Full wwPDB X-ray Structure Validation Report (i)

Mar 24, 2022 – 03:28 pm GMT

PDB ID	:	6SG8
Title	:	Structure of Sosuga virus receptor binding protein
Authors	:	Bowden, T.A.; Stelfox, A.J.
Deposited on	:	2019-08-02
Resolution	:	2.50 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
https://www.wwpdb.org/validation/2017/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:

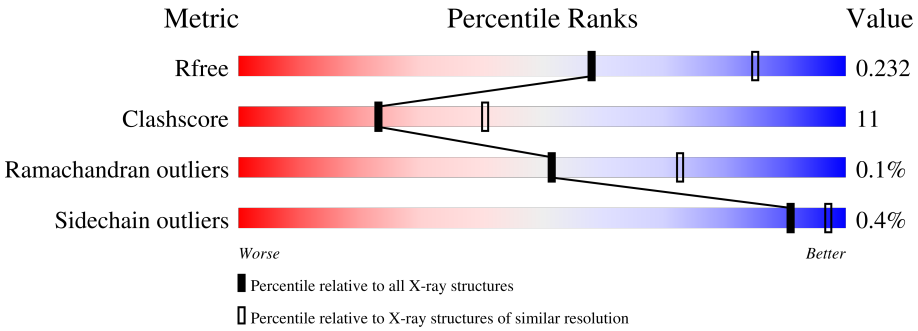
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.27
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

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 2.50 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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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%

Mol	Chain	Length	Quality of chain
1	A	468	62% 16% 21%
1	B	468	65% 16% 19%

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	602	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 6121 atoms, of which 30 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.

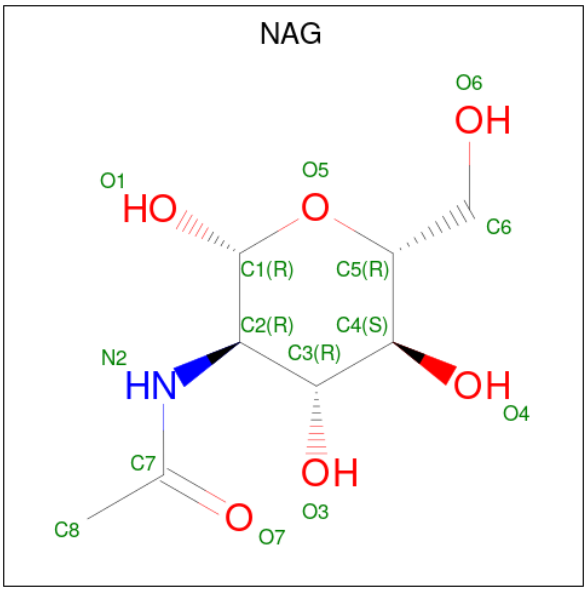
- Molecule 1 is a protein called Hemagglutinin-neuraminidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	370	Total	C	N	O	S	0	0	0
			2891	1839	476	553	23			
1	B	381	Total	C	N	O	S	0	0	0
			2979	1894	491	571	23			

There are 20 discrepancies between the modelled and reference sequences:

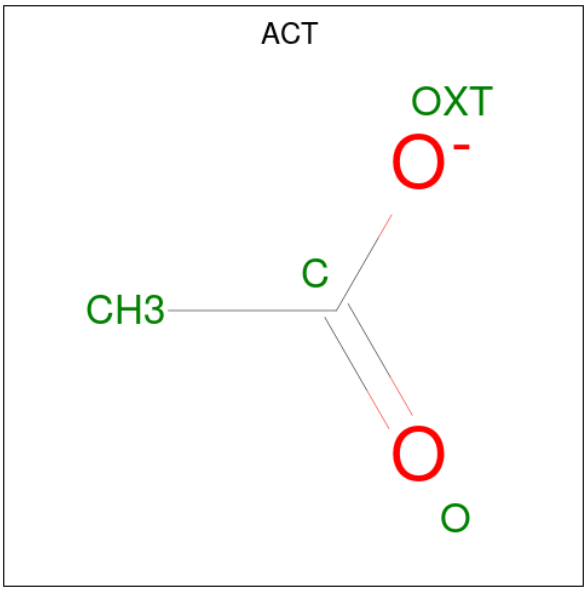
Chain	Residue	Modelled	Actual	Comment	Reference
A	583	GLY	-	expression tag	UNP W5SB61
A	584	THR	-	expression tag	UNP W5SB61
A	585	GLU	-	expression tag	UNP W5SB61
A	586	THR	-	expression tag	UNP W5SB61
A	587	SER	-	expression tag	UNP W5SB61
A	588	GLN	-	expression tag	UNP W5SB61
A	589	VAL	-	expression tag	UNP W5SB61
A	590	ALA	-	expression tag	UNP W5SB61
A	591	PRO	-	expression tag	UNP W5SB61
A	592	ALA	-	expression tag	UNP W5SB61
B	583	GLY	-	expression tag	UNP W5SB61
B	584	THR	-	expression tag	UNP W5SB61
B	585	GLU	-	expression tag	UNP W5SB61
B	586	THR	-	expression tag	UNP W5SB61
B	587	SER	-	expression tag	UNP W5SB61
B	588	GLN	-	expression tag	UNP W5SB61
B	589	VAL	-	expression tag	UNP W5SB61
B	590	ALA	-	expression tag	UNP W5SB61
B	591	PRO	-	expression tag	UNP W5SB61
B	592	ALA	-	expression tag	UNP W5SB61

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C H O 7 2 3 2	0	0
3	A	1	Total C H O 7 2 3 2	0	0
3	A	1	Total C H O 7 2 3 2	0	0
3	A	1	Total C H O 7 2 3 2	0	0
3	B	1	Total C H O 7 2 3 2	0	0
3	B	1	Total C H O 7 2 3 2	0	0
3	B	1	Total C H O 7 2 3 2	0	0
3	B	1	Total C H O 7 2 3 2	0	0
3	B	1	Total C H O 7 2 3 2	0	0
3	B	1	Total C H O 7 2 3 2	0	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 5 is water.

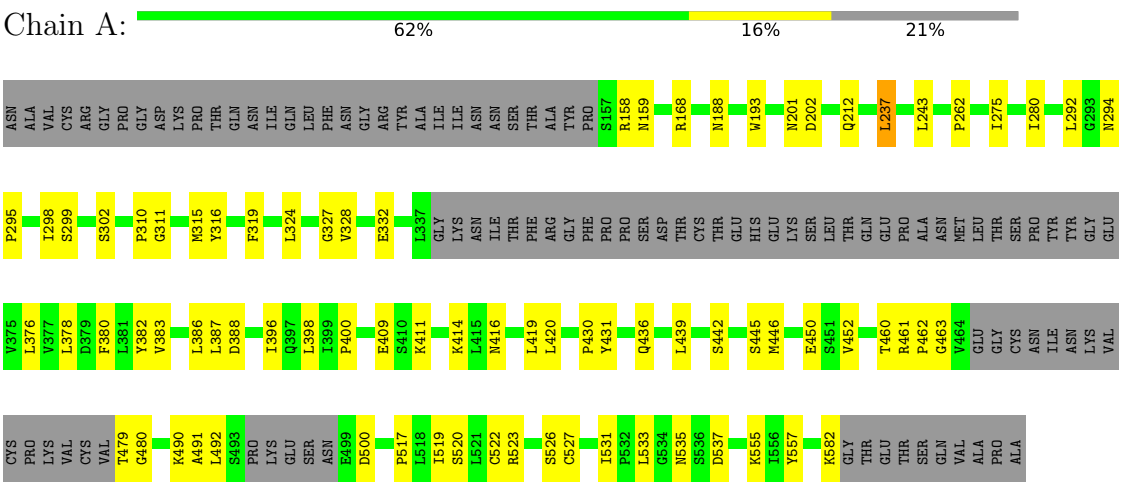
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	17	Total O 17 17	0	0
5	B	22	Total O 22 22	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

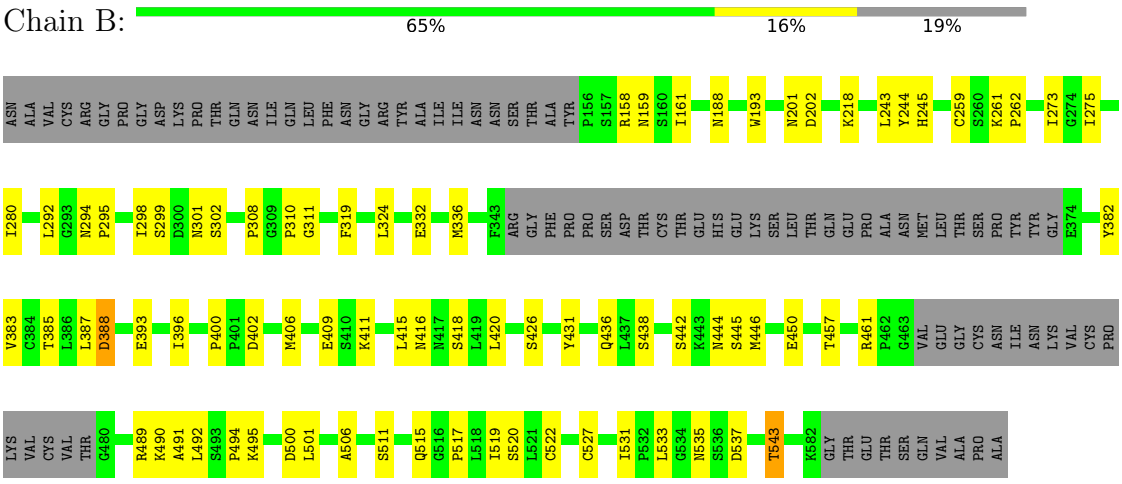
• Molecule 1: Hemagglutinin-neuraminidase

Chain A:



• Molecule 1: Hemagglutinin-neuraminidase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	75.70Å 84.04Å 81.69Å 90.00° 112.85° 90.00°	Depositor
Resolution (Å)	51.60 – 2.50 51.60 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.7 (51.60-2.50) 99.7 (51.60-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.52 (at 2.51Å)	Xtriage
Refinement program	PHENIX dev_3488	Depositor
R, R_{free}	0.194 , 0.231 0.194 , 0.232	Depositor DCC
R_{free} test set	1532 reflections (4.68%)	wwPDB-VP
Wilson B-factor (Å^2)	63.4	Xtriage
Anisotropy	0.352	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6121	wwPDB-VP
Average B, all atoms (Å^2)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.92% 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, 0.333 respectively for untwinned datasets, and 0.375, 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, NAG, ACT

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	0.29	0/2955	0.50	0/4011
1	B	0.28	0/3047	0.49	0/4135
All	All	0.28	0/6002	0.50	0/8146

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	2891	0	2840	65	0
1	B	2979	0	2924	61	0
2	A	56	0	52	10	0
2	B	84	0	78	13	0
3	A	16	12	12	1	0
3	B	24	18	18	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	17	0	0	0	0
5	B	22	0	0	3	0
All	All	6091	30	5924	136	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 11.

All (136) 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:416:ASN:HB2	1:B:490:LYS:HD3	1.28	1.09
2:A:602:NAG:H3	2:A:602:NAG:H83	1.43	0.97
1:B:158:ARG:HG2	1:B:159:ASN:H	1.34	0.90
2:B:604:NAG:H3	2:B:604:NAG:H83	1.52	0.89
1:A:452:VAL:HG22	2:A:602:NAG:H82	1.56	0.86
1:B:298:ILE:HG22	1:B:396:ILE:HD11	1.55	0.86
1:A:299:SER:HG	1:A:302:SER:HG	1.12	0.85
1:B:402:ASP:HB2	2:B:602:NAG:H82	1.59	0.83
1:A:324:LEU:HD11	1:A:382:TYR:HB2	1.65	0.79
1:B:492:LEU:HB2	2:B:605:NAG:O6	1.83	0.79
1:A:158:ARG:HG2	1:A:159:ASN:H	1.50	0.75
2:A:602:NAG:H3	2:A:602:NAG:C8	2.17	0.74
3:A:608:ACT:H2	2:B:603:NAG:H82	1.70	0.73
1:B:438:SER:OG	1:B:450:GLU:HG2	1.88	0.72
1:A:158:ARG:HB3	1:A:582:LYS:C	2.09	0.72
1:B:158:ARG:HG2	1:B:159:ASN:N	2.06	0.71
1:B:506:ALA:O	1:B:543:THR:HG21	1.90	0.71
1:B:415:LEU:HD22	2:B:605:NAG:H81	1.72	0.71
1:A:490:LYS:HE2	1:A:492:LEU:HA	1.72	0.70
1:A:420:LEU:HD23	1:A:436:GLN:HA	1.73	0.70
1:B:218:LYS:NZ	5:B:701:HOH:O	2.25	0.70
1:B:387:LEU:HD12	1:B:387:LEU:O	1.93	0.69
1:A:452:VAL:HG22	2:A:602:NAG:C8	2.23	0.68
1:A:302:SER:CB	1:A:332:GLU:HG2	2.22	0.68
1:A:387:LEU:HD12	1:A:388:ASP:N	2.08	0.68
1:B:418:SER:OG	1:B:490:LYS:NZ	2.21	0.68
1:B:273:ILE:HD11	1:B:301:ASN:O	1.93	0.68
1:B:535:ASN:HB2	1:B:537:ASP:OD1	1.94	0.67
1:B:442:SER:HB3	1:B:445:SER:HB3	1.78	0.66
1:B:436:GLN:HG2	1:B:494:PRO:HG3	1.79	0.64
1:B:491:ALA:HA	1:B:500:ASP:OD1	1.97	0.64
1:B:275:ILE:HD11	1:B:298:ILE:HD12	1.80	0.63
1:B:324:LEU:HD11	1:B:382:TYR:HB2	1.80	0.63
1:A:491:ALA:HA	1:A:500:ASP:OD1	1.98	0.63
1:B:280:ILE:HG23	1:B:292:LEU:HB2	1.81	0.63
1:B:450:GLU:HB2	2:B:602:NAG:O7	1.99	0.63
1:A:158:ARG:HB3	1:A:582:LYS:O	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:416:ASN:HB2	1:A:490:LYS:HD3	1.82	0.62
1:B:489:ARG:NH1	5:B:702:HOH:O	2.33	0.62
1:A:158:ARG:HG2	1:A:159:ASN:N	2.14	0.62
1:A:243:LEU:O	1:A:262:PRO:HD2	2.00	0.61
1:B:495:LYS:HE2	2:B:602:NAG:H61	1.83	0.60
1:B:302:SER:HB2	1:B:332:GLU:HG2	1.83	0.60
1:A:522:CYS:HA	1:A:527:CYS:HA	1.82	0.60
1:A:387:LEU:HD12	1:A:388:ASP:H	1.66	0.60
2:A:602:NAG:H83	2:A:602:NAG:C3	2.27	0.60
1:A:450:GLU:CB	2:A:602:NAG:H62	2.31	0.60
1:B:299:SER:OG	1:B:302:SER:OG	2.14	0.59
1:B:517:PRO:HG2	1:B:533:LEU:HB2	1.85	0.58
2:B:604:NAG:H3	2:B:604:NAG:C8	2.28	0.58
1:A:275:ILE:CD1	1:A:298:ILE:HG21	2.33	0.58
1:B:402:ASP:CB	2:B:602:NAG:H82	2.33	0.57
1:B:522:CYS:HA	1:B:527:CYS:HA	1.86	0.56
1:A:450:GLU:HB3	2:A:602:NAG:H62	1.86	0.56
1:B:298:ILE:HG22	1:B:396:ILE:CD1	2.30	0.56
1:B:387:LEU:O	1:B:388:ASP:HB2	2.05	0.56
1:B:311:GLY:HA3	1:B:411:LYS:HB2	1.88	0.56
1:B:393:GLU:HG3	1:B:444:ASN:ND2	2.21	0.56
1:A:275:ILE:HD11	1:A:298:ILE:HG21	1.87	0.56
1:A:535:ASN:HB2	1:A:537:ASP:OD1	2.06	0.56
1:A:316:TYR:O	1:A:319:PHE:HB2	2.05	0.55
1:A:490:LYS:HE2	1:A:492:LEU:CA	2.36	0.55
1:B:302:SER:CB	1:B:332:GLU:HG2	2.37	0.55
1:B:383:VAL:HG11	1:B:446:MET:HB3	1.88	0.54
1:A:400:PRO:HG3	1:A:450:GLU:HA	1.89	0.54
1:A:416:ASN:HB2	1:A:490:LYS:CD	2.38	0.54
1:A:275:ILE:HD11	1:A:298:ILE:HD13	1.89	0.54
1:A:319:PHE:CD2	1:A:446:MET:HE3	2.42	0.54
1:A:302:SER:HB2	1:A:332:GLU:HG2	1.90	0.53
1:A:212:GLN:HB3	1:A:237:LEU:HD22	1.91	0.53
1:B:520:SER:HB3	1:B:522:CYS:SG	2.48	0.53
1:A:419:LEU:HD12	1:A:439:LEU:HD11	1.91	0.53
1:B:420:LEU:HD23	1:B:436:GLN:HA	1.90	0.53
1:A:383:VAL:HG11	1:A:446:MET:HB3	1.90	0.53
1:B:319:PHE:CD2	1:B:446:MET:HE3	2.44	0.53
1:A:555:LYS:HE2	1:A:557:TYR:OH	2.08	0.52
1:B:161:ILE:HG23	1:B:531:ILE:HD11	1.92	0.52
1:B:491:ALA:HA	1:B:500:ASP:CG	2.31	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:604:NAG:H82	2:B:604:NAG:C1	2.41	0.51
1:A:450:GLU:HB2	2:A:602:NAG:H5	1.93	0.51
1:B:310:PRO:HD2	1:B:409:GLU:HB3	1.93	0.51
1:B:406:MET:CE	1:B:426:SER:HB3	2.41	0.50
1:A:310:PRO:CD	1:A:409:GLU:HB3	2.41	0.50
1:B:517:PRO:HB2	1:B:533:LEU:HD12	1.93	0.50
1:A:461:ARG:HG3	1:A:462:PRO:HD2	1.94	0.50
1:A:479:THR:OG1	1:A:480:GLY:N	2.42	0.50
1:A:520:SER:HB3	1:A:522:CYS:SG	2.52	0.49
1:B:244:TYR:CE1	1:B:261:LYS:HE2	2.47	0.49
1:A:327:GLY:HA2	1:A:376:LEU:O	2.13	0.49
1:A:310:PRO:HD2	1:A:409:GLU:HB3	1.94	0.48
1:B:308:PRO:HB3	1:B:324:LEU:HD23	1.95	0.48
1:B:319:PHE:CE1	1:B:385:THR:HG22	2.48	0.48
1:B:406:MET:HE3	1:B:426:SER:HB3	1.95	0.48
1:A:275:ILE:CD1	1:A:298:ILE:HD13	2.44	0.48
1:A:328:VAL:CG1	1:A:378:LEU:HD12	2.43	0.48
1:A:442:SER:HB2	1:A:445:SER:HB3	1.96	0.47
1:B:332:GLU:O	1:B:336:MET:HG3	2.15	0.47
1:A:188:ASN:HA	1:A:193:TRP:HA	1.97	0.47
1:A:517:PRO:HG2	1:A:533:LEU:HB2	1.95	0.46
1:A:450:GLU:OE1	2:A:602:NAG:H5	2.15	0.46
1:A:461:ARG:CG	1:A:462:PRO:HD2	2.46	0.46
1:A:380:PHE:CE2	1:A:398:LEU:HD13	2.51	0.46
1:B:245:HIS:O	1:B:259:CYS:HA	2.16	0.45
1:A:519:ILE:HB	1:A:531:ILE:HB	1.99	0.45
1:B:489:ARG:O	1:B:501:LEU:HA	2.16	0.45
2:B:604:NAG:H83	2:B:604:NAG:C3	2.36	0.45
1:A:461:ARG:HG2	1:A:463:GLY:H	1.81	0.44
1:B:310:PRO:CD	1:B:409:GLU:HB3	2.47	0.44
1:B:519:ILE:HB	1:B:531:ILE:HB	1.99	0.44
1:B:188:ASN:HA	1:B:193:TRP:HA	2.00	0.44
1:A:201:ASN:O	1:A:202:ASP:HB3	2.18	0.44
1:A:168:ARG:HD3	1:A:168:ARG:HA	1.86	0.44
1:B:511:SER:O	1:B:515:GLN:HG3	2.18	0.44
1:A:315:MET:HE1	1:A:386:LEU:HB2	2.00	0.43
1:A:316:TYR:HD2	1:A:446:MET:HE2	1.83	0.43
1:A:450:GLU:HB2	2:A:602:NAG:H62	2.00	0.43
1:B:319:PHE:CG	1:B:446:MET:HE3	2.54	0.42
1:B:491:ALA:HA	1:B:500:ASP:OD2	2.20	0.42
1:A:386:LEU:HD12	1:A:386:LEU:HA	1.76	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:400:PRO:HB2	2:B:602:NAG:H81	2.01	0.42
1:A:294:ASN:OD1	1:A:295:PRO:HD2	2.19	0.42
1:A:311:GLY:HA3	1:A:411:LYS:HB2	2.02	0.41
1:A:431:TYR:CD1	1:A:460:THR:HG22	2.55	0.41
1:B:543:THR:CG2	5:B:710:HOH:O	2.68	0.41
1:A:298:ILE:HG12	1:A:396:ILE:HD11	2.01	0.41
1:B:431:TYR:CD1	1:B:457:THR:HA	2.56	0.41
1:A:523:ARG:N	1:A:526:SER:O	2.49	0.41
1:A:280:ILE:HG23	1:A:292:LEU:HB2	2.03	0.41
1:A:430:PRO:HG2	1:A:431:TYR:CE2	2.56	0.41
2:B:604:NAG:C8	2:B:604:NAG:C1	2.99	0.41
3:B:608:ACT:H2	3:B:611:ACT:OXT	2.20	0.41
1:A:275:ILE:HD13	1:A:298:ILE:HG21	2.03	0.41
1:A:315:MET:O	1:A:414:LYS:HD3	2.21	0.40
1:B:294:ASN:OD1	1:B:295:PRO:HD2	2.21	0.40
1:B:243:LEU:O	1:B:262:PRO:HD2	2.20	0.40
1:B:201:ASN:O	1:B:202:ASP:HB3	2.21	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	362/468 (77%)	350 (97%)	12 (3%)	0	100	100
1	B	375/468 (80%)	362 (96%)	12 (3%)	1 (0%)	41	61
All	All	737/936 (79%)	712 (97%)	24 (3%)	1 (0%)	51	73

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	388	ASP

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	334/418 (80%)	333 (100%)	1 (0%)	92 97
1	B	344/418 (82%)	342 (99%)	2 (1%)	86 95
All	All	678/836 (81%)	675 (100%)	3 (0%)	91 97

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	237	LEU
1	B	461	ARG
1	B	543	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 22 ligands modelled in this entry, 2 are monoatomic - leaving 20 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	$\#\|Z\| > 2$
3	ACT	B	607	-	1,3,3	5.88	1 (100%)	0,3,3	-	-
2	NAG	B	606	1	14,14,15	0.27	0	17,19,21	0.47	0
3	ACT	B	612	-	1,3,3	5.61	1 (100%)	0,3,3	-	-
3	ACT	B	611	-	1,3,3	6.61	1 (100%)	0,3,3	-	-
2	NAG	B	605	1	14,14,15	0.35	0	17,19,21	0.49	0
3	ACT	B	610	-	1,3,3	6.04	1 (100%)	0,3,3	-	-
2	NAG	A	601	1	14,14,15	0.25	0	17,19,21	0.43	0
3	ACT	B	608	-	1,3,3	6.43	1 (100%)	0,3,3	-	-
2	NAG	B	601	1	14,14,15	0.26	0	17,19,21	0.43	0
3	ACT	A	608	-	1,3,3	5.53	1 (100%)	0,3,3	-	-
2	NAG	B	604	1	14,14,15	0.20	0	17,19,21	0.54	0
3	ACT	A	607	-	1,3,3	5.56	1 (100%)	0,3,3	-	-
2	NAG	A	602	1	14,14,15	0.26	0	17,19,21	0.66	0
2	NAG	B	603	1	14,14,15	0.22	0	17,19,21	0.34	0
2	NAG	A	603	1	14,14,15	0.22	0	17,19,21	0.34	0
2	NAG	B	602	1	14,14,15	0.26	0	17,19,21	0.58	0
3	ACT	A	605	-	1,3,3	5.98	1 (100%)	0,3,3	-	-
3	ACT	B	609	-	1,3,3	5.06	1 (100%)	0,3,3	-	-
3	ACT	A	606	-	1,3,3	5.88	1 (100%)	0,3,3	-	-
2	NAG	A	604	1	14,14,15	0.19	0	17,19,21	0.46	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	B	601	1	-	0/6/23/26	0/1/1/1
2	NAG	A	603	1	-	1/6/23/26	0/1/1/1
2	NAG	B	602	1	-	2/6/23/26	0/1/1/1
2	NAG	B	605	1	-	2/6/23/26	0/1/1/1
2	NAG	B	604	1	-	5/6/23/26	0/1/1/1
2	NAG	B	606	1	-	2/6/23/26	0/1/1/1
2	NAG	A	601	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	602	1	-	5/6/23/26	0/1/1/1
2	NAG	B	603	1	-	2/6/23/26	0/1/1/1
2	NAG	A	604	1	-	2/6/23/26	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	611	ACT	CH3-C	6.61	1.57	1.48
3	B	608	ACT	CH3-C	6.43	1.56	1.48
3	B	610	ACT	CH3-C	6.04	1.56	1.48
3	A	605	ACT	CH3-C	5.98	1.56	1.48
3	B	607	ACT	CH3-C	5.88	1.56	1.48
3	A	606	ACT	CH3-C	5.88	1.56	1.48
3	B	612	ACT	CH3-C	5.61	1.55	1.48
3	A	607	ACT	CH3-C	5.56	1.55	1.48
3	A	608	ACT	CH3-C	5.53	1.55	1.48
3	B	609	ACT	CH3-C	5.06	1.55	1.48

There are no bond angle outliers.

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	602	NAG	O5-C5-C6-O6
2	A	604	NAG	C4-C5-C6-O6
2	A	601	NAG	C4-C5-C6-O6
2	A	602	NAG	C4-C5-C6-O6
2	B	602	NAG	O5-C5-C6-O6
2	A	604	NAG	O5-C5-C6-O6
2	A	601	NAG	O5-C5-C6-O6
2	B	603	NAG	O5-C5-C6-O6
2	A	602	NAG	C8-C7-N2-C2
2	A	602	NAG	O7-C7-N2-C2
2	B	604	NAG	C8-C7-N2-C2
2	B	604	NAG	O7-C7-N2-C2
2	B	602	NAG	C4-C5-C6-O6
2	B	603	NAG	C4-C5-C6-O6
2	B	606	NAG	O5-C5-C6-O6
2	B	606	NAG	C4-C5-C6-O6
2	B	605	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	B	605	NAG	O5-C5-C6-O6
2	B	604	NAG	C4-C5-C6-O6
2	A	602	NAG	C3-C2-N2-C7
2	B	604	NAG	C3-C2-N2-C7
2	B	604	NAG	O5-C5-C6-O6
2	A	603	NAG	O5-C5-C6-O6

There are no ring outliers.

8 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	611	ACT	1	0
2	B	605	NAG	2	0
3	B	608	ACT	1	0
3	A	608	ACT	1	0
2	B	604	NAG	5	0
2	A	602	NAG	10	0
2	B	603	NAG	1	0
2	B	602	NAG	5	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.