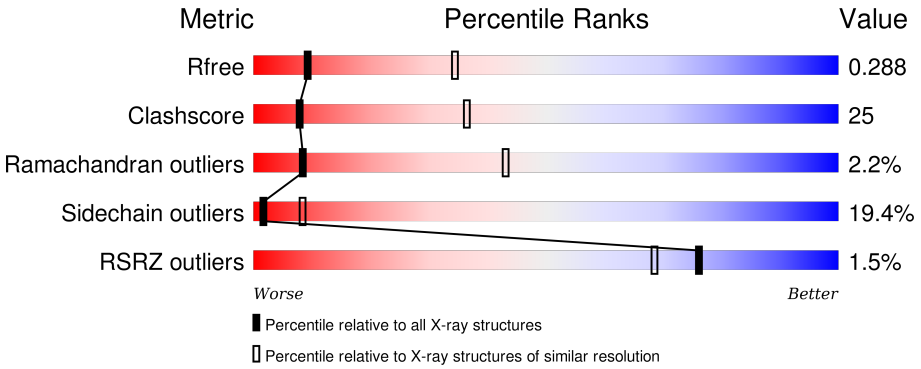
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.27 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	1756 (3.36-3.20)
Clashscore	102246	1941 (3.36-3.20)
Ramachandran outliers	100387	1905 (3.36-3.20)
Sidechain outliers	100360	1903 (3.36-3.20)
RSRZ outliers	91569	1764 (3.36-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	253	51% 36% 6% 7%
1	B	253	2% 43% 39% 11% 6%

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
2	NAG	A	2405	-	-	-	X
4	IUM	B	2410	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 3974 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 Envelope glycoprotein E2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	235	Total	C	N	O	S	0	0	0
			1858	1180	310	348	20			
1	B	237	Total	C	N	O	S	0	0	0
			1876	1191	313	352	20			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	778	LEU	-	EXPRESSION TAG	UNP P19711
A	779	LEU	-	EXPRESSION TAG	UNP P19711
A	780	GLU	-	EXPRESSION TAG	UNP P19711
A	788	ASP	ASN	CONFLICT	UNP P19711
B	778	LEU	-	EXPRESSION TAG	UNP P19711
B	779	LEU	-	EXPRESSION TAG	UNP P19711
B	780	GLU	-	EXPRESSION TAG	UNP P19711
B	788	ASP	ASN	CONFLICT	UNP P19711

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

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

Continued on next page...

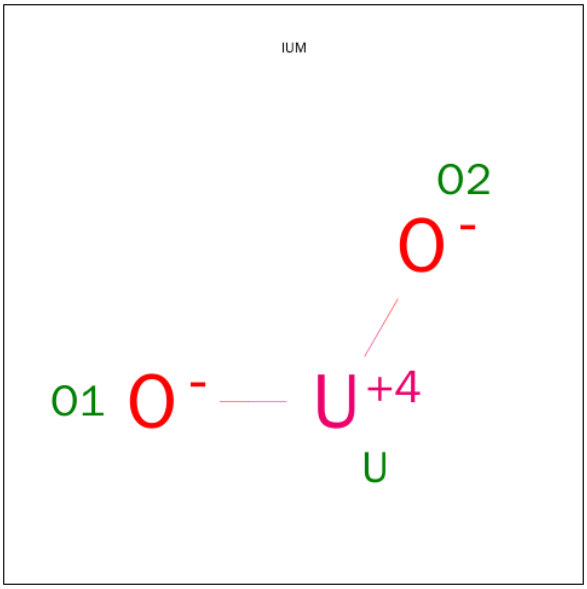
Continued from previous page...

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

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Ca 1 1	0	0
3	A	3	Total Ca 3 3	0	0

- Molecule 4 is URANYL (VI) ION (three-letter code: IUM) (formula: O_2U).



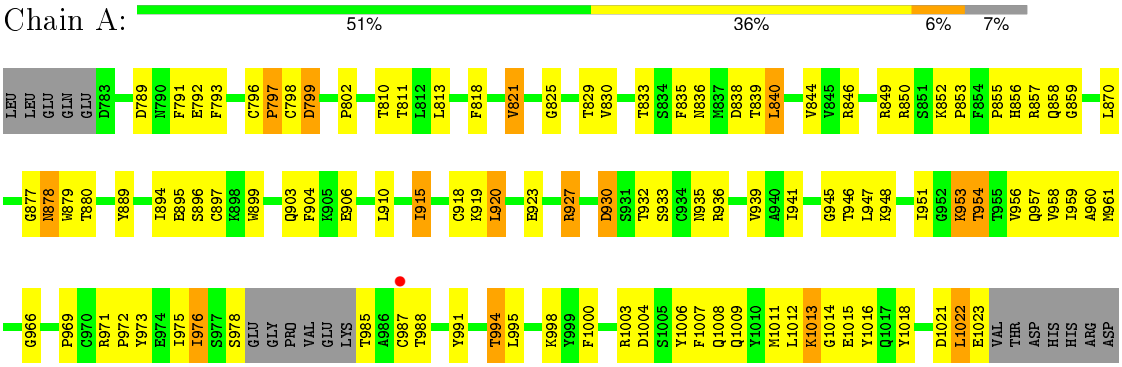
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total O U 3 2 1	0	0
4	B	1	Total O U 3 2 1	0	0
4	B	1	Total O U 3 2 1	0	0
4	B	1	Total O U 3 2 1	0	0

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.

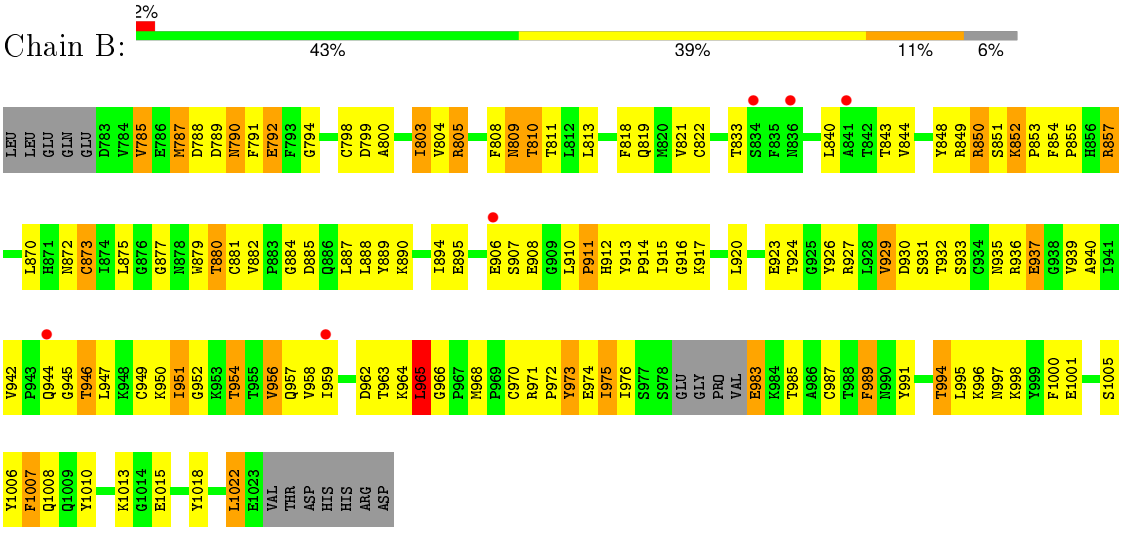
- Molecule 1: Envelope glycoprotein E2

Chain A:



- Molecule 1: Envelope glycoprotein E2

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	136.72Å 54.45Å 95.92Å 90.00° 92.23° 90.00°	Depositor
Resolution (Å)	47.97 – 3.27 47.92 – 3.27	Depositor EDS
% Data completeness (in resolution range)	99.1 (47.97-3.27) 99.5 (47.92-3.27)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	2.07 (at 3.25Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.246 , 0.289 0.246 , 0.288	Depositor DCC
R_{free} test set	556 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	40.4	Xtriage
Anisotropy	0.477	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 31.6	EDS
Estimated twinning fraction	0.034 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 11093 reflections	Xtriage
F_o,F_c correlation	0.84	EDS
Total number of atoms	3974	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.89% 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: CA, IUM, NAG

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	0.53	0/1904	0.77	0/2577
1	B	0.50	1/1922 (0.1%)	0.78	2/2600 (0.1%)
All	All	0.51	1/3826 (0.0%)	0.78	2/5177 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	873	CYS	CB-SG	-5.27	1.73	1.81

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	873	CYS	CB-CA-C	-5.42	99.55	110.40
1	B	965	LEU	CA-CB-CG	5.24	127.36	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	1858	0	1792	76	3
1	B	1876	0	1816	119	1
2	A	112	0	100	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	112	0	100	4	0
3	A	3	0	0	0	0
3	B	1	0	0	0	0
4	B	12	0	0	2	2
All	All	3974	0	3808	194	3

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 25.

All (194) 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:B:976:ILE:HD11	1:B:991:TYR:CZ	1.22	1.69
1:B:976:ILE:CD1	1:B:991:TYR:CE1	1.94	1.50
1:B:976:ILE:CD1	1:B:991:TYR:CZ	1.96	1.48
1:B:976:ILE:HD11	1:B:991:TYR:CE1	1.59	1.27
1:B:976:ILE:HD12	1:B:991:TYR:CE1	1.71	1.18
1:B:951:ILE:HG23	1:B:956:VAL:HG11	1.30	1.14
1:B:951:ILE:CG2	1:B:956:VAL:HG11	1.78	1.11
1:B:976:ILE:HD11	1:B:991:TYR:CE2	1.88	1.08
1:B:791:PHE:O	1:B:857:ARG:NH2	1.93	1.02
1:A:923:GLU:OE2	1:A:927:ARG:NH2	1.96	0.98
1:B:849:ARG:NH1	1:B:851:SER:HB2	1.80	0.95
1:B:850:ARG:NH2	1:B:852:LYS:O	2.01	0.93
1:A:935:ASN:ND2	1:A:961:MET:SD	2.42	0.92
1:B:877:GLY:HA3	1:B:880:THR:HG23	1.55	0.88
1:B:790:ASN:ND2	1:B:790:ASN:O	2.06	0.88
1:B:983:GLU:N	1:B:983:GLU:OE1	2.09	0.85
1:B:976:ILE:HD12	1:B:991:TYR:HE1	1.43	0.84
1:A:994:THR:N	1:A:1015:GLU:O	2.10	0.84
1:B:850:ARG:HG3	1:B:854:PHE:HE1	1.43	0.83
2:B:2406:NAG:H3	2:B:2406:NAG:C8	2.10	0.82
1:A:987:CYS:SG	1:B:987:CYS:O	2.38	0.82
1:B:974:GLU:OE1	4:B:2410:IUM:O2	1.97	0.82
1:B:951:ILE:HG22	1:B:956:VAL:HG11	1.62	0.81
1:A:906:GLU:OE2	1:A:953:LYS:NZ	2.14	0.80
1:B:857:ARG:HG3	1:B:857:ARG:HH11	1.45	0.80
1:B:849:ARG:CZ	1:B:851:SER:HB2	2.10	0.80
1:B:850:ARG:HG3	1:B:854:PHE:CE1	2.16	0.80
1:B:976:ILE:CD1	1:B:991:TYR:OH	2.30	0.79
1:A:939:VAL:HG11	1:A:969:PRO:HD3	1.63	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:976:ILE:CG1	1:B:991:TYR:CE1	2.65	0.79
1:B:962:ASP:OD2	1:B:964:LYS:HG3	1.83	0.78
2:B:2406:NAG:H3	2:B:2406:NAG:H83	1.64	0.78
1:B:787:MET:HG3	1:B:791:PHE:CD2	2.19	0.78
1:A:994:THR:OG1	1:A:1000:PHE:CE2	2.38	0.77
1:A:877:GLY:O	1:A:880:THR:OG1	2.07	0.73
1:B:951:ILE:HD12	1:B:952:GLY:H	1.52	0.73
1:B:805:ARG:HD3	1:B:805:ARG:N	2.05	0.71
1:B:908:GLU:OE2	4:B:2411:IUM:U	1.69	0.71
1:B:889:TYR:HA	1:B:927:ARG:HD3	1.72	0.71
1:B:791:PHE:CD1	1:B:792:GLU:N	2.58	0.71
1:B:877:GLY:CA	1:B:880:THR:HG23	2.21	0.70
1:A:939:VAL:CG1	1:A:969:PRO:HD3	2.22	0.70
1:B:822:CYS:CB	1:B:877:GLY:HA2	2.20	0.70
1:B:951:ILE:HD12	1:B:952:GLY:N	2.06	0.69
1:B:809:ASN:HD22	2:B:2401:NAG:H83	1.56	0.68
1:B:976:ILE:HG13	1:B:991:TYR:CD1	2.28	0.68
1:B:788:ASP:OD1	1:B:789:ASP:N	2.28	0.67
1:A:835:PHE:CE1	1:A:836:ASN:O	2.48	0.66
1:B:962:ASP:OD2	1:B:964:LYS:CG	2.44	0.66
1:B:933:SER:OG	1:B:935:ASN:N	2.28	0.65
1:B:975:ILE:HD12	1:B:975:ILE:N	2.11	0.65
1:A:1022:LEU:N	1:A:1022:LEU:HD22	2.12	0.65
1:B:889:TYR:OH	1:B:894:ILE:HD11	1.97	0.63
1:B:946:THR:HG22	1:B:959:ILE:HD13	1.82	0.62
1:B:945:GLY:HA3	1:B:957:GLN:HG2	1.81	0.62
1:B:907:SER:HB2	1:B:913:TYR:CD1	2.34	0.62
1:B:968:MET:CE	1:B:1000:PHE:CE1	2.82	0.62
1:A:919:LYS:NZ	1:A:920:LEU:O	2.30	0.60
1:B:822:CYS:HB2	1:B:877:GLY:HA2	1.84	0.60
1:B:937:GLU:HA	1:B:937:GLU:OE1	2.00	0.59
1:A:889:TYR:CZ	1:A:894:ILE:HD11	2.37	0.59
1:A:1004:ASP:OD2	1:A:1011:MET:HE1	2.03	0.59
1:B:1005:SER:O	1:B:1008:GLN:NE2	2.35	0.59
1:A:930:ASP:OD2	1:A:932:THR:HG23	2.03	0.59
1:B:857:ARG:NH1	1:B:857:ARG:HG3	2.17	0.58
1:A:904:PHE:HD1	1:A:954:THR:HG21	1.68	0.58
1:B:994:THR:N	1:B:1015:GLU:O	2.35	0.58
1:A:840:LEU:HD22	1:A:840:LEU:N	2.19	0.57
1:B:968:MET:HE2	1:B:1000:PHE:CE1	2.39	0.57
1:A:850:ARG:NE	1:A:852:LYS:O	2.34	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:836:ASN:HB3	1:A:839:THR:O	2.05	0.56
1:A:899:TRP:CD2	1:A:915:ILE:HD13	2.40	0.56
1:B:968:MET:HE3	1:B:1000:PHE:CE1	2.40	0.56
1:A:939:VAL:HG21	1:A:995:LEU:CD2	2.35	0.56
1:A:904:PHE:HE1	1:A:954:THR:HG1	1.54	0.56
1:A:1013:LYS:HD3	1:B:1006:TYR:CE1	2.41	0.55
1:B:879:TRP:O	1:B:879:TRP:HE3	1.89	0.55
1:B:875:LEU:HB2	1:B:882:VAL:CG2	2.37	0.55
1:A:840:LEU:CD2	1:A:840:LEU:N	2.69	0.55
1:B:917:LYS:HB3	1:B:926:TYR:HB3	1.87	0.55
1:B:950:LYS:CD	1:B:971:ARG:NH2	2.70	0.54
1:A:829:THR:HG22	1:A:849:ARG:HG2	1.88	0.54
1:B:976:ILE:HD12	1:B:991:TYR:CZ	2.06	0.53
1:B:907:SER:OG	1:B:907:SER:O	2.19	0.53
1:B:850:ARG:CG	1:B:854:PHE:CE1	2.91	0.53
1:A:894:ILE:HG23	1:A:918:CYS:HB3	1.89	0.53
1:B:873:CYS:HB3	1:B:881:CYS:HA	1.90	0.53
1:B:968:MET:HE2	1:B:1000:PHE:CZ	2.44	0.53
1:A:939:VAL:CG2	1:A:995:LEU:CD2	2.87	0.52
1:B:1022:LEU:N	1:B:1022:LEU:HD12	2.24	0.52
1:A:923:GLU:CD	1:A:927:ARG:HH21	2.05	0.52
1:B:822:CYS:HB3	1:B:877:GLY:HA2	1.90	0.52
1:B:976:ILE:CG1	1:B:991:TYR:CD1	2.92	0.52
1:B:976:ILE:HG13	1:B:976:ILE:O	2.10	0.52
1:B:976:ILE:HG13	1:B:991:TYR:CE1	2.39	0.52
1:B:789:ASP:HA	1:B:850:ARG:NH1	2.25	0.52
1:A:946:THR:HG23	1:A:959:ILE:HD13	1.91	0.51
1:A:1013:LYS:HD3	1:B:1006:TYR:CZ	2.46	0.51
1:B:885:ASP:OD1	1:B:885:ASP:N	2.43	0.51
1:B:910:LEU:HD23	1:B:951:ILE:HD11	1.91	0.51
1:A:1006:TYR:CZ	1:B:1013:LYS:HG2	2.46	0.51
1:B:951:ILE:HG22	1:B:956:VAL:CG1	2.37	0.51
1:B:950:LYS:HD2	1:B:971:ARG:NH2	2.26	0.51
1:A:858:GLN:CG	1:A:859:GLY:H	2.23	0.51
1:B:963:THR:O	1:B:997:ASN:ND2	2.43	0.50
1:B:879:TRP:O	1:B:879:TRP:CE3	2.66	0.49
1:A:994:THR:HG22	1:A:995:LEU:O	2.12	0.49
1:A:810:THR:OG1	1:A:821:VAL:O	2.29	0.49
1:B:907:SER:HB2	1:B:913:TYR:HB2	1.95	0.49
1:B:972:PRO:HD3	1:B:1000:PHE:CG	2.48	0.49
1:B:911:PRO:HG3	1:B:936:ARG:NH2	2.27	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:994:THR:OG1	1:A:1000:PHE:HE2	1.95	0.48
1:B:996:LYS:O	1:B:997:ASN:HB2	2.14	0.47
1:B:1006:TYR:HD1	1:B:1007:PHE:CD1	2.32	0.47
1:A:988:THR:O	1:A:1021:ASP:N	2.44	0.47
1:A:959:ILE:HD12	1:A:960:ALA:H	1.79	0.47
1:A:818:PHE:CE1	1:A:830:VAL:HG21	2.50	0.47
1:A:960:ALA:HB2	1:A:995:LEU:HG	1.97	0.46
1:B:1007:PHE:N	1:B:1007:PHE:CD1	2.81	0.46
1:A:1003:ARG:NH1	1:A:1009:GLN:HA	2.30	0.46
2:B:2406:NAG:C1	2:B:2406:NAG:H82	2.46	0.46
1:B:805:ARG:CD	1:B:805:ARG:N	2.78	0.46
1:B:968:MET:HG2	1:B:998:LYS:HB3	1.98	0.46
1:B:966:GLY:O	1:B:998:LYS:HA	2.16	0.46
1:A:904:PHE:CD1	1:A:954:THR:HG21	2.50	0.46
1:A:818:PHE:CE2	1:A:830:VAL:HG11	2.51	0.46
1:A:972:PRO:CG	1:A:975:ILE:HD11	2.46	0.46
1:B:791:PHE:HD1	1:B:792:GLU:N	2.10	0.46
1:B:968:MET:CE	1:B:1000:PHE:CZ	2.99	0.46
1:A:1016:TYR:CD1	1:A:1016:TYR:N	2.82	0.45
1:B:989:PHE:CD2	1:B:1018:TYR:HD2	2.35	0.45
1:B:803:ILE:HD11	1:B:805:ARG:CZ	2.46	0.45
1:A:1013:LYS:HE2	1:A:1018:TYR:OH	2.16	0.45
1:A:879:TRP:HE3	1:A:879:TRP:O	2.00	0.45
1:B:870:LEU:HB3	1:B:887:LEU:HD13	1.98	0.45
1:B:930:ASP:OD2	1:B:932:THR:HG23	2.17	0.45
1:A:956:VAL:HG12	1:A:957:GLN:N	2.31	0.45
1:A:994:THR:HG23	1:A:995:LEU:N	2.32	0.44
1:B:940:ALA:O	1:B:958:VAL:HG23	2.17	0.44
1:A:956:VAL:HG12	1:A:957:GLN:H	1.83	0.44
1:B:808:PHE:HE2	1:B:810:THR:HG1	1.63	0.44
1:A:1013:LYS:HB3	1:A:1013:LYS:HE3	1.68	0.44
1:B:1007:PHE:HD1	1:B:1007:PHE:N	2.16	0.44
1:A:946:THR:CG2	1:A:959:ILE:HD13	2.48	0.44
1:B:1001:GLU:OE2	1:B:1010:TYR:OH	2.25	0.44
1:A:1022:LEU:CD2	1:A:1022:LEU:N	2.80	0.44
1:B:917:LYS:CB	1:B:926:TYR:HB3	2.47	0.44
1:B:798:CYS:C	1:B:800:ALA:N	2.70	0.44
1:B:954:THR:O	1:B:956:VAL:HG12	2.18	0.43
1:B:972:PRO:HD3	1:B:1000:PHE:HB3	1.99	0.43
1:B:857:ARG:CG	1:B:857:ARG:HH11	2.25	0.43
1:B:965:LEU:HA	1:B:997:ASN:O	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:855:PRO:O	1:A:857:ARG:HG3	2.18	0.43
1:B:1006:TYR:CD1	1:B:1007:PHE:CD1	3.06	0.43
1:A:1007:PHE:CD1	1:A:1007:PHE:N	2.86	0.43
1:B:803:ILE:HD12	1:B:803:ILE:C	2.39	0.43
1:B:803:ILE:HD12	1:B:803:ILE:O	2.19	0.43
1:A:796:CYS:SG	1:A:802:PRO:HB3	2.58	0.43
1:A:939:VAL:HG22	1:A:958:VAL:CG2	2.49	0.43
1:A:839:THR:C	1:A:840:LEU:HD22	2.39	0.43
1:A:1004:ASP:O	1:A:1008:GLN:HA	2.19	0.43
1:A:797:PRO:O	1:A:799:ASP:N	2.51	0.42
1:A:994:THR:HG21	1:A:998:LYS:O	2.19	0.42
1:B:973:TYR:HD1	1:B:973:TYR:O	2.03	0.42
1:B:787:MET:CG	1:B:791:PHE:CD2	2.98	0.42
1:A:825:GLY:HA2	1:A:853:PRO:HB3	2.01	0.42
1:A:994:THR:CG2	1:A:995:LEU:N	2.82	0.42
1:B:973:TYR:CD1	1:B:973:TYR:C	2.93	0.42
1:A:966:GLY:O	1:A:998:LYS:HA	2.19	0.42
1:B:950:LYS:HD3	1:B:971:ARG:NH2	2.34	0.42
1:A:939:VAL:CG2	1:A:995:LEU:HD21	2.49	0.42
1:A:897:CYS:HA	1:A:918:CYS:HA	2.01	0.42
1:B:794:GLY:HA3	1:B:818:PHE:CZ	2.54	0.42
1:A:835:PHE:CD1	1:A:836:ASN:N	2.88	0.42
1:A:910:LEU:CD2	1:A:951:ILE:HG21	2.50	0.42
1:B:945:GLY:HA2	1:B:959:ILE:HG12	2.01	0.42
1:A:878:ASN:O	1:A:879:TRP:CD1	2.73	0.42
1:A:878:ASN:N	1:A:878:ASN:OD1	2.43	0.42
1:B:923:GLU:CD	1:B:927:ARG:HH12	2.23	0.41
1:A:951:ILE:HG12	1:A:956:VAL:HG21	2.02	0.41
1:A:791:PHE:CZ	1:A:793:PHE:O	2.73	0.41
1:B:785:VAL:HG12	1:B:848:TYR:HA	2.03	0.41
1:B:857:ARG:NH1	1:B:857:ARG:CG	2.83	0.41
1:A:1015:GLU:C	1:A:1016:TYR:CD1	2.94	0.41
1:A:939:VAL:HG23	1:A:995:LEU:HD21	2.03	0.41
1:B:920:LEU:HD12	1:B:923:GLU:OE2	2.20	0.40
1:B:906:GLU:O	1:B:913:TYR:HE1	2.04	0.40
1:B:994:THR:HG22	1:B:995:LEU:O	2.21	0.40
1:A:895:GLU:OE1	1:A:896:SER:HB3	2.21	0.40
1:A:976:ILE:HG12	1:A:991:TYR:CE1	2.56	0.40
1:B:916:GLY:O	1:B:929:VAL:HG13	2.21	0.40
1:A:818:PHE:CZ	1:A:830:VAL:HG21	2.56	0.40
1:B:819:GLN:HG2	1:B:821:VAL:HG12	2.02	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:894:ILE:HD12	1:B:894:ILE:N	2.36	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1023:GLU:OE1	4:B:2410:IUM:O2[2_555]	1.67	0.53
1:A:985:THR:OG1	4:B:2410:IUM:U[2_555]	1.87	0.33
1:A:792:GLU:OE2	1:B:805:ARG:NH1[4_545]	2.08	0.12

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	231/253 (91%)	200 (87%)	28 (12%)	3 (1%)	15 55
1	B	233/253 (92%)	195 (84%)	31 (13%)	7 (3%)	5 35
All	All	464/506 (92%)	395 (85%)	59 (13%)	10 (2%)	8 43

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	911	PRO
1	A	797	PRO
1	A	1014	GLY
1	B	799	ASP
1	B	809	ASN
1	B	884	GLY
1	B	914	PRO
1	A	945	GLY
1	B	855	PRO
1	B	853	PRO

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	208/225 (92%)	174 (84%)	34 (16%)	3 14
1	B	210/225 (93%)	163 (78%)	47 (22%)	1 5
All	All	418/450 (93%)	337 (81%)	81 (19%)	2 8

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	789	ASP
1	A	798	CYS
1	A	799	ASP
1	A	811	THR
1	A	813	LEU
1	A	821	VAL
1	A	833	THR
1	A	838	ASP
1	A	840	LEU
1	A	844	VAL
1	A	846	ARG
1	A	856	HIS
1	A	870	LEU
1	A	878	ASN
1	A	903	GLN
1	A	915	ILE
1	A	920	LEU
1	A	927	ARG
1	A	930	ASP
1	A	933	SER
1	A	936	ARG
1	A	941	ILE
1	A	947	LEU
1	A	948	LYS
1	A	953	LYS
1	A	954	THR
1	A	971	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	973	TYR
1	A	976	ILE
1	A	978	SER
1	A	994	THR
1	A	1012	LEU
1	A	1013	LYS
1	A	1022	LEU
1	B	785	VAL
1	B	787	MET
1	B	790	ASN
1	B	792	GLU
1	B	803	ILE
1	B	804	VAL
1	B	805	ARG
1	B	810	THR
1	B	811	THR
1	B	813	LEU
1	B	833	THR
1	B	840	LEU
1	B	843	THR
1	B	844	VAL
1	B	850	ARG
1	B	852	LYS
1	B	857	ARG
1	B	872	ASN
1	B	880	THR
1	B	888	LEU
1	B	890	LYS
1	B	895	GLU
1	B	912	HIS
1	B	915	ILE
1	B	924	THR
1	B	929	VAL
1	B	931	SER
1	B	937	GLU
1	B	939	VAL
1	B	942	VAL
1	B	944	GLN
1	B	946	THR
1	B	947	LEU
1	B	949	CYS
1	B	951	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	954	THR
1	B	956	VAL
1	B	965	LEU
1	B	970	CYS
1	B	973	TYR
1	B	975	ILE
1	B	983	GLU
1	B	985	THR
1	B	989	PHE
1	B	994	THR
1	B	1007	PHE
1	B	1022	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	790	ASN
1	B	856	HIS
1	B	871	HIS
1	B	872	ASN
1	B	886	GLN
1	B	1008	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

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	$\#\|Z\| > 2$
2	NAG	A	2401	1,2	14,14,15	0.47	0	15,19,21	2.13	6 (40%)
2	NAG	A	2402	2	14,14,15	0.70	0	15,19,21	1.34	1 (6%)
2	NAG	A	2403	1,2	14,14,15	0.60	0	15,19,21	2.21	6 (40%)
2	NAG	A	2404	2	14,14,15	0.75	0	15,19,21	0.99	1 (6%)
2	NAG	A	2405	1,2	14,14,15	0.46	0	15,19,21	1.53	3 (20%)
2	NAG	A	2406	2	14,14,15	0.57	0	15,19,21	1.55	1 (6%)
2	NAG	A	2407	1,2	14,14,15	0.58	0	15,19,21	1.45	4 (26%)
2	NAG	A	2408	2	14,14,15	0.41	0	15,19,21	2.66	1 (6%)
2	NAG	B	2401	1,2	14,14,15	0.46	0	15,19,21	2.41	6 (40%)
2	NAG	B	2402	2	14,14,15	0.39	0	15,19,21	2.55	2 (13%)
2	NAG	B	2403	1,2	14,14,15	0.47	0	15,19,21	1.65	4 (26%)
2	NAG	B	2404	2	14,14,15	0.71	0	15,19,21	1.15	1 (6%)
2	NAG	B	2405	1,2	14,14,15	0.60	0	15,19,21	1.70	2 (13%)
2	NAG	B	2406	2	14,14,15	0.55	0	15,19,21	1.31	2 (13%)
2	NAG	B	2407	1,2	14,14,15	0.54	0	15,19,21	1.77	6 (40%)
2	NAG	B	2408	2	14,14,15	0.47	0	15,19,21	2.76	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	NAG	A	2401	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	2402	2	-	0/6/23/26	0/1/1/1
2	NAG	A	2403	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	2404	2	-	0/6/23/26	0/1/1/1
2	NAG	A	2405	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	2406	2	-	0/6/23/26	0/1/1/1
2	NAG	A	2407	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	2408	2	-	0/6/23/26	0/1/1/1
2	NAG	B	2401	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	2402	2	-	0/6/23/26	0/1/1/1
2	NAG	B	2403	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	2404	2	-	0/6/23/26	0/1/1/1
2	NAG	B	2405	1,2	-	0/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	2406	2	-	0/6/23/26	0/1/1/1
2	NAG	B	2407	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	2408	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	2402	NAG	C4-C3-C2	-3.71	105.46	111.23
2	B	2407	NAG	C3-C4-C5	-2.94	105.07	110.20
2	B	2401	NAG	O7-C7-C8	-2.87	116.80	122.06
2	B	2404	NAG	C3-C4-C5	-2.59	105.68	110.20
2	A	2401	NAG	C4-C3-C2	-2.49	107.36	111.23
2	A	2407	NAG	O7-C7-C8	-2.48	117.50	122.06
2	A	2401	NAG	O7-C7-C8	-2.43	117.61	122.06
2	A	2403	NAG	O7-C7-C8	-2.40	117.66	122.06
2	B	2407	NAG	O7-C7-C8	-2.39	117.68	122.06
2	B	2406	NAG	C3-C2-N2	-2.35	104.94	110.56
2	B	2403	NAG	O7-C7-C8	-2.23	117.98	122.06
2	B	2401	NAG	C4-C3-C2	-2.17	107.86	111.23
2	A	2405	NAG	C3-C4-C5	-2.17	106.41	110.20
2	A	2407	NAG	C1-O5-C5	2.03	114.82	112.25
2	A	2401	NAG	C3-C2-N2	2.04	115.44	110.56
2	A	2401	NAG	C2-N2-C7	2.04	125.66	123.04
2	B	2405	NAG	C2-N2-C7	2.07	125.69	123.04
2	B	2407	NAG	O4-C4-C3	2.10	115.07	110.34
2	B	2403	NAG	C2-N2-C7	2.19	125.85	123.04
2	A	2405	NAG	C2-N2-C7	2.24	125.92	123.04
2	B	2407	NAG	C2-N2-C7	2.26	125.95	123.04
2	A	2403	NAG	C2-N2-C7	2.41	126.13	123.04
2	A	2403	NAG	C3-C4-C5	2.44	114.46	110.20
2	B	2403	NAG	C8-C7-N2	2.63	121.14	116.11
2	A	2407	NAG	C2-N2-C7	2.64	126.43	123.04
2	A	2404	NAG	C4-C3-C2	2.65	115.36	111.23
2	B	2401	NAG	C3-C4-C5	2.65	114.83	110.20
2	B	2407	NAG	C8-C7-N2	2.72	121.31	116.11
2	A	2403	NAG	C4-C3-C2	2.72	115.47	111.23
2	B	2407	NAG	C1-O5-C5	2.80	115.80	112.25
2	A	2401	NAG	C8-C7-N2	2.88	121.62	116.11
2	A	2405	NAG	C1-O5-C5	2.89	115.92	112.25
2	A	2407	NAG	C8-C7-N2	2.93	121.71	116.11
2	B	2406	NAG	C4-C3-C2	2.99	115.88	111.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	2403	NAG	C8-C7-N2	3.06	121.96	116.11
2	B	2401	NAG	C2-N2-C7	3.44	127.46	123.04
2	B	2401	NAG	C8-C7-N2	3.84	123.45	116.11
2	A	2402	NAG	C1-O5-C5	3.89	117.19	112.25
2	B	2403	NAG	C1-O5-C5	4.47	117.92	112.25
2	A	2406	NAG	C1-O5-C5	5.03	118.63	112.25
2	B	2405	NAG	C4-C3-C2	5.14	119.22	111.23
2	A	2401	NAG	C1-O5-C5	5.57	119.31	112.25
2	B	2401	NAG	C1-O5-C5	5.58	119.33	112.25
2	A	2403	NAG	C1-O5-C5	5.78	119.58	112.25
2	B	2402	NAG	C1-O5-C5	8.64	123.21	112.25
2	A	2408	NAG	C1-O5-C5	9.98	124.91	112.25
2	B	2408	NAG	C1-O5-C5	10.22	125.22	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2401	NAG	1	0
2	B	2406	NAG	3	0

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	IUM	B	2410	1	0,2,2	0.00	-	0,1,1	0.00	-
4	IUM	B	2411	1,4	0,2,2	0.00	-	0,1,1	0.00	-
4	IUM	B	2412	4	0,2,2	0.00	-	0,1,1	0.00	-
4	IUM	B	2413	1	0,2,2	0.00	-	0,1,1	0.00	-

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	IUM	B	2410	1	-	0/0/0/0	0/0/0/0
4	IUM	B	2411	1,4	-	0/0/0/0	0/0/0/0
4	IUM	B	2412	4	-	0/0/0/0	0/0/0/0
4	IUM	B	2413	1	-	0/0/0/0	0/0/0/0

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.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	2410	IUM	1	2
4	B	2411	IUM	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	235/253 (92%)	-0.07	1 (0%)	93	91	20, 36, 61, 83	0
1	B	237/253 (93%)	0.14	6 (2%)	61	52	19, 49, 87, 128	0
All	All	472/506 (93%)	0.04	7 (1%)	76	68	19, 43, 75, 128	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	944	GLN	3.4
1	B	834	SER	3.0
1	B	836	ASN	2.7
1	B	841	ALA	2.6
1	A	987	CYS	2.2
1	B	906	GLU	2.0
1	B	959	ILE	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

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
2	NAG	A	2405	14/15	0.73	0.34	2.18	92,105,118,130	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	NAG	B	2401	14/15	0.91	0.20	0.23	33,40,44,46	0
2	NAG	A	2403	14/15	0.82	0.20	-0.24	54,61,70,77	0
2	NAG	B	2403	14/15	0.92	0.18	-0.96	53,59,67,75	0
2	NAG	B	2402	14/15	0.83	0.26	-	55,61,67,70	0
2	NAG	A	2402	14/15	0.61	0.38	-	97,111,123,124	0
2	NAG	B	2407	14/15	0.85	0.43	-	83,95,113,132	0
2	NAG	B	2405	14/15	0.70	0.29	-	92,105,118,130	0
2	NAG	A	2407	14/15	0.69	0.33	-	94,108,130,140	0
2	NAG	B	2408	14/15	0.57	0.77	-	137,150,157,158	0
2	NAG	B	2406	14/15	0.68	0.40	-	136,143,145,146	0
2	NAG	A	2408	14/15	0.57	0.38	-	127,137,142,144	0
2	NAG	A	2406	14/15	0.53	0.52	-	136,143,145,146	0
2	NAG	A	2404	14/15	0.72	0.37	-	84,95,99,108	0
2	NAG	B	2404	14/15	0.71	0.30	-	82,90,101,104	0
2	NAG	A	2401	14/15	0.63	0.30	-	60,76,88,99	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, 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	IUM	B	2411	3/3	0.96	0.14	-1.13	56,56,68,93	3
3	CA	B	2409	1/1	0.94	0.18	-	30,30,30,30	0
4	IUM	B	2412	3/3	0.98	0.10	-	60,60,72,80	3
3	CA	A	2409	1/1	0.92	0.10	-	41,41,41,41	0
4	IUM	B	2413	3/3	0.81	0.28	-	63,63,65,116	3
3	CA	A	2410	1/1	0.97	0.10	-	14,14,14,14	0
4	IUM	B	2410	3/3	0.99	0.21	-	12,12,15,17	3
3	CA	A	2411	1/1	0.93	0.09	-	30,30,30,30	0

6.5 Other polymers (i)

There are no such residues in this entry.