Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:22 AM GMT

PDB ID	:	3ECQ
Title	:	Endo-alpha-N-acetylgalactosaminidase from Streptococcus pneumoniae: SeMet structure
Authors	:	Caines, M.E.C.; Zhu, H.; Vuckovic, M.; Strynadka, N.C.J.
Deposited on	:	2008-09-01
Resolution	:	2.90 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 ①) were used in the production of this report:

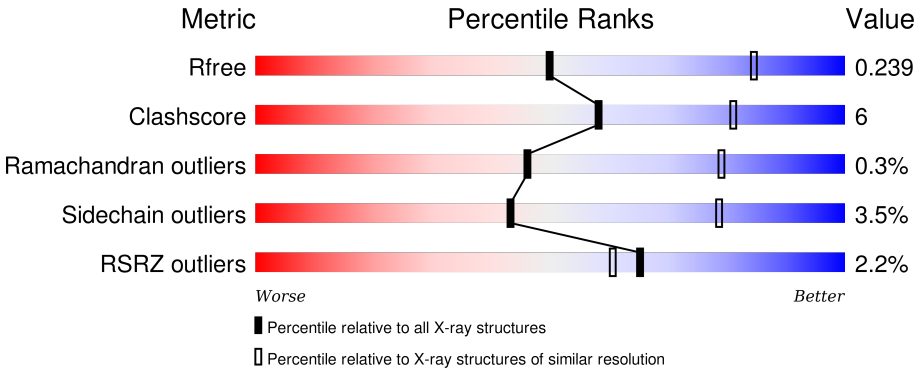
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.90 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	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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	1531	74% 13% 13%
1	B	1531	3% 74% 14% • 12%

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
4	GOL	A	2003	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 21372 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 Endo-alpha-N-acetylgalactosaminidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1336	Total	C	N	O	Se	0	1	0
			10586	6644	1831	2088	23			
1	B	1347	Total	C	N	O	Se	0	0	0
			10671	6695	1844	2108	24			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	37	GLY	-	EXPRESSION TAG	UNP Q8DR60
A	38	SER	-	EXPRESSION TAG	UNP Q8DR60
A	39	MSE	-	EXPRESSION TAG	UNP Q8DR60
B	37	GLY	-	EXPRESSION TAG	UNP Q8DR60
B	38	SER	-	EXPRESSION TAG	UNP Q8DR60
B	39	MSE	-	EXPRESSION TAG	UNP Q8DR60

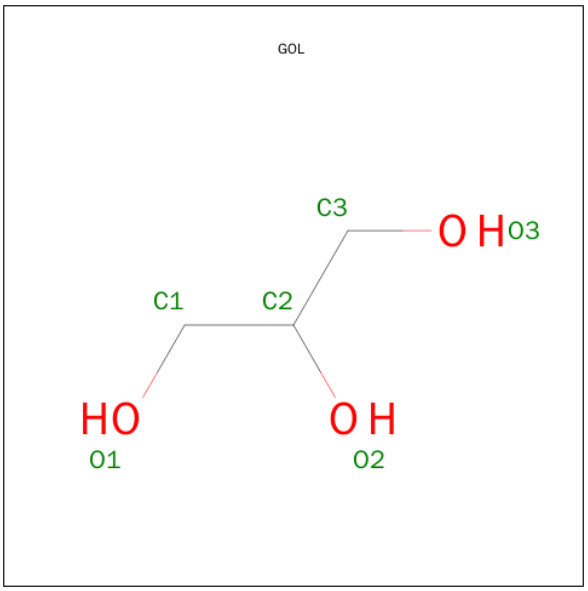
- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Ca	0	0
			2	2		
2	A	2	Total	Ca	0	0
			2	2		

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 5 is water.

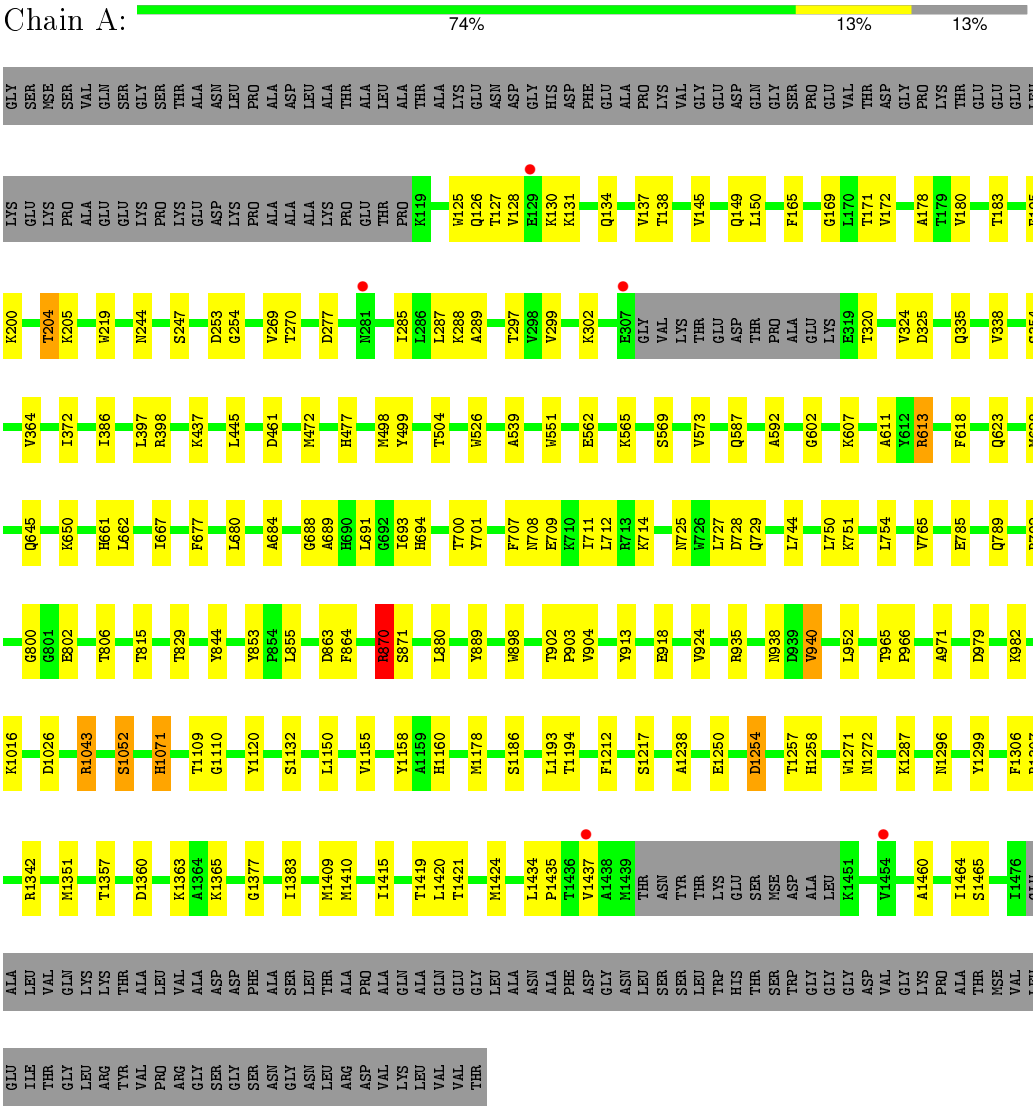
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	53	Total O 53 53	0	0
5	B	44	Total O 44 44	0	0

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.

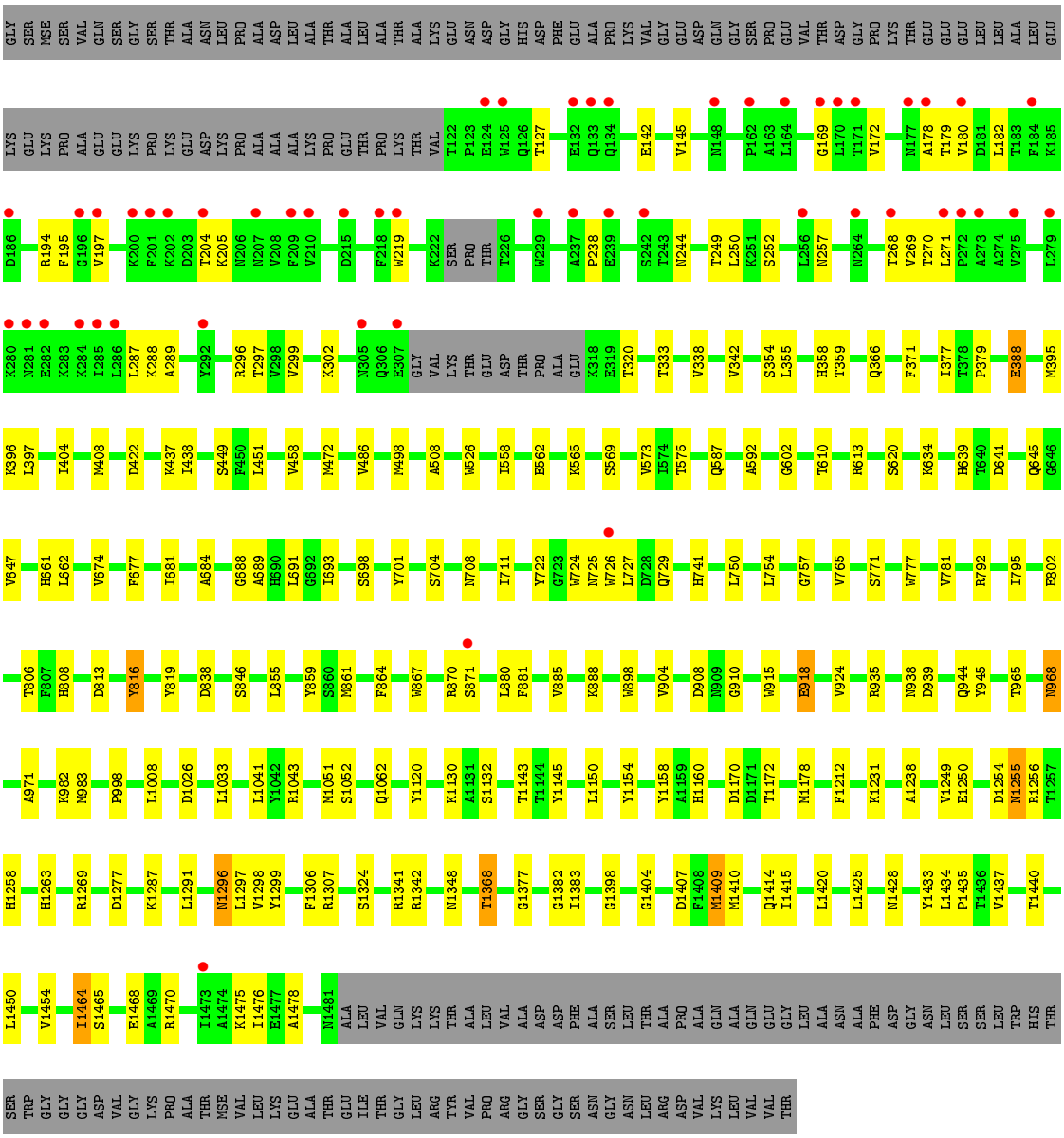
- Molecule 1: Endo-alpha-N-acetylgalactosaminidase

Chain A:



- Molecule 1: Endo-alpha-N-acetylgalactosaminidase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	210.61Å 158.21Å 112.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	112.51 – 2.90 112.44 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.4 (112.51-2.90) 99.4 (112.44-2.90)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	2.30 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.190 , 0.235 0.198 , 0.239	Depositor DCC
R_{free} test set	4164 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	56.7	Xtriage
Anisotropy	0.136	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 43.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	2 of 83382 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	21372	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.80% 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: GOL, CA, NA

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	0.52	0/10800	0.64	4/14588 (0.0%)
1	B	0.50	0/10880	0.62	1/14691 (0.0%)
All	All	0.51	0/21680	0.63	5/29279 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	607	LYS	CB-CA-C	-5.33	99.74	110.40
1	B	1307	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	A	870	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	A	1307	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	A	613	ARG	NE-CZ-NH1	5.07	122.83	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1377	GLY	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	B	1377	GLY	Peptide

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	10586	0	10172	123	0
1	B	10671	0	10253	124	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	6	0	8	0	0
4	B	6	0	8	0	0
5	A	53	0	0	0	0
5	B	44	0	0	0	0
All	All	21372	0	20441	247	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 6.

All (247) 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:472:MSE:HE2	1:A:498:MSE:HE1	1.31	1.09
1:B:472:MSE:HE2	1:B:498:MSE:HE1	1.10	1.07
1:A:1419:THR:O	1:A:1424:MSE:HE3	1.73	0.87
1:B:219:TRP:CZ2	1:B:269:VAL:HG21	2.14	0.81
1:B:795:ILE:HD11	1:B:808:HIS:CD2	2.19	0.78
1:B:855:LEU:HD21	1:B:935:ARG:HB2	1.68	0.76
1:B:219:TRP:CE2	1:B:269:VAL:HG21	2.20	0.75
1:A:324:VAL:HG21	1:A:364:VAL:CG1	2.18	0.74
1:B:472:MSE:CE	1:B:498:MSE:HE1	2.05	0.72
1:A:751:LYS:NZ	1:A:789:GLN:O	2.22	0.72
1:B:1454:VAL:HG22	1:B:1476:ILE:HD13	1.71	0.71
1:A:815:THR:HG22	1:A:844:TYR:OH	1.91	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:904:VAL:CG2	1:A:940:VAL:HG22	2.22	0.69
1:B:693:ILE:HD11	1:B:750:LEU:HD21	1.75	0.67
1:A:684:ALA:HB1	1:A:689:ALA:HB3	1.76	0.67
1:A:1383:ILE:HD13	1:A:1410:MSE:HE1	1.76	0.66
1:A:1313:THR:HG21	1:A:1420:LEU:HD13	1.75	0.66
1:A:918:GLU:O	1:A:935:ARG:NH1	2.28	0.66
1:A:324:VAL:HG21	1:A:364:VAL:HG13	1.77	0.66
1:A:219:TRP:NE1	1:A:269:VAL:HG21	2.12	0.65
1:B:688:GLY:HA3	1:B:971:ALA:HB1	1.79	0.63
1:A:219:TRP:CE2	1:A:269:VAL:HG21	2.33	0.63
1:B:968:ASN:N	1:B:968:ASN:HD22	1.97	0.63
1:A:855:LEU:HD21	1:A:935:ARG:HB2	1.81	0.62
1:B:195:PHE:CE1	1:B:299:VAL:HG21	2.34	0.62
1:A:461:ASP:OD2	1:A:539:ALA:HB2	2.00	0.61
1:A:870:ARG:HH11	1:A:870:ARG:HG3	1.65	0.61
1:B:498:MSE:HE3	1:B:526:TRP:HB2	1.83	0.60
1:B:498:MSE:HE3	1:B:526:TRP:CD1	2.35	0.60
1:A:1360:ASP:OD1	1:A:1365:LYS:NZ	2.34	0.60
1:A:792:ARG:HD2	1:A:806:THR:OG1	2.02	0.60
1:A:338:VAL:HG12	1:A:355:LEU:CD1	2.31	0.60
1:A:904:VAL:HG21	1:A:940:VAL:HG22	1.82	0.60
1:A:1193:LEU:HD23	1:A:1194:THR:N	2.15	0.60
1:A:338:VAL:HG12	1:A:355:LEU:HD11	1.83	0.60
1:A:145:VAL:HG11	1:A:302:LYS:HD3	1.83	0.59
1:B:968:ASN:H	1:B:968:ASN:ND2	2.01	0.59
1:B:864:PHE:HA	1:B:871:SER:HA	1.84	0.59
1:B:1420:LEU:HD11	1:B:1425:LEU:HG	1.85	0.59
1:B:968:ASN:HD22	1:B:968:ASN:H	1.51	0.58
1:A:708:ASN:O	1:A:711:ILE:HG22	2.03	0.58
1:B:792:ARG:HD2	1:B:806:THR:OG1	2.03	0.58
1:B:1249:VAL:HG11	1:B:1291:LEU:HD13	1.86	0.57
1:B:795:ILE:CD1	1:B:808:HIS:CD2	2.86	0.57
1:A:611:ALA:HB2	1:A:880:LEU:HD21	1.87	0.57
1:A:688:GLY:HA3	1:A:971:ALA:HB1	1.86	0.57
1:B:1383:ILE:HD13	1:B:1410:MSE:HE1	1.86	0.57
1:B:727:LEU:HD22	1:B:1258:HIS:CG	2.40	0.56
1:A:693:ILE:HD11	1:A:750:LEU:HD21	1.88	0.56
1:A:1460:ALA:HB1	1:A:1464:ILE:CD1	2.35	0.56
1:A:902:THR:HG22	1:A:903:PRO:O	2.06	0.56
1:A:1460:ALA:HB1	1:A:1464:ILE:HD11	1.86	0.56
1:B:145:VAL:HG11	1:B:302:LYS:HD3	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1383:ILE:CD1	1:A:1410:MSE:HE1	2.36	0.56
1:A:853:TYR:O	1:A:935:ARG:NH2	2.39	0.56
1:B:1383:ILE:CD1	1:B:1410:MSE:HE1	2.36	0.55
1:B:661:HIS:CD2	1:B:701:TYR:HE2	2.23	0.55
1:A:1193:LEU:HD23	1:A:1193:LEU:C	2.26	0.55
1:B:1008:LEU:HD21	1:B:1033:LEU:HD11	1.89	0.55
1:B:333:THR:HG22	1:B:342:VAL:HG22	1.89	0.54
1:B:898:TRP:CZ2	1:B:918:GLU:HG2	2.42	0.54
1:B:1212:PHE:CZ	1:B:1238:ALA:HB1	2.43	0.54
1:B:397:LEU:HD11	1:B:408:MSE:HE2	1.90	0.54
1:B:881:PHE:CD1	1:B:885:VAL:HG21	2.43	0.54
1:A:498:MSE:HE3	1:A:526:TRP:HB2	1.90	0.54
1:B:498:MSE:CE	1:B:802:GLU:HG3	2.38	0.54
1:B:661:HIS:CD2	1:B:701:TYR:CE2	2.96	0.54
1:A:815:THR:HG22	1:A:844:TYR:CZ	2.43	0.54
1:B:684:ALA:HB1	1:B:689:ALA:HB3	1.90	0.53
1:B:726:TRP:CZ3	1:B:1256:ARG:HD2	2.44	0.53
1:A:1212:PHE:CE2	1:A:1238:ALA:HB1	2.43	0.53
1:A:125:TRP:O	1:A:137:VAL:HG11	2.09	0.53
1:B:180:VAL:HG21	1:B:197:VAL:HG11	1.89	0.53
1:B:613:ARG:N	1:B:861:MSE:HE3	2.24	0.53
1:B:968:ASN:N	1:B:968:ASN:ND2	2.56	0.53
1:B:904:VAL:HG22	1:B:915:TRP:O	2.09	0.53
1:B:1434:LEU:N	1:B:1435:PRO:HD2	2.25	0.52
1:A:150:LEU:HD13	1:A:165:PHE:CG	2.44	0.52
1:A:195:PHE:CE1	1:A:299:VAL:HG21	2.45	0.52
1:B:634:LYS:HB3	1:B:1051:MSE:HE2	1.92	0.52
1:A:1287:LYS:HE3	1:A:1409:MSE:HE3	1.92	0.51
1:A:197:VAL:HG22	1:A:287:LEU:HD22	1.92	0.51
1:A:1464:ILE:HG22	1:A:1465:SER:O	2.09	0.51
1:B:1298:VAL:HG12	1:B:1299:TYR:CD2	2.46	0.51
1:B:613:ARG:NH2	1:B:645:GLN:OE1	2.41	0.51
1:B:182:LEU:HD22	1:B:287:LEU:HD21	1.93	0.51
1:A:1001:TRP:CD2	1:A:1043:ARG:HD3	2.45	0.51
1:A:725:ASN:HB2	1:A:729:GLN:OE1	2.11	0.51
1:A:661:HIS:CD2	1:A:701:TYR:HE2	2.29	0.50
1:A:904:VAL:HG11	1:A:940:VAL:CG1	2.41	0.50
1:B:602:GLY:HA3	1:B:792:ARG:HG3	1.93	0.50
1:B:1475:LYS:O	1:B:1478:ALA:HB3	2.11	0.50
1:A:700:THR:HG23	1:A:707:PHE:HD2	1.76	0.50
1:A:709:GLU:HA	1:A:712:LEU:HD12	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:GLN:HA	1:A:137:VAL:HG21	1.94	0.49
1:A:573:VAL:HG21	1:A:592:ALA:HB1	1.93	0.49
1:B:377:ILE:HD11	1:B:404:ILE:HD13	1.95	0.49
1:A:650:LYS:HE2	1:A:694:HIS:ND1	2.27	0.49
1:A:727:LEU:HD22	1:A:1258:HIS:ND1	2.28	0.49
1:B:204:THR:HG23	1:B:205:LYS:HG3	1.94	0.49
1:A:904:VAL:HG11	1:A:940:VAL:HG13	1.94	0.49
1:A:338:VAL:CG1	1:A:355:LEU:HD11	2.41	0.49
1:A:795:ILE:HD11	1:A:800:GLY:O	2.12	0.49
1:A:197:VAL:HG22	1:A:287:LEU:CD2	2.43	0.48
1:B:1296:ASN:HD22	1:B:1297:LEU:H	1.61	0.48
1:A:634:LYS:NZ	1:A:1052:SER:O	2.46	0.48
1:B:708:ASN:O	1:B:711:ILE:HG22	2.13	0.48
1:B:1368:THR:HG22	1:B:1428:ASN:HD21	1.78	0.48
1:B:647:VAL:HB	1:B:691:LEU:HD23	1.94	0.48
1:B:1341:ARG:O	1:B:1342:ARG:C	2.51	0.48
1:B:1212:PHE:CE2	1:B:1238:ALA:HB1	2.48	0.48
1:A:1158:TYR:CE2	1:A:1160:HIS:HB2	2.48	0.48
1:A:979:ASP:N	1:A:979:ASP:OD1	2.47	0.48
1:B:371:PHE:HB2	1:B:449:SER:HB3	1.94	0.48
1:A:498:MSE:CE	1:A:802:GLU:HG3	2.44	0.48
1:B:354:SER:HB3	1:B:359:THR:HG22	1.96	0.48
1:A:1212:PHE:CZ	1:A:1238:ALA:HB1	2.49	0.47
1:A:587:GLN:OE1	1:A:898:TRP:N	2.44	0.47
1:B:558:ILE:HD12	1:B:741:HIS:CE1	2.49	0.47
1:B:498:MSE:HE2	1:B:802:GLU:HG3	1.96	0.47
1:B:725:ASN:HA	1:B:729:GLN:HA	1.97	0.47
1:A:1306:PHE:CZ	1:A:1415:ILE:HG21	2.50	0.47
1:B:1231:LYS:HG2	1:B:1414:GLN:HG3	1.96	0.47
1:A:904:VAL:HG21	1:A:940:VAL:HG13	1.96	0.47
1:A:870:ARG:HH11	1:A:870:ARG:CG	2.26	0.47
1:A:613:ARG:NH2	1:A:645:GLN:OE1	2.46	0.47
1:B:498:MSE:CE	1:B:526:TRP:HB2	2.46	0.47
1:A:180:VAL:HG21	1:A:197:VAL:HG11	1.97	0.46
1:A:904:VAL:HG22	1:A:940:VAL:HG22	1.97	0.46
1:B:1269:ARG:HG3	1:B:1277:ASP:OD1	2.16	0.46
1:B:379:PRO:HG2	1:B:395:MSE:HE2	1.98	0.46
1:B:867:TRP:O	1:B:870:ARG:HB2	2.15	0.46
1:A:178:ALA:HB1	1:A:199:LEU:HD23	1.97	0.46
1:A:254:GLY:O	1:A:270:THR:HA	2.16	0.46
1:A:864:PHE:HA	1:A:871:SER:HA	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:680:LEU:HG	1:A:691:LEU:HD11	1.96	0.46
1:B:1306:PHE:CZ	1:B:1415:ILE:HG21	2.50	0.46
1:B:1130:LYS:HD2	1:B:1145:TYR:CD1	2.51	0.46
1:B:172:VAL:HG22	1:B:178:ALA:HB2	1.97	0.46
1:B:1464:ILE:HG23	1:B:1468:GLU:HB2	1.98	0.46
1:B:610:THR:O	1:B:859:TYR:HE1	1.99	0.46
1:A:744:LEU:HD13	1:A:785:GLU:HG2	1.97	0.46
1:B:179:THR:HG21	1:B:819:TYR:CE1	2.50	0.46
1:B:145:VAL:HG11	1:B:302:LYS:CD	2.45	0.45
1:B:677:PHE:CD2	1:B:754:LEU:HD11	2.52	0.45
1:A:289:ALA:HB1	1:A:297:THR:HB	1.97	0.45
1:B:498:MSE:HE3	1:B:526:TRP:CG	2.50	0.45
1:A:904:VAL:CG2	1:A:940:VAL:CG2	2.93	0.45
1:B:1287:LYS:HD2	1:B:1409:MSE:HE3	1.99	0.45
1:B:1154:TYR:O	1:B:1255:ASN:ND2	2.49	0.45
1:A:1357:THR:HG22	1:A:1365:LYS:HD2	1.99	0.45
1:B:1368:THR:HG22	1:B:1428:ASN:ND2	2.31	0.45
1:B:681:ILE:HG21	1:B:757:GLY:HA3	1.99	0.45
1:B:437:LYS:HG3	1:B:438:ILE:N	2.30	0.45
1:B:1249:VAL:HG13	1:B:1250:GLU:HG3	1.99	0.45
1:A:1437:VAL:O	1:A:1437:VAL:CG1	2.65	0.45
1:A:1120:TYR:HA	1:A:1178:MSE:O	2.16	0.45
1:A:498:MSE:HE3	1:A:526:TRP:CD1	2.52	0.45
1:B:498:MSE:HE3	1:B:526:TRP:CB	2.47	0.45
1:B:145:VAL:CG1	1:B:302:LYS:CD	2.95	0.45
1:A:499:TYR:CE2	1:A:829:THR:HG23	2.52	0.45
1:B:704:SER:O	1:B:1263:HIS:ND1	2.51	0.44
1:A:1331:VAL:HG11	1:A:1351:MSE:HE2	1.99	0.44
1:B:338:VAL:O	1:B:355:LEU:HD12	2.17	0.44
1:B:1382:GLY:C	1:B:1383:ILE:HD12	2.38	0.44
1:B:677:PHE:CE2	1:B:754:LEU:HD11	2.52	0.44
1:B:722:TYR:CD2	1:B:1398:GLY:HA3	2.53	0.44
1:A:360:LEU:HD21	1:A:504:THR:HG23	1.99	0.44
1:A:904:VAL:HG22	1:A:940:VAL:CG2	2.48	0.44
1:A:727:LEU:HD22	1:A:1258:HIS:CG	2.51	0.44
1:A:138:THR:HG23	1:A:149:GLN:HB3	1.98	0.44
1:B:1158:TYR:CE2	1:B:1160:HIS:HB2	2.52	0.44
1:A:1299:TYR:OH	1:A:1410:MSE:HE3	2.18	0.44
1:A:618:PHE:CE2	1:A:1254:ASP:HB3	2.53	0.44
1:B:838:ASP:OD2	1:B:888:LYS:NZ	2.49	0.44
1:B:777:TRP:O	1:B:781:VAL:HG23	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:354:SER:HA	1:B:358:HIS:O	2.18	0.44
1:B:1170:ASP:O	1:B:1172:THR:HG23	2.18	0.44
1:A:641:ASP:O	1:A:982:LYS:NZ	2.51	0.44
1:A:667:ILE:N	1:A:667:ILE:HD12	2.32	0.44
1:A:1424:MSE:HE2	1:A:1424:MSE:HB2	2.00	0.43
1:A:372:ILE:HG12	1:A:397:LEU:HD13	2.00	0.43
1:A:1271:TRP:CE3	1:A:1272:ASN:HB2	2.53	0.43
1:A:169:GLY:O	1:A:171:THR:HG22	2.17	0.43
1:A:172:VAL:HG21	1:A:200:LYS:HG2	2.01	0.43
1:A:324:VAL:HG21	1:A:364:VAL:HG12	1.97	0.43
1:B:587:GLN:NE2	1:B:898:TRP:O	2.45	0.43
1:B:458:VAL:CG1	1:B:486:VAL:HG21	2.48	0.43
1:B:1041:LEU:HD12	1:B:1041:LEU:N	2.33	0.43
1:B:169:GLY:C	1:B:910:GLY:HA2	2.39	0.43
1:B:145:VAL:CG1	1:B:302:LYS:HD2	2.49	0.43
1:A:1109:THR:CG2	1:A:1110:GLY:N	2.81	0.43
1:A:204:THR:HG23	1:A:205:LYS:HG3	1.99	0.43
1:B:698:SER:HA	1:B:771:SER:HB3	2.00	0.43
1:A:677:PHE:CD2	1:A:754:LEU:HD21	2.54	0.42
1:B:508:ALA:O	1:B:575:THR:HG22	2.19	0.42
1:A:661:HIS:CD2	1:A:701:TYR:CE2	3.07	0.42
1:B:1464:ILE:HG22	1:B:1465:SER:O	2.19	0.42
1:B:195:PHE:CD1	1:B:299:VAL:HG11	2.55	0.42
1:A:372:ILE:HG23	1:A:445:LEU:CD1	2.50	0.42
1:A:324:VAL:CG1	1:A:325:ASP:N	2.83	0.42
1:A:1257:THR:HG21	1:A:1299:TYR:CD2	2.55	0.42
1:B:727:LEU:HD22	1:B:1258:HIS:ND1	2.35	0.42
1:B:1120:TYR:HA	1:B:1178:MSE:O	2.19	0.42
1:B:289:ALA:HB1	1:B:297:THR:HB	2.01	0.42
1:A:171:THR:CA	1:A:285:ILE:HD12	2.50	0.42
1:B:813:ASP:OD1	1:B:813:ASP:C	2.56	0.42
1:A:623:GLN:HE21	1:A:1155:VAL:CG1	2.33	0.42
1:A:1001:TRP:CE2	1:A:1043:ARG:HD3	2.55	0.42
1:B:377:ILE:HD11	1:B:404:ILE:CD1	2.50	0.42
1:B:983:MSE:HE1	1:B:998:PRO:CD	2.50	0.42
1:A:1383:ILE:CD1	1:A:1410:MSE:CE	2.98	0.41
1:A:130:LYS:O	1:A:134:GLN:HG3	2.20	0.41
1:B:939:ASP:O	1:B:945:TYR:HB2	2.20	0.41
1:A:889:TYR:OH	1:A:952:LEU:HD22	2.19	0.41
1:B:238:PRO:HB3	1:B:244:ASN:HD21	1.85	0.41
1:A:1421:THR:O	1:A:1424:MSE:HB3	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:573:VAL:HG21	1:B:592:ALA:HB1	2.01	0.41
1:A:1299:TYR:HE1	1:A:1383:ILE:HD13	1.85	0.41
1:B:1298:VAL:HG12	1:B:1299:TYR:HD2	1.84	0.41
1:A:1212:PHE:N	1:A:1212:PHE:CD1	2.88	0.41
1:B:1404:GLY:HA2	1:B:1407:ASP:OD2	2.20	0.41
1:B:498:MSE:CE	1:B:526:TRP:CD1	3.04	0.41
1:B:1450:LEU:O	1:B:1454:VAL:HG23	2.20	0.41
1:A:562:GLU:OE2	1:A:565:LYS:NZ	2.48	0.41
1:A:602:GLY:HA3	1:A:792:ARG:HG3	2.02	0.41
1:A:477:HIS:CE1	1:A:913:TYR:CE1	3.09	0.41
1:B:250:LEU:HD11	1:B:271:LEU:CD1	2.51	0.41
1:A:150:LEU:HD22	1:A:165:PHE:CD2	2.55	0.41
1:A:650:LYS:HA	1:A:694:HIS:HB3	2.03	0.41
1:A:965:THR:HG22	1:A:966:PRO:O	2.21	0.41
1:B:257:ASN:OD1	1:B:268:THR:HG23	2.21	0.41
1:A:1434:LEU:N	1:A:1435:PRO:HD2	2.36	0.41
1:A:498:MSE:HE1	1:A:802:GLU:HG3	2.02	0.41
1:A:1383:ILE:HD13	1:A:1410:MSE:CE	2.49	0.41
1:A:183:THR:HA	1:A:244:ASN:O	2.21	0.41
1:B:219:TRP:NE1	1:B:269:VAL:HG21	2.36	0.40
1:A:1071[B]:HIS:CD2	1:A:1071[B]:HIS:H	2.39	0.40
1:A:127:THR:HG23	1:A:128:VAL:O	2.21	0.40
1:B:562:GLU:OE2	1:B:565:LYS:NZ	2.45	0.40
1:B:422:ASP:OD1	1:B:569:SER:OG	2.29	0.40
1:B:1383:ILE:CD1	1:B:1410:MSE:CE	2.99	0.40
1:B:726:TRP:CH2	1:B:1256:ARG:HD2	2.57	0.40
1:B:641:ASP:O	1:B:982:LYS:NZ	2.54	0.40
1:B:1433:TYR:O	1:B:1437:VAL:HG23	2.21	0.40
1:B:1212:PHE:CD1	1:B:1212:PHE:N	2.90	0.40
1:B:388:GLU:N	1:B:388:GLU:OE2	2.53	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	1331/1531 (87%)	1272 (96%)	55 (4%)	4 (0%)	46 79
1	B	1341/1531 (88%)	1276 (95%)	60 (4%)	5 (0%)	39 74
All	All	2672/3062 (87%)	2548 (95%)	115 (4%)	9 (0%)	46 79

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1254	ASP
1	B	1254	ASP
1	B	662	LEU
1	B	816	TYR
1	A	662	LEU
1	A	551	TRP
1	B	1062	GLN
1	B	765	VAL
1	A	765	VAL

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	1132/1257 (90%)	1094 (97%)	38 (3%)	44 79
1	B	1140/1257 (91%)	1098 (96%)	42 (4%)	41 77
All	All	2272/2514 (90%)	2192 (96%)	80 (4%)	43 78

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	131	LYS
1	A	204	THR
1	A	247	SER
1	A	253	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	277	ASP
1	A	288	LYS
1	A	320	THR
1	A	335	GLN
1	A	354	SER
1	A	359	THR
1	A	386	ILE
1	A	398	ARG
1	A	437	LYS
1	A	569	SER
1	A	628	MSE
1	A	714	LYS
1	A	728	ASP
1	A	797	TRP
1	A	863	ASP
1	A	870	ARG
1	A	924	VAL
1	A	938	ASN
1	A	940	VAL
1	A	989	GLN
1	A	1016	LYS
1	A	1026	ASP
1	A	1043	ARG
1	A	1052	SER
1	A	1071[A]	HIS
1	A	1071[B]	HIS
1	A	1132	SER
1	A	1150	LEU
1	A	1186	SER
1	A	1217	SER
1	A	1250	GLU
1	A	1296	ASN
1	A	1342	ARG
1	A	1363	LYS
1	B	127	THR
1	B	142	GLU
1	B	194	ARG
1	B	249	THR
1	B	252	SER
1	B	270	THR
1	B	288	LYS
1	B	296	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	320	THR
1	B	366	GLN
1	B	388	GLU
1	B	396	LYS
1	B	451	LEU
1	B	620	SER
1	B	639	HIS
1	B	674	VAL
1	B	724	TRP
1	B	816	TYR
1	B	846	SER
1	B	880	LEU
1	B	908	ASP
1	B	918	GLU
1	B	924	VAL
1	B	938	ASN
1	B	944	GLN
1	B	965	THR
1	B	968	ASN
1	B	1026	ASP
1	B	1043	ARG
1	B	1052	SER
1	B	1132	SER
1	B	1143	THR
1	B	1150	LEU
1	B	1255	ASN
1	B	1296	ASN
1	B	1324	SER
1	B	1348	ASN
1	B	1368	THR
1	B	1409	MSE
1	B	1440	THR
1	B	1464	ILE
1	B	1470	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	413	GLN
1	A	787	ASN
1	A	821	ASN
1	A	909	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1296	ASN
1	B	148	ASN
1	B	175	ASN
1	B	413	GLN
1	B	657	HIS
1	B	661	HIS
1	B	694	HIS
1	B	787	ASN
1	B	953	ASN
1	B	968	ASN
1	B	1296	ASN
1	B	1300	GLN
1	B	1428	ASN
1	B	1432	ASN
1	B	1456	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 6 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	GOL	A	2003	-	5,5,5	0.40	0	5,5,5	0.56	0
4	GOL	B	2003	-	5,5,5	0.41	0	5,5,5	0.33	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	GOL	A	2003	-	-	0/4/4/4	0/0/0/0
4	GOL	B	2003	-	-	0/4/4/4	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.

No monomer is involved in short contacts.

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	1313/1531 (85%)	0.02	5 (0%) 93 92	29, 49, 83, 128	0
1	B	1323/1531 (86%)	0.23	52 (3%) 43 36	32, 55, 103, 146	0
All	All	2636/3062 (86%)	0.13	57 (2%) 65 60	29, 52, 96, 146	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	281	ASN	5.6
1	B	271	LEU	5.0
1	B	202	LYS	4.2
1	B	275	VAL	4.0
1	B	282	GLU	3.9
1	B	197	VAL	3.8
1	B	229	TRP	3.8
1	B	170	LEU	3.6
1	B	210	VAL	3.5
1	B	169	GLY	3.3
1	B	133	GLN	3.2
1	B	239	GLU	3.2
1	B	285	ILE	3.1
1	B	215	ASP	3.1
1	B	201	PHE	3.1
1	B	286	LEU	3.0
1	B	280	LYS	2.9
1	B	726	TRP	2.9
1	B	200	LYS	2.9
1	B	1473	ILE	2.9
1	A	1454	VAL	2.9
1	B	268	THR	2.8
1	B	273	ALA	2.8
1	B	272	PRO	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	237	ALA	2.7
1	B	284	LYS	2.7
1	A	129	GLU	2.7
1	B	132	GLU	2.6
1	B	186	ASP	2.6
1	B	171	THR	2.5
1	B	184	PHE	2.5
1	B	124	GLU	2.5
1	B	148	ASN	2.5
1	B	264	ASN	2.4
1	B	256	LEU	2.4
1	B	209	PHE	2.4
1	B	162	PRO	2.4
1	B	219	TRP	2.4
1	B	134	GLN	2.3
1	B	177	ASN	2.3
1	A	307	GLU	2.3
1	B	218	PHE	2.3
1	B	164	LEU	2.3
1	A	1437	VAL	2.3
1	B	242	SER	2.2
1	B	307	GLU	2.2
1	B	871	SER	2.2
1	B	204	THR	2.2
1	B	207	ASN	2.2
1	B	292	TYR	2.2
1	B	125	TRP	2.2
1	B	196	GLY	2.1
1	B	279	LEU	2.1
1	B	180	VAL	2.0
1	A	281	ASN	2.0
1	B	305	ASN	2.0
1	B	178	ALA	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

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, 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
4	GOL	A	2003	6/6	0.73	0.30	2.23	81,82,82,82	0
2	CA	A	2000	1/1	0.84	0.15	-0.52	63,63,63,63	0
4	GOL	B	2003	6/6	0.79	0.21	-0.68	60,64,65,66	0
2	CA	B	2000	1/1	0.98	0.13	-0.75	54,54,54,54	0
2	CA	B	2001	1/1	0.99	0.14	-1.52	36,36,36,36	0
3	NA	B	2002	1/1	0.79	0.15	-1.61	41,41,41,41	0
3	NA	A	2002	1/1	0.95	0.14	-2.01	20,20,20,20	0
2	CA	A	2001	1/1	0.99	0.14	-2.08	42,42,42,42	0

6.5 Other polymers

There are no such residues in this entry.