Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 09:13 PM GMT

PDB ID	:	1O0V
Title	:	The crystal structure of IgE Fc reveals an asymmetrically bent conformation
Authors	:	Wan, T.; Beavil, R.L.; Fabiane, S.M.; Beavil, A.J.; Sohi, M.K.; Keown, M.; Young, R.J.; Henry, A.J.; Owens, R.J.; Gould, H.J.; Sutton, B.J.
Deposited on	:	2002-09-06
Resolution	:	2.60 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:

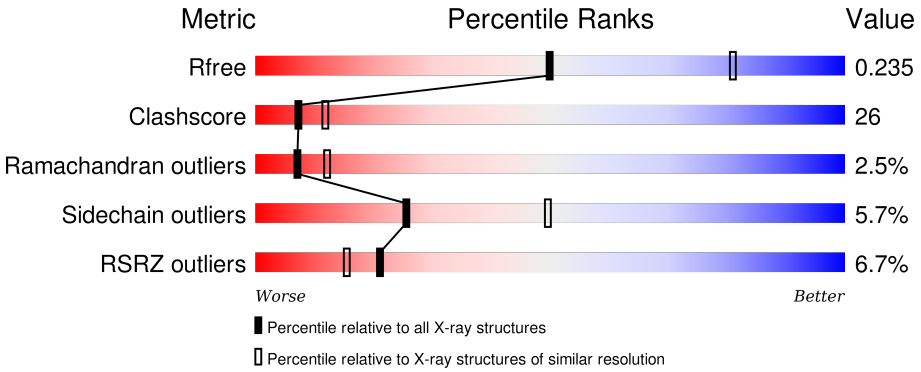
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

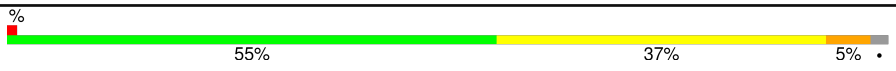
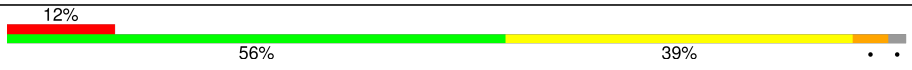
The reported resolution of this entry is 2.60 Å.

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	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	327	
1	B	327	

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	MAN	A	7	-	-	-	X
3	BMA	B	7	-	-	-	X
4	SO4	A	1012	-	-	-	X
5	GOL	A	1001	-	X	-	X
5	GOL	A	1002	-	X	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5436 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 Immunoglobulin heavy chain epsilon-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	319	Total	C	N	O	S	0	0	0
			2495	1557	443	484	11			
1	B	320	Total	C	N	O	S	0	0	0
			2499	1559	444	485	11			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	225	ALA	CYS	ENGINEERED	GB 386807
A	265	GLN	ASN	ENGINEERED	GB 386807
A	371	GLN	ASN	ENGINEERED	GB 386807
B	225	ALA	CYS	ENGINEERED	GB 386807
B	265	GLN	ASN	ENGINEERED	GB 386807
B	371	GLN	ASN	ENGINEERED	GB 386807

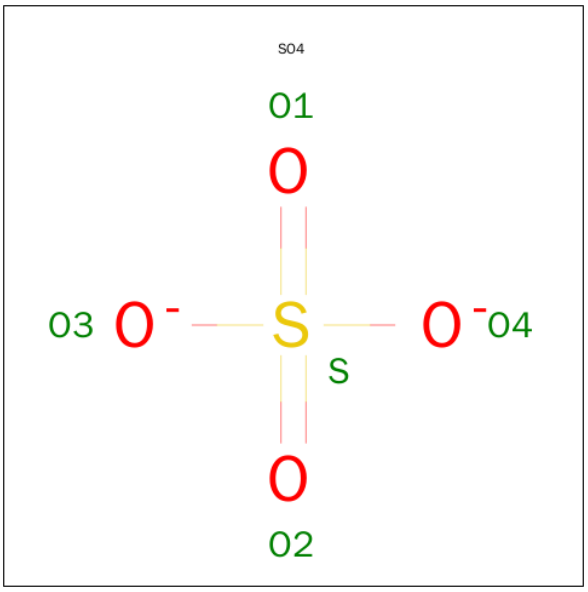
- Molecule 2 is a polymer of unknown type called SUGAR (7-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	7	Total	C	N	O	0	0
			83	46	2	35		

- Molecule 3 is a polymer of unknown type called NAG-NAG-MAN-MAN-MAN-MAN-MAN (7-MER).

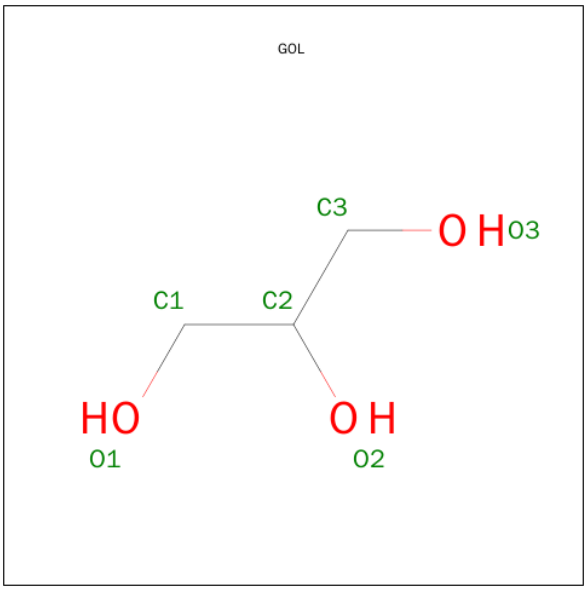
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	7	Total	C	N	O	0	0
			83	46	2	35		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 6 is water.

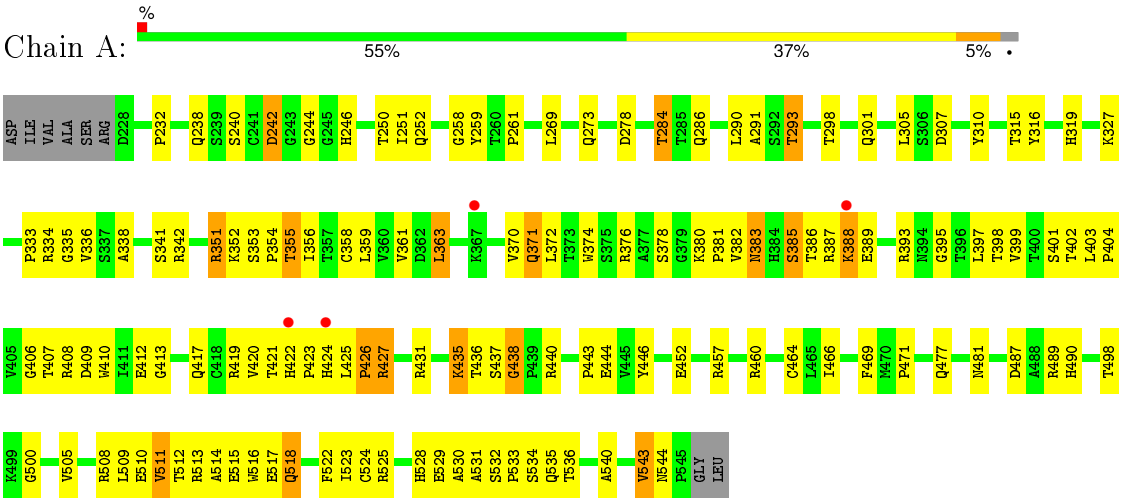
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	120	Total O 120 120	0	0
6	B	124	Total O 124 124	0	0

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.

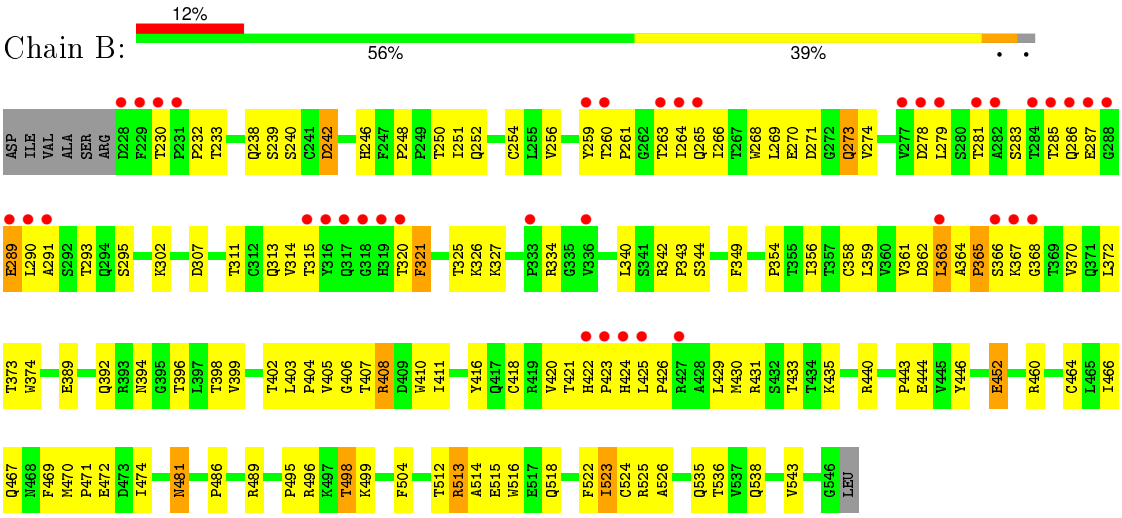
- Molecule 1: Immunoglobulin heavy chain epsilon-1

Chain A:



- Molecule 1: Immunoglobulin heavy chain epsilon-1

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	129.31Å 74.83Å 78.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	54.00 – 2.60 50.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.7 (54.00-2.60) 99.8 (50.00-2.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	4.61 (at 2.61Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.218 , 0.297 0.221 , 0.235	Depositor DCC
R_{free} test set	1230 reflections (5.11%)	DCC
Wilson B-factor (Å^2)	40.8	Xtriage
Anisotropy	0.100	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 65.3	EDS
Estimated twinning fraction	0.023 for -h,l,k	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 24083 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	5436	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.44% 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: MAN, GOL, BMA, NAG, SO4

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	0.42	0/2557	0.67	0/3486
1	B	0.41	0/2561	0.67	0/3491
All	All	0.42	0/5118	0.67	0/6977

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	2495	0	2434	135	0
1	B	2499	0	2437	135	0
2	A	83	0	70	4	0
3	B	83	0	70	3	0
4	A	20	0	0	1	0
5	A	12	0	8	0	0
6	A	120	0	0	2	0
6	B	124	0	0	4	0
All	All	5436	0	5019	264	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 26.

All (264) 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:284:THR:HB	1:A:293:THR:HB	1.34	1.06
1:B:523:ILE:HD13	1:B:538:GLN:HB2	1.39	1.03
1:B:422:HIS:HB3	1:B:425:LEU:HD13	1.41	1.01
1:B:315:THR:HG22	1:B:320:THR:HG22	1.48	0.94
1:B:232:PRO:HG3	1:B:259:TYR:HB2	1.54	0.89
1:A:351:ARG:HB2	1:A:351:ARG:NH1	1.89	0.88
1:A:356:ILE:HD11	1:A:403:LEU:HD23	1.55	0.85
1:B:523:ILE:CD1	1:B:538:GLN:HB2	2.08	0.84
1:A:403:LEU:HD12	1:A:404:PRO:HD2	1.61	0.83
1:A:351:ARG:HB2	1:A:351:ARG:HH11	1.43	0.82
1:A:238:GLN:HE21	1:B:240:SER:HA	1.44	0.81
1:A:342:ARG:HH12	1:B:302:LYS:HD3	1.48	0.79
1:A:427:ARG:HD2	1:A:427:ARG:H	1.46	0.79
1:A:452:GLU:OE2	1:A:457:ARG:HG3	1.82	0.79
1:A:408:ARG:O	1:A:412:GLU:HG2	1.85	0.77
1:A:370:VAL:HG11	1:A:399:VAL:HG21	1.67	0.77
1:A:242:ASP:HB2	1:A:246:HIS:HB2	1.67	0.76
1:A:334:ARG:HG3	1:A:334:ARG:HH11	1.50	0.76
1:B:307:ASP:OD1	1:B:327:LYS:HE3	1.86	0.75
1:A:238:GLN:NE2	1:B:240:SER:HA	2.02	0.75
1:A:252:GLN:HE21	1:A:298:THR:HG23	1.52	0.75
1:B:514:ALA:O	1:B:518:GLN:HG2	1.88	0.74
1:B:512:THR:OG1	1:B:515:GLU:HG3	1.87	0.74
1:B:269:LEU:HD23	1:B:274:VAL:HA	1.70	0.74
1:B:513:ARG:HB2	1:B:513:ARG:HH11	1.54	0.73
1:A:477:GLN:HE21	1:A:525:ARG:HD2	1.56	0.70
1:B:452:GLU:HG3	1:B:460:ARG:NH2	2.06	0.70
1:B:523:ILE:HD11	1:B:525:ARG:HB2	1.74	0.70
1:A:358:CYS:HB2	1:A:374:TRP:CH2	2.27	0.69
1:B:315:THR:HG22	1:B:320:THR:CG2	2.21	0.69
1:A:471:PRO:O	1:A:528:HIS:HE1	1.73	0.69
1:B:232:PRO:HG3	1:B:259:TYR:CB	2.23	0.69
1:B:523:ILE:HD12	1:B:524:CYS:N	2.08	0.68
1:A:422:HIS:HD2	1:A:423:PRO:HD2	1.56	0.68
1:A:305:LEU:HD23	1:A:327:LYS:HD3	1.75	0.68
1:B:408:ARG:HD3	1:B:408:ARG:H	1.58	0.68
1:A:422:HIS:CE1	1:A:424:HIS:HB3	2.30	0.67
1:A:341:SER:OG	2:A:7:MAN:H62	1.95	0.66
1:B:361:VAL:HG12	1:B:362:ASP:N	2.12	0.65
1:B:261:PRO:HD3	1:B:290:LEU:HA	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:GLN:HG3	1:A:290:LEU:O	1.98	0.64
1:A:513:ARG:O	1:A:517:GLU:HG3	1.99	0.63
1:A:389:GLU:HB2	1:A:397:LEU:HD11	1.81	0.63
1:B:407:THR:OG1	1:B:408:ARG:HD3	1.99	0.63
1:A:489:ARG:HG2	1:A:489:ARG:HH11	1.63	0.63
1:B:242:ASP:HB3	1:B:246:HIS:H	1.64	0.62
1:A:242:ASP:CB	1:A:246:HIS:H	2.12	0.62
1:B:344:SER:HB3	3:B:7:BMA:H4	1.80	0.62
1:B:326:LYS:HG2	1:B:327:LYS:N	2.15	0.61
1:B:499:LYS:O	1:B:499:LYS:HG3	2.00	0.61
1:A:242:ASP:HB3	1:A:246:HIS:H	1.66	0.61
1:A:334:ARG:HG3	1:A:334:ARG:NH1	2.13	0.60
1:B:523:ILE:C	1:B:523:ILE:HD12	2.22	0.60
1:A:534:SER:O	1:A:536:THR:HG23	2.02	0.60
1:A:376:ARG:HG3	1:A:382:VAL:CG1	2.31	0.60
1:A:336:VAL:HG22	1:A:363:LEU:HB3	1.84	0.59
1:B:269:LEU:HB2	1:B:311:THR:HB	1.84	0.59
1:B:230:THR:OG1	1:B:260:THR:HG23	2.03	0.59
1:A:315:THR:HA	1:A:319:HIS:O	2.03	0.59
1:B:422:HIS:O	1:B:425:LEU:HB2	2.03	0.59
1:A:386:THR:O	1:A:401:SER:HA	2.02	0.58
1:A:419:ARG:HG3	1:A:419:ARG:HH11	1.68	0.58
1:A:372:LEU:HD23	1:A:420:VAL:HB	1.84	0.58
1:A:422:HIS:HB3	1:A:425:LEU:HB2	1.85	0.58
1:A:376:ARG:HG3	1:A:382:VAL:HG12	1.86	0.58
1:B:321:PHE:N	1:B:321:PHE:CD2	2.69	0.57
1:A:511:VAL:HG21	1:A:522:PHE:CE2	2.39	0.57
1:A:413:GLY:HA2	1:A:435:LYS:HG2	1.84	0.57
1:A:386:THR:O	1:A:386:THR:HG23	2.03	0.57
1:B:343:PRO:HD3	1:B:356:ILE:HG22	1.85	0.57
1:B:359:LEU:CD1	1:B:398:THR:HG23	2.34	0.57
1:A:406:GLY:O	1:A:409:ASP:HB2	2.05	0.57
1:B:523:ILE:HD12	1:B:524:CYS:C	2.25	0.57
1:A:419:ARG:NH1	1:A:419:ARG:HG3	2.20	0.56
1:A:435:LYS:HB2	1:A:435:LYS:NZ	2.20	0.56
1:A:422:HIS:HB3	1:A:425:LEU:CB	2.34	0.56
1:A:528:HIS:CD2	1:A:530:ALA:H	2.24	0.56
1:B:279:LEU:N	1:B:279:LEU:HD12	2.21	0.56
1:B:285:THR:HG22	1:B:287:GLU:HG2	1.88	0.56
1:B:286:GLN:HB3	1:B:291:ALA:HA	1.87	0.56
1:A:543:VAL:CG2	1:A:544:ASN:N	2.68	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:362:ASP:HA	1:B:396:THR:HB	1.87	0.56
1:B:286:GLN:CB	1:B:291:ALA:HA	2.36	0.56
1:B:261:PRO:HB3	1:B:286:GLN:OE1	2.06	0.56
1:A:232:PRO:HG3	1:A:316:TYR:CB	2.35	0.55
1:A:284:THR:CB	1:A:293:THR:HB	2.22	0.55
1:A:351:ARG:HD2	1:A:353:SER:HB2	1.87	0.55
1:B:408:ARG:HD3	1:B:408:ARG:N	2.21	0.55
1:B:361:VAL:HG12	1:B:362:ASP:H	1.71	0.55
1:A:361:VAL:HG12	1:A:398:THR:HG23	1.87	0.55
1:A:269:LEU:HA	1:A:273:GLN:O	2.07	0.55
1:A:387:ARG:O	1:A:388:LYS:HB2	2.07	0.55
1:B:513:ARG:HA	1:B:516:TRP:CE2	2.42	0.55
1:A:374:TRP:CD1	1:A:385:SER:HB3	2.42	0.54
1:B:264:ILE:HD11	1:B:314:VAL:HG13	1.89	0.54
1:A:425:LEU:HG	1:A:426:PRO:HD2	1.88	0.54
1:B:498:THR:OG1	1:B:499:LYS:N	2.34	0.54
1:A:513:ARG:HA	1:A:516:TRP:CD2	2.42	0.54
1:A:531:ALA:O	1:A:535:GLN:HA	2.07	0.54
1:A:284:THR:HB	1:A:293:THR:CB	2.24	0.54
1:B:440:ARG:HA	1:B:470:MET:O	2.07	0.54
1:A:398:THR:HG21	2:A:2:NAG:H82	1.90	0.54
1:A:389:GLU:OE1	1:A:397:LEU:HD21	2.08	0.54
1:B:265:GLN:HB2	1:B:315:THR:OG1	2.08	0.53
1:B:370:VAL:CG2	1:B:420:VAL:HG13	2.38	0.53
1:B:269:LEU:CD2	1:B:274:VAL:HG22	2.38	0.53
1:A:514:ALA:O	1:A:518:GLN:HB2	2.08	0.53
1:B:349:PHE:CG	1:B:535:GLN:HG2	2.43	0.53
1:B:248:PRO:HD2	1:B:251:ILE:CD1	2.39	0.53
1:B:516:TRP:CD2	1:B:543:VAL:HG21	2.43	0.53
1:B:326:LYS:HG2	1:B:327:LYS:H	1.74	0.52
1:B:422:HIS:CB	1:B:425:LEU:HD13	2.29	0.52
1:B:232:PRO:CG	1:B:259:TYR:HB2	2.35	0.52
1:A:422:HIS:CD2	1:A:423:PRO:HD2	2.42	0.52
1:B:408:ARG:CD	1:B:408:ARG:H	2.22	0.52
1:A:523:ILE:HG12	1:A:540:ALA:HB2	1.91	0.52
1:B:286:GLN:HA	1:B:291:ALA:HA	1.91	0.52
1:B:370:VAL:CG1	1:B:399:VAL:HG21	2.40	0.52
1:B:389:GLU:HG2	1:B:399:VAL:HG22	1.92	0.51
1:B:392:GLN:HA	1:B:392:GLN:NE2	2.24	0.51
1:A:528:HIS:HD2	1:A:530:ALA:H	1.58	0.51
1:B:242:ASP:CB	1:B:246:HIS:H	2.23	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:354:PRO:HG2	1:A:407:THR:HA	1.91	0.51
1:B:256:VAL:O	1:B:256:VAL:HG13	2.11	0.51
1:A:446:TYR:O	1:A:464:CYS:HA	2.11	0.50
1:B:281:THR:HG23	1:B:281:THR:O	2.10	0.50
1:A:242:ASP:CB	1:A:246:HIS:HB2	2.40	0.50
4:A:1014:SO4:O4	1:B:496:ARG:HD2	2.12	0.50
1:B:270:GLU:HB3	1:B:273:GLN:NE2	2.27	0.50
1:B:422:HIS:ND1	1:B:423:PRO:HD2	2.26	0.49
1:A:371:GLN:O	1:A:420:VAL:HA	2.12	0.49
1:B:446:TYR:O	1:B:464:CYS:HA	2.12	0.49
1:A:532:SER:HB2	1:A:533:PRO:HA	1.94	0.49
1:A:240:SER:HB2	1:B:325:THR:OG1	2.12	0.49
1:B:349:PHE:CD1	1:B:535:GLN:HG2	2.48	0.49
1:B:466:ILE:N	1:B:466:ILE:HD12	2.28	0.49
1:A:437:SER:O	1:A:438:GLY:O	2.30	0.48
1:A:342:ARG:HH11	1:A:342:ARG:HG3	1.77	0.48
1:B:342:ARG:HG3	1:B:410:TRP:CZ2	2.48	0.48
1:B:431:ARG:HG3	6:B:636:HOH:O	2.13	0.48
1:B:256:VAL:CG1	1:B:293:THR:HG23	2.43	0.48
1:B:344:SER:CB	3:B:7:BMA:H4	2.42	0.48
3:B:7:BMA:H62	6:B:645:HOH:O	2.13	0.48
1:B:513:ARG:HA	1:B:516:TRP:CD2	2.49	0.48
1:B:359:LEU:HD11	1:B:398:THR:HG23	1.96	0.48
1:B:411:ILE:O	1:B:435:LYS:HE2	2.14	0.48
1:A:355:THR:HG23	1:A:402:THR:HG23	1.94	0.48
1:B:403:LEU:HD12	1:B:404:PRO:HD2	1.95	0.47
1:A:508:ARG:NH1	1:B:467:GLN:OE1	2.48	0.47
1:A:372:LEU:CD2	1:A:420:VAL:HB	2.45	0.47
1:A:387:ARG:HH11	1:A:387:ARG:HB2	1.78	0.47
1:B:342:ARG:HG3	1:B:410:TRP:CH2	2.48	0.47
1:A:232:PRO:HA	1:A:259:TYR:HB3	1.96	0.47
1:B:283:SER:O	1:B:293:THR:HA	2.14	0.47
1:A:363:LEU:H	1:A:363:LEU:HD13	1.80	0.47
1:A:489:ARG:NH1	1:A:489:ARG:HG2	2.29	0.47
1:A:342:ARG:HG2	1:A:410:TRP:CH2	2.49	0.47
1:A:436:THR:HG21	1:A:471:PRO:HB3	1.97	0.47
1:B:486:PRO:HD2	1:B:489:ARG:CG	2.45	0.47
1:B:239:SER:OG	1:B:252:GLN:HG2	2.14	0.47
1:A:490:HIS:HB3	1:A:509:LEU:HD12	1.96	0.46
1:B:242:ASP:HB2	1:B:246:HIS:O	2.16	0.46
1:A:378:SER:C	1:A:380:LYS:H	2.18	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:270:GLU:HB3	1:B:273:GLN:HE22	1.81	0.46
1:B:422:HIS:ND1	1:B:423:PRO:CD	2.79	0.46
1:A:376:ARG:HD3	1:A:381:PRO:O	2.16	0.46
1:A:398:THR:HG21	2:A:2:NAG:C8	2.46	0.46
1:B:443:PRO:HB3	1:B:469:PHE:HB3	1.97	0.46
1:B:233:THR:O	1:B:256:VAL:HA	2.15	0.46
1:A:334:ARG:C	1:A:336:VAL:H	2.19	0.46
1:B:259:TYR:O	1:B:291:ALA:HB3	2.15	0.46
1:B:259:TYR:O	1:B:259:TYR:CG	2.68	0.46
1:B:361:VAL:CG1	1:B:362:ASP:N	2.79	0.46
1:B:363:LEU:HD23	1:B:364:ALA:H	1.80	0.46
1:A:359:LEU:HD11	1:A:398:THR:HG23	1.98	0.46
1:A:333:PRO:HB2	1:A:425:LEU:HD11	1.99	0.45
1:A:508:ARG:NH2	1:B:498:THR:HB	2.31	0.45
1:A:376:ARG:HD3	1:A:380:LYS:O	2.16	0.45
1:B:429:LEU:O	1:B:430:MET:HG3	2.17	0.45
1:A:242:ASP:C	1:A:244:GLY:N	2.68	0.45
1:B:286:GLN:HB3	1:B:291:ALA:CB	2.46	0.45
1:B:444:GLU:O	1:B:466:ILE:HA	2.16	0.45
1:A:444:GLU:O	1:A:466:ILE:HA	2.16	0.45
1:A:351:ARG:CG	1:A:353:SER:HB2	2.47	0.45
1:A:383:ASN:HB2	1:A:404:PRO:HG2	1.98	0.45
1:B:367:LYS:HD2	1:B:368:GLY:N	2.31	0.45
1:A:435:LYS:CB	1:A:435:LYS:NZ	2.80	0.45
1:B:367:LYS:HB3	1:B:424:HIS:HE1	1.82	0.45
1:A:528:HIS:HD2	1:A:530:ALA:HB3	1.81	0.45
1:B:340:LEU:HD21	1:B:433:THR:HG22	1.98	0.44
1:B:486:PRO:HD2	1:B:489:ARG:HG3	1.98	0.44
1:A:440:ARG:HB3	1:A:530:ALA:HB2	1.98	0.44
1:B:394:ASN:OD1	1:B:396:THR:HG23	2.17	0.44
1:B:343:PRO:HD3	1:B:356:ILE:CG2	2.46	0.44
1:B:266:ILE:N	1:B:266:ILE:HD12	2.32	0.44
1:B:269:LEU:HD11	1:B:313:GLN:CD	2.38	0.44
1:B:496:ARG:HG3	6:B:589:HOH:O	2.17	0.44
1:A:490:HIS:HB3	1:A:509:LEU:CD1	2.47	0.44
1:A:393:ARG:C	1:A:395:GLY:H	2.21	0.44
1:A:435:LYS:HB2	1:A:435:LYS:HZ2	1.83	0.44
1:B:363:LEU:HD11	1:B:370:VAL:HB	1.99	0.44
1:A:477:GLN:HG3	1:A:525:ARG:HB3	2.00	0.44
1:A:387:ARG:NH1	1:A:387:ARG:HB2	2.32	0.44
1:A:363:LEU:CD1	1:A:363:LEU:N	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:278:ASP:C	1:B:279:LEU:HD12	2.38	0.43
1:B:420:VAL:HB	1:B:429:LEU:HB2	2.00	0.43
1:A:443:PRO:CA	1:A:469:PHE:HB3	2.49	0.43
1:B:372:LEU:HD21	1:B:418:CYS:SG	2.59	0.43
1:A:513:ARG:HA	1:A:516:TRP:CE3	2.54	0.43
1:A:251:ILE:HD13	1:A:301:GLN:HA	2.00	0.43
1:A:443:PRO:HB2	1:A:466:ILE:CG2	2.49	0.43
1:A:250:THR:C	1:A:251:ILE:HD12	2.39	0.43
1:B:398:THR:HG22	6:B:665:HOH:O	2.18	0.43
1:A:338:ALA:HB3	1:A:431:ARG:NH1	2.34	0.43
1:B:281:THR:O	1:B:295:SER:HA	2.18	0.43
1:B:271:ASP:C	1:B:273:GLN:H	2.21	0.43
1:B:286:GLN:HB3	1:B:291:ALA:CA	2.49	0.43
1:A:351:ARG:O	1:A:352:LYS:HB2	2.19	0.43
1:B:440:ARG:HD3	1:B:471:PRO:HD3	2.00	0.43
1:A:341:SER:HG	2:A:7:MAN:H62	1.82	0.42
1:A:333:PRO:HG3	1:A:427:ARG:HH12	1.83	0.42
1:B:405:VAL:HG13	1:B:416:TYR:OH	2.20	0.42
1:B:481:ASN:HD22	1:B:481:ASN:HA	1.67	0.42
1:B:522:PHE:CD1	1:B:522:PHE:N	2.87	0.42
1:B:286:GLN:CA	1:B:291:ALA:HA	2.50	0.42
1:A:342:ARG:NH1	1:A:342:ARG:HG3	2.34	0.42
1:A:269:LEU:O	1:A:310:TYR:HA	2.19	0.42
1:B:254:CYS:HB2	1:B:268:TRP:CZ2	2.55	0.42
1:A:422:HIS:NE2	1:A:424:HIS:HB3	2.34	0.42
1:A:242:ASP:C	1:A:244:GLY:H	2.23	0.42
1:B:354:PRO:HG3	1:B:407:THR:HG22	2.02	0.42
1:A:363:LEU:HD22	1:A:363:LEU:C	2.40	0.41
1:A:489:ARG:NH1	1:A:489:ARG:CG	2.81	0.41
1:A:437:SER:HB3	6:A:1120:HOH:O	2.19	0.41
1:B:358:CYS:HB2	1:B:374:TRP:CH2	2.55	0.41
1:A:376:ARG:CZ	1:A:380:LYS:HB2	2.51	0.41
1:B:361:VAL:CG1	1:B:362:ASP:H	2.33	0.41
1:B:405:VAL:CG1	1:B:406:GLY:N	2.84	0.41
1:B:289:GLU:HA	1:B:289:GLU:OE1	2.21	0.41
1:B:232:PRO:HD2	1:B:321:PHE:HE1	1.85	0.41
1:A:408:ARG:HB2	1:A:408:ARG:HE	1.49	0.41
1:A:510:GLU:OE2	1:B:499:LYS:HG2	2.20	0.41
1:A:387:ARG:CB	1:A:387:ARG:NH1	2.84	0.41
1:A:355:THR:HG23	1:A:402:THR:CG2	2.51	0.41
1:A:512:THR:O	1:A:515:GLU:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:263:THR:HG22	1:B:264:ILE:N	2.36	0.41
1:B:370:VAL:HG11	1:B:399:VAL:HG21	2.03	0.41
1:A:529:GLU:HB3	6:A:1020:HOH:O	2.21	0.41
1:B:259:TYR:CE2	1:B:293:THR:HG22	2.55	0.41
1:B:498:THR:HG22	1:B:504:PHE:HB3	2.03	0.41
1:A:333:PRO:O	1:A:336:VAL:HB	2.21	0.41
1:A:363:LEU:HD13	1:A:363:LEU:N	2.34	0.41
1:A:543:VAL:HG23	1:A:544:ASN:N	2.36	0.41
1:A:261:PRO:HG3	1:A:291:ALA:HB2	2.03	0.41
1:A:334:ARG:NH1	1:A:424:HIS:CE1	2.89	0.40
1:B:474:ILE:HD11	1:B:526:ALA:HB1	2.02	0.40
1:B:421:THR:O	1:B:422:HIS:HB2	2.21	0.40
1:A:498:THR:C	1:A:500:GLY:H	2.23	0.40
1:B:525:ARG:HG3	1:B:538:GLN:HB3	2.03	0.40
1:B:363:LEU:O	1:B:365:PRO:HD3	2.21	0.40
1:A:443:PRO:HA	1:A:469:PHE:HB3	2.03	0.40
1:B:472:GLU:HG3	1:B:495:PRO:HB2	2.03	0.40
1:A:389:GLU:HA	1:A:399:VAL:HA	2.04	0.40
1:A:471:PRO:O	1:A:528:HIS:CE1	2.63	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	317/327 (97%)	289 (91%)	19 (6%)	9 (3%)	6 10
1	B	318/327 (97%)	283 (89%)	28 (9%)	7 (2%)	8 15
All	All	635/654 (97%)	572 (90%)	47 (7%)	16 (2%)	7 12

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	385	SER
1	B	242	ASP
1	B	334	ARG
1	B	365	PRO
1	B	426	PRO
1	A	258	GLY
1	A	383	ASN
1	A	388	LYS
1	A	426	PRO
1	A	438	GLY
1	B	289	GLU
1	A	242	ASP
1	A	518	GLN
1	B	498	THR
1	B	366	SER
1	A	335	GLY

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	283/289 (98%)	264 (93%)	19 (7%)	20	40
1	B	283/289 (98%)	270 (95%)	13 (5%)	33	61
All	All	566/578 (98%)	534 (94%)	32 (6%)	25	49

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	278	ASP
1	A	284	THR
1	A	293	THR
1	A	307	ASP
1	A	351	ARG
1	A	355	THR
1	A	363	LEU
1	A	371	GLN

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Mol	Chain	Res	Type
1	A	417	GLN
1	A	421	THR
1	A	427	ARG
1	A	435	LYS
1	A	460	ARG
1	A	481	ASN
1	A	487	ASP
1	A	505	VAL
1	A	511	VAL
1	A	524	CYS
1	A	543	VAL
1	B	238	GLN
1	B	250	THR
1	B	273	GLN
1	B	321	PHE
1	B	363	LEU
1	B	373	THR
1	B	402	THR
1	B	408	ARG
1	B	452	GLU
1	B	481	ASN
1	B	513	ARG
1	B	523	ILE
1	B	536	THR

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	238	GLN
1	A	252	GLN
1	A	286	GLN
1	A	383	ASN
1	A	417	GLN
1	A	422	HIS
1	A	477	GLN
1	A	528	HIS
1	B	238	GLN
1	B	273	GLN
1	B	294	GLN
1	B	371	GLN
1	B	383	ASN
1	B	392	GLN

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Mol	Chain	Res	Type
1	B	424	HIS
1	B	481	ASN
1	B	494	GLN
1	B	518	GLN
1	B	538	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

14 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	1	1,2	14,14,15	0.70	0	15,19,21	0.69	0
2	NAG	A	2	2	14,14,15	0.50	0	15,19,21	0.82	1 (6%)
2	BMA	A	3	2	11,11,12	0.43	0	14,15,17	0.66	0
2	MAN	A	4	2	11,11,12	0.48	0	14,15,17	0.60	0
2	MAN	A	5	2	11,11,12	0.68	0	14,15,17	0.69	0
2	MAN	A	6	2	11,11,12	0.57	0	14,15,17	0.60	0
2	MAN	A	7	2	11,11,12	0.42	0	14,15,17	0.75	1 (7%)
3	NAG	B	1	1,3	14,14,15	0.46	0	15,19,21	0.92	1 (6%)
3	NAG	B	2	3	14,14,15	0.57	0	15,19,21	0.81	0
3	BMA	B	3	3	11,11,12	0.41	0	14,15,17	0.44	0
3	MAN	B	4	3	11,11,12	0.67	0	14,15,17	0.66	0
3	MAN	B	5	3	11,11,12	0.64	0	14,15,17	0.46	0
3	MAN	B	6	3	11,11,12	0.52	0	14,15,17	0.76	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	BMA	B	7	3	11,11,12	0.59	0	14,15,17	0.64	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
2	NAG	A	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	2	2	-	0/6/23/26	0/1/1/1
2	BMA	A	3	2	-	0/2/19/22	0/1/1/1
2	MAN	A	4	2	-	0/2/19/22	0/1/1/1
2	MAN	A	5	2	-	0/2/19/22	0/1/1/1
2	MAN	A	6	2	-	0/2/19/22	0/1/1/1
2	MAN	A	7	2	-	0/2/19/22	0/1/1/1
3	NAG	B	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	2	3	-	0/6/23/26	0/1/1/1
3	BMA	B	3	3	-	0/2/19/22	0/1/1/1
3	MAN	B	4	3	-	0/2/19/22	0/1/1/1
3	MAN	B	5	3	-	0/2/19/22	0/1/1/1
3	MAN	B	6	3	-	0/2/19/22	0/1/1/1
3	BMA	B	7	3	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1	NAG	C2-N2-C7	-2.51	119.81	123.04
2	A	2	NAG	C2-N2-C7	-2.48	119.85	123.04
2	A	7	MAN	C1-O5-C5	2.34	115.22	112.25
3	B	6	MAN	C1-O5-C5	2.37	115.25	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2	NAG	2	0
2	A	7	MAN	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	7	BMA	3	0

5.6 Ligand geometry (i)

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	GOL	A	1001	-	5,5,5	4.87	5 (100%)	5,5,5	5.69	3 (60%)
5	GOL	A	1002	-	5,5,5	4.76	5 (100%)	5,5,5	5.68	3 (60%)
4	SO4	A	1011	-	4,4,4	0.25	0	6,6,6	0.10	0
4	SO4	A	1012	-	4,4,4	0.25	0	6,6,6	0.22	0
4	SO4	A	1013	-	4,4,4	0.21	0	6,6,6	0.10	0
4	SO4	A	1014	-	4,4,4	0.25	0	6,6,6	0.16	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
5	GOL	A	1001	-	-	0/4/4/4	0/0/0/0
5	GOL	A	1002	-	-	0/4/4/4	0/0/0/0
4	SO4	A	1011	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1012	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1013	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1014	-	-	0/0/0/0	0/0/0/0

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1001	GOL	C3-C2	-8.30	1.20	1.52
5	A	1002	GOL	C3-C2	-7.96	1.21	1.52
5	A	1001	GOL	C1-C2	-3.13	1.40	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1002	GOL	C1-C2	-3.10	1.40	1.52
5	A	1001	GOL	O2-C2	-2.87	1.34	1.43
5	A	1002	GOL	O2-C2	-2.71	1.35	1.43
5	A	1001	GOL	O3-C3	3.22	1.56	1.42
5	A	1002	GOL	O3-C3	3.49	1.57	1.42
5	A	1002	GOL	O1-C1	4.54	1.61	1.42
5	A	1001	GOL	O1-C1	4.59	1.62	1.42

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1001	GOL	O1-C1-C2	3.27	126.04	110.18
5	A	1002	GOL	O1-C1-C2	3.35	126.45	110.18
5	A	1002	GOL	O2-C2-C3	6.59	138.85	108.65
5	A	1001	GOL	O2-C2-C3	6.60	138.90	108.65
5	A	1002	GOL	O3-C3-C2	10.31	160.18	110.18
5	A	1001	GOL	O3-C3-C2	10.34	160.33	110.18

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1014	SO4	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	319/327 (97%)	-0.09	4 (1%) 79 75	17, 38, 85, 100	0
1	B	320/327 (97%)	0.34	39 (12%) 5 3	12, 40, 100, 122	0
All	All	639/654 (97%)	0.12	43 (6%) 21 15	12, 39, 93, 122	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	286	GLN	9.5
1	B	423	PRO	5.2
1	B	317	GLN	4.7
1	B	229	PHE	4.5
1	B	230	THR	4.5
1	B	366	SER	4.1
1	B	424	HIS	4.0
1	B	285	THR	3.9
1	B	231	PRO	3.8
1	B	288	GLY	3.7
1	B	287	GLU	3.7
1	B	259	TYR	3.6
1	A	367	LYS	3.6
1	B	290	LEU	3.5
1	B	228	ASP	3.5
1	B	289	GLU	3.4
1	B	425	LEU	3.4
1	B	333	PRO	3.3
1	B	368	GLY	3.3
1	B	284	THR	3.3
1	B	278	ASP	3.3
1	B	265	GLN	3.2
1	A	424	HIS	3.1
1	B	367	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	264	ILE	3.0
1	B	263	THR	2.8
1	B	427	ARG	2.8
1	B	260	THR	2.8
1	B	316	TYR	2.6
1	A	422	HIS	2.6
1	B	422	HIS	2.6
1	B	319	HIS	2.6
1	B	318	GLY	2.5
1	B	291	ALA	2.4
1	A	388	LYS	2.3
1	B	363	LEU	2.2
1	B	320	THR	2.2
1	B	279	LEU	2.2
1	B	281	THR	2.2
1	B	315	THR	2.2
1	B	282	ALA	2.1
1	B	336	VAL	2.1
1	B	277	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
3	BMA	B	7	11/12	0.68	0.40	19.62	86,88,88,89	0
2	MAN	A	7	11/12	0.74	0.34	5.15	103,104,106,106	0
2	NAG	A	1	14/15	0.82	0.22	-0.12	84,86,88,89	0
3	NAG	B	1	14/15	0.88	0.18	-0.15	55,57,59,59	0
2	NAG	A	2	14/15	0.89	0.20	-0.46	84,86,86,88	0
3	NAG	B	2	14/15	0.94	0.13	-1.77	58,60,62,64	0
3	MAN	B	4	11/12	0.89	0.19	-	80,84,87,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	BMA	B	3	11/12	0.90	0.11	-	67,69,74,77	0
2	BMA	A	3	11/12	0.83	0.22	-	90,91,93,97	0
2	MAN	A	6	11/12	0.67	0.30	-	101,101,103,103	0
3	MAN	B	6	11/12	0.69	0.31	-	94,96,98,98	0
2	MAN	A	5	11/12	0.62	0.26	-	100,101,102,102	0
2	MAN	A	4	11/12	0.83	0.19	-	93,95,99,102	0
3	MAN	B	5	11/12	0.69	0.28	-	76,78,80,80	0

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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
5	GOL	A	1001	6/6	0.87	0.32	8.13	79,79,80,81	0
5	GOL	A	1002	6/6	0.72	0.46	7.08	83,84,85,85	0
4	SO4	A	1012	5/5	0.88	0.24	2.35	69,69,70,72	0
4	SO4	A	1011	5/5	0.76	0.22	0.31	119,120,120,120	0
4	SO4	A	1014	5/5	0.95	0.15	-0.99	44,45,47,47	0
4	SO4	A	1013	5/5	0.71	0.34	-	118,119,120,120	0

6.5 Other polymers

There are no such residues in this entry.