



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:00 PM GMT

PDB ID : 4B7Q
Title : H1N1 2009 Pandemic Influenza Virus: Resistance of the I223R Neuraminidase Mutant Explained by Kinetic and Structural Analysis
Authors : Liu, J.; Van Der Vries, E.; Vachieri, S.G.; Xiong, X.; Collins, P.J.; Walker, P.A.; Haire, L.F.; Hay, A.J.; Schutten, M.; Osterhaus, A.D.M.E.; Martin, S.R.; Boucher, C.A.B.; Skehel, J.J.; Gamblin, S.J.
Deposited on : 2012-08-21
Resolution : 2.73 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

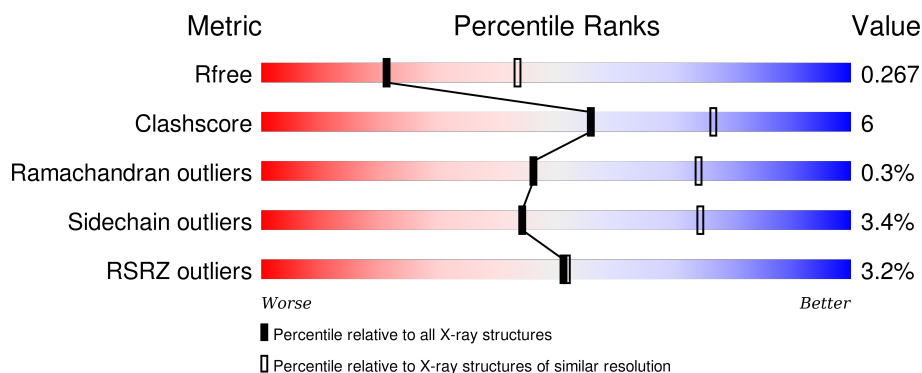
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.73 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	2439 (2.74-2.70)
Clashscore	102246	2771 (2.74-2.70)
Ramachandran outliers	100387	2726 (2.74-2.70)
Sidechain outliers	100360	2727 (2.74-2.70)
RSRZ outliers	91569	2443 (2.74-2.70)

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 $\leq 5\%$. 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	469	<div> <div>7%</div> <div>68% 14% 17%</div> </div>
1	B	469	<div> <div>69% 13% 17%</div> </div>
1	C	469	<div> <div>69% 13% 17%</div> </div>
1	D	469	<div> <div>3%</div> <div>66% 15% 17%</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12571 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.

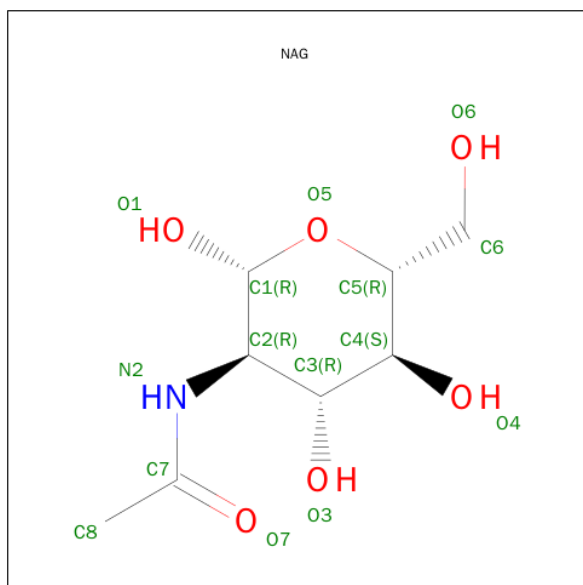
- Molecule 1 is a protein called NEURAMINIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	387	Total	C	N	O	S	0	0	0
			2994	1880	517	576	21			
1	B	387	Total	C	N	O	S	0	0	0
			2994	1880	517	576	21			
1	C	387	Total	C	N	O	S	0	0	0
			2994	1880	517	576	21			
1	D	387	Total	C	N	O	S	0	0	0
			2994	1880	517	576	21			

There are 4 discrepancies between the modelled and reference sequences:

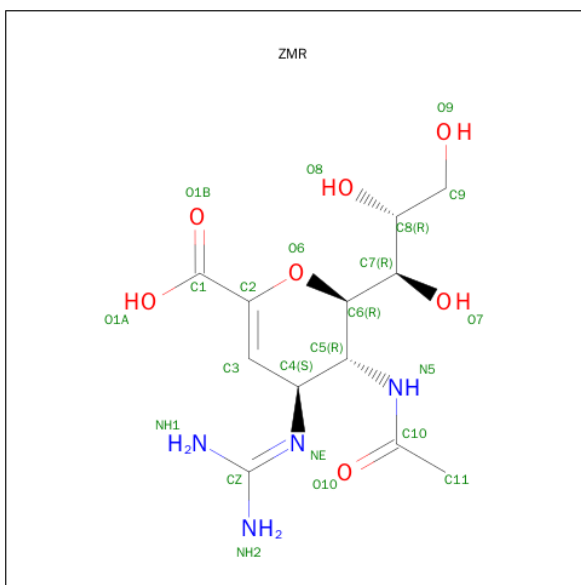
Chain	Residue	Modelled	Actual	Comment	Reference
A	351	PHE	TYR	CONFLICT	UNP C7FH46
B	351	PHE	TYR	CONFLICT	UNP C7FH46
C	351	PHE	TYR	CONFLICT	UNP C7FH46
D	351	PHE	TYR	CONFLICT	UNP C7FH46

- Molecule 2 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 3 is ZANAMIVIR (three-letter code: ZMR) (formula: $C_{12}H_{20}N_4O_7$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			23	12	4	7		
3	B	1	Total	C	N	O	0	0
			23	12	4	7		
3	C	1	Total	C	N	O	0	0
			23	12	4	7		
3	D	1	Total	C	N	O	0	0
			23	12	4	7		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Ca	0	0
			1	1		
4	A	2	Total	Ca	0	0
			2	2		
4	D	1	Total	Ca	0	0
			1	1		
4	C	1	Total	Ca	0	0
			1	1		

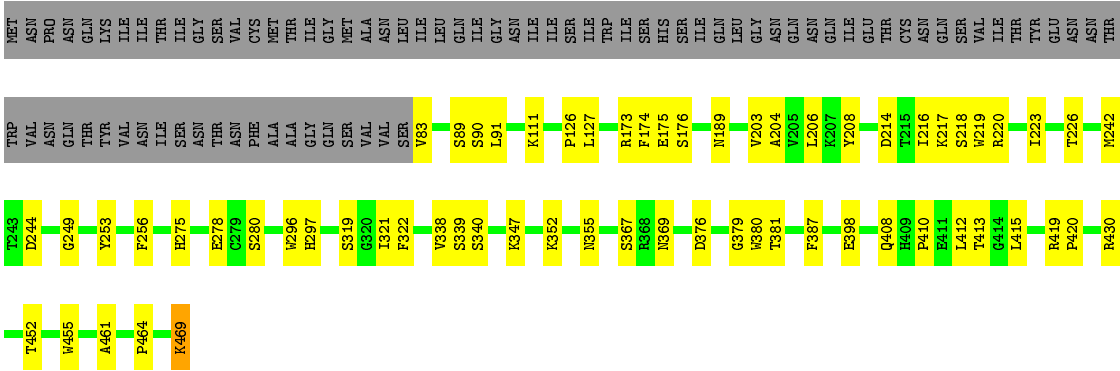
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	86	Total	O	0	0
			86	86		

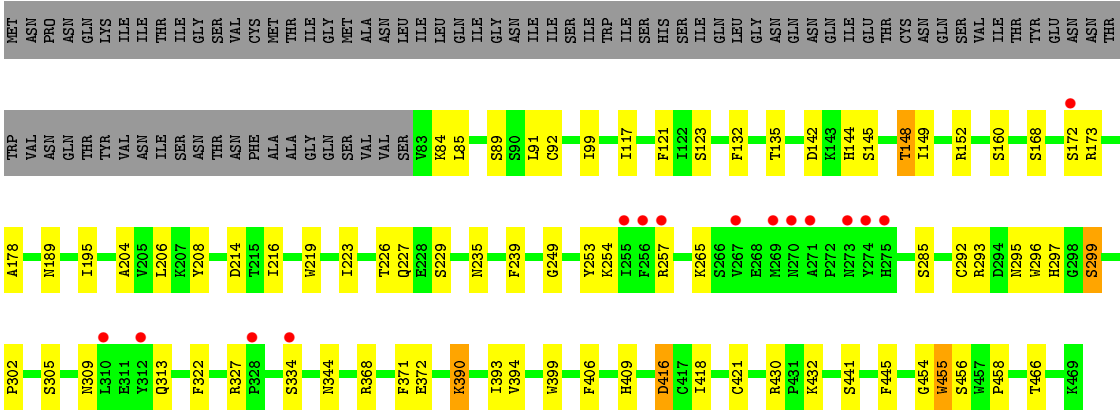
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	94	Total 94	O 94	0	0
5	C	120	Total 120	O 120	0	0
5	D	86	Total 86	O 86	0	0



● Molecule 1: NEURAMINIDASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	82.65Å 148.82Å 166.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	55.49 – 2.73 66.29 – 2.73	Depositor EDS
% Data completeness (in resolution range)	99.0 (55.49-2.73) 99.1 (66.29-2.73)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.53 (at 2.73Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8_1069)	Depositor
R, R_{free}	0.174 , 0.258 0.194 , 0.267	Depositor DCC
R_{free} test set	2790 reflections (5.35%)	DCC
Wilson B-factor (Å ²)	35.1	Xtriage
Anisotropy	0.150	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 49.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 54994 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	12571	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.39% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZMR, CA, 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	0.40	0/3076	0.56	0/4180
1	B	0.40	0/3076	0.58	0/4180
1	C	0.44	0/3076	0.58	0/4180
1	D	0.41	0/3076	0.56	0/4180
All	All	0.41	0/12304	0.57	0/16720

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 [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	2994	0	2829	43	0
1	B	2994	0	2827	40	0
1	C	2994	0	2827	35	0
1	D	2994	0	2828	37	0
2	A	14	0	13	1	0
2	B	28	0	26	0	0
2	C	42	0	39	0	0
2	D	28	0	26	0	0
3	A	23	0	19	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	23	0	19	0	0
3	C	23	0	19	0	0
3	D	23	0	19	1	0
4	A	2	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	86	0	0	6	0
5	B	94	0	0	5	0
5	C	120	0	0	4	0
5	D	86	0	0	4	0
All	All	12571	0	11491	146	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 (146) 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:C:355:ASN:OD1	1:C:381:THR:OG1	2.03	0.76
1:D:265:LYS:NZ	1:D:309:ASN:O	2.22	0.72
1:C:91:LEU:HD22	1:C:420:PRO:HG3	1.72	0.72
1:A:87:GLY:HA3	1:A:234:VAL:HG13	1.71	0.71
1:B:265:LYS:HG2	1:B:310:LEU:HD12	1.72	0.70
1:D:173:ARG:NH1	5:D:2018:HOH:O	2.22	0.70
1:A:157:THR:O	5:A:2018:HOH:O	2.09	0.70
1:D:206:LEU:HD13	1:D:214:ASP:HB3	1.75	0.69
1:D:285:SER:O	5:D:2052:HOH:O	2.11	0.68
1:B:398:GLU:HG2	1:B:458:PRO:CB	2.24	0.68
1:D:416:ASP:OD1	1:D:416:ASP:N	2.25	0.67
1:C:204:ALA:HB3	1:C:216:ILE:HG23	1.75	0.67
1:B:257:ARG:NH2	1:B:259:GLU:OE2	2.27	0.66
1:B:443:ILE:HD12	1:B:445:PHE:HE1	1.60	0.66
1:B:398:GLU:HG2	1:B:458:PRO:HB3	1.77	0.65
1:C:206:LEU:HD13	1:C:214:ASP:HB3	1.78	0.65
1:A:133:PHE:O	5:A:2018:HOH:O	2.12	0.65
1:D:204:ALA:HB3	1:D:216:ILE:HG23	1.79	0.65
1:A:393:ILE:HG22	1:A:394:VAL:HG23	1.81	0.63
1:D:121:PHE:CG	1:D:229:SER:HA	2.34	0.62
1:A:271:ALA:HB1	1:A:274:TYR:HB2	1.82	0.61
1:A:105:SER:HA	1:A:166:VAL:HG22	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:ARG:HG2	1:B:144:HIS:HD2	1.64	0.61
1:C:376:ASP:OD1	5:C:2089:HOH:O	2.16	0.60
1:A:113:ASP:O	1:A:168:SER:HB2	2.01	0.60
1:C:242:MET:HB2	1:C:256:PHE:HE1	1.67	0.59
1:D:219:TRP:CE2	1:D:254:LYS:HE3	2.37	0.58
1:B:430:ARG:NH2	5:B:2088:HOH:O	2.37	0.58
1:C:398:GLU:OE1	5:C:2097:HOH:O	2.17	0.57
1:A:324:ASP:OD1	1:A:325:ASN:N	2.37	0.57
1:A:146:ASN:HD22	2:A:511:NAG:H83	1.68	0.57
1:D:117:ILE:HG22	1:D:135:THR:HA	1.85	0.57
1:D:152:ARG:NH1	3:D:601:ZMR:O10	2.38	0.56
1:A:344:ASN:HB3	5:A:2071:HOH:O	2.06	0.56
1:B:113:ASP:O	1:B:168:SER:HB2	2.06	0.56
1:C:218:SER:OG	1:C:244:ASP:OD2	2.21	0.56
1:C:367:SER:OG	1:C:369:ASN:OD1	2.24	0.56
1:C:464:PRO:HG2	1:C:469:LYS:HE3	1.88	0.55
1:D:91:LEU:HD12	1:D:418:ILE:O	2.07	0.55
1:A:402:TYR:HB2	1:A:425:GLU:OE1	2.05	0.55
1:A:102:LYS:HG3	1:A:443:ILE:HG22	1.88	0.55
1:A:322:PHE:HB2	1:A:327:ARG:HD2	1.89	0.55
1:C:278:GLU:OE1	1:C:347:LYS:HB2	2.08	0.54
1:B:226:THR:HB	1:B:242:MET:HG2	1.91	0.53
1:D:84:LYS:NZ	1:D:235:ASN:OD1	2.39	0.53
1:A:107:ARG:HG2	1:B:144:HIS:CD2	2.42	0.53
1:A:122:ILE:HD12	1:A:423:TRP:HB3	1.89	0.53
1:B:398:GLU:HG2	1:B:458:PRO:HB2	1.91	0.53
1:A:249:GLY:HA2	1:A:296:TRP:CD1	2.43	0.52
1:B:226:THR:OG1	1:B:227:GLN:N	2.41	0.52
1:C:203:VAL:HG22	1:C:217:LYS:HG3	1.92	0.52
1:B:193:ILE:HG12	1:B:206:LEU:HG	1.91	0.52
1:B:451:ASP:HB3	1:C:217:LYS:HB2	1.90	0.52
1:B:465:PHE:N	1:B:468:ASP:OD2	2.39	0.52
1:D:372:GLU:OE1	1:D:390:LYS:NZ	2.30	0.52
1:A:384:ASP:OD2	1:A:386:ASN:HB2	2.10	0.51
1:C:321:ILE:HD11	1:C:387:PHE:HB3	1.92	0.51
1:D:456:SER:O	1:D:458:PRO:HD3	2.11	0.51
1:A:278:GLU:OE2	1:A:402:TYR:OH	2.25	0.51
1:B:234:VAL:HG11	1:B:286:SER:HA	1.93	0.51
1:D:313:GLN:NE2	5:D:2057:HOH:O	2.32	0.51
1:B:87:GLY:HA3	1:B:234:VAL:HG22	1.92	0.51
1:B:101:SER:HA	1:C:174:PHE:CZ	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:THR:HG23	5:A:2018:HOH:O	2.13	0.48
1:A:195:ILE:HG12	1:A:204:ALA:HB2	1.94	0.48
1:C:219:TRP:CD1	1:C:220:ARG:HG2	2.48	0.48
1:D:168:SER:O	1:D:172:SER:HB3	2.12	0.48
1:B:381:THR:OG1	5:B:2072:HOH:O	2.20	0.48
1:D:393:ILE:HG22	1:D:394:VAL:HG23	1.96	0.48
1:D:189:ASN:HB2	1:D:208:TYR:CZ	2.49	0.47
1:B:331:LYS:NZ	5:B:2063:HOH:O	2.47	0.47
1:A:133:PHE:CE2	1:A:159:MET:HB2	2.50	0.47
1:A:133:PHE:CZ	1:A:167:PRO:HB3	2.50	0.47
1:A:464:PRO:HB2	1:A:468:ASP:HB2	1.96	0.47
1:D:371:PHE:O	1:D:393:ILE:HB	2.15	0.47
1:C:111:LYS:HB2	1:D:142:ASP:HB2	1.97	0.47
1:C:189:ASN:HB2	1:C:208:TYR:CZ	2.49	0.47
1:D:406:PHE:CZ	1:D:421:CYS:HB3	2.51	0.46
1:B:271:ALA:HB1	1:B:274:TYR:HB2	1.97	0.46
1:D:239:PHE:CE2	1:D:257:ARG:HG3	2.51	0.46
1:B:133:PHE:CE1	1:B:159:MET:HB2	2.51	0.45
1:A:158:LEU:HD22	1:A:181:ALA:HB1	1.99	0.45
1:B:400:SER:O	1:B:427:ILE:HG12	2.17	0.45
1:D:226:THR:OG1	1:D:227:GLN:N	2.50	0.45
1:D:293:ARG:NH2	1:D:295:ASN:OD1	2.42	0.45
1:D:454:GLY:HA3	5:D:2070:HOH:O	2.16	0.45
1:D:299:SER:OG	1:D:327:ARG:HA	2.17	0.45
1:C:352:LYS:HD2	1:C:380:TRP:CE2	2.52	0.45
1:A:85:LEU:HD13	1:A:409:HIS:CE1	2.51	0.44
1:B:228:GLU:O	1:B:347:LYS:HE2	2.17	0.44
1:D:292:CYS:HB2	1:D:302:PRO:HG2	1.98	0.44
1:C:249:GLY:HA2	1:C:296:TRP:CE2	2.52	0.44
1:D:99:ILE:HD12	1:D:445:PHE:CZ	2.53	0.44
1:A:222:ASN:ND2	1:A:245:GLY:O	2.49	0.44
1:A:220:ARG:NE	5:A:2047:HOH:O	2.46	0.44
1:D:399:TRP:CH2	1:D:432:LYS:HB3	2.52	0.44
1:A:147:GLY:CA	1:A:430:ARG:HH22	2.31	0.44
1:A:363:LYS:HB2	1:A:370:GLY:HA3	2.00	0.44
1:C:322:PHE:CE1	1:C:338:VAL:HG21	2.52	0.44
1:A:197:GLY:HA2	1:D:455:TRP:CE3	2.53	0.44
1:D:132:PHE:CD2	1:D:160:SER:HB3	2.53	0.43
1:C:430:ARG:NE	5:C:2108:HOH:O	2.40	0.43
1:C:408:GLN:HB3	1:C:412:LEU:HD23	2.01	0.43
1:C:352:LYS:HB2	1:C:380:TRP:CZ3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:145:SER:O	1:D:148:THR:OG1	2.29	0.43
1:A:327:ARG:O	5:A:2065:HOH:O	2.21	0.43
1:B:316:TYR:CE1	1:B:337:PRO:HG3	2.53	0.43
1:C:253:TYR:OH	1:C:275:HIS:HA	2.19	0.43
1:A:219:TRP:CD1	1:A:220:ARG:HG2	2.54	0.43
1:C:220:ARG:HB2	1:C:244:ASP:CG	2.39	0.43
1:A:249:GLY:HA2	1:A:296:TRP:CG	2.54	0.43
1:B:222:ASN:HB3	1:B:245:GLY:HA2	2.01	0.43
1:B:343:ALA:O	1:B:344:ASN:HB2	2.19	0.43
1:C:173:ARG:HD2	1:C:175:GLU:OE2	2.19	0.43
1:C:461:ALA:HA	1:D:144:HIS:NE2	2.33	0.42
1:C:419:ARG:HA	1:C:420:PRO:HD3	1.87	0.42
1:A:413:THR:OG1	1:A:415:LEU:HB2	2.20	0.42
1:B:249:GLY:HA2	1:B:296:TRP:CE2	2.55	0.42
1:A:234:VAL:HG11	1:A:286:SER:HA	2.01	0.42
1:A:104:ASN:O	1:A:108:ILE:HG12	2.19	0.42
1:C:413:THR:HG23	1:C:415:LEU:HB2	2.00	0.42
1:B:227:GLN:HB3	1:B:229:SER:HB2	2.01	0.42
1:A:191:LEU:HD11	1:A:206:LEU:HD23	2.01	0.42
1:A:163:ILE:HG13	1:A:164:GLY:N	2.35	0.42
1:C:126:PRO:O	1:C:127:LEU:HD23	2.19	0.42
1:B:398:GLU:HG3	5:B:2081:HOH:O	2.20	0.41
1:C:226:THR:HB	1:C:242:MET:HG2	2.03	0.41
1:B:294:ASP:OD1	1:B:297:HIS:N	2.49	0.41
1:B:301:ARG:HA	1:B:302:PRO:HD2	1.93	0.41
1:A:451:ASP:HB3	1:B:217:LYS:HB2	2.02	0.41
1:B:451:ASP:CB	1:C:217:LYS:HB2	2.51	0.41
1:D:85:LEU:HD13	1:D:409:HIS:CG	2.55	0.41
1:D:322:PHE:HB2	1:D:327:ARG:HD2	2.02	0.41
1:A:430:ARG:HE	1:A:430:ARG:HB2	1.56	0.41
1:B:219:TRP:CD1	1:B:220:ARG:HG2	2.56	0.41
1:A:322:PHE:CD2	1:A:328:PRO:HD2	2.56	0.41
1:B:427:ILE:O	1:B:427:ILE:HG13	2.20	0.41
1:B:352:LYS:HB2	1:B:380:TRP:CE3	2.56	0.41
1:B:277:GLU:OE1	1:B:295:ASN:HB2	2.21	0.41
1:D:178:ALA:HA	1:D:195:ILE:O	2.20	0.41
1:D:249:GLY:HA2	1:D:296:TRP:CE2	2.56	0.40
1:C:319:SER:HB2	1:C:379:GLY:CA	2.52	0.40
1:B:390:LYS:NZ	5:B:2075:HOH:O	2.46	0.40
1:B:262:LYS:O	1:B:264:VAL:HG13	2.22	0.40
1:A:188:ILE:HG22	1:A:189:ASN:ND2	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:339:SER:O	5:C:2081:HOH:O	2.22	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	385/469 (82%)	358 (93%)	26 (7%)	1 (0%)	46	74
1	B	385/469 (82%)	365 (95%)	19 (5%)	1 (0%)	46	74
1	C	385/469 (82%)	365 (95%)	19 (5%)	1 (0%)	46	74
1	D	385/469 (82%)	363 (94%)	20 (5%)	2 (0%)	34	62
All	All	1540/1876 (82%)	1451 (94%)	84 (6%)	5 (0%)	46	74

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	223	ILE
1	D	148	THR
1	B	201	GLY
1	C	223	ILE
1	A	223	ILE

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	334/408 (82%)	326 (98%)	8 (2%)	57	84
1	B	334/408 (82%)	324 (97%)	10 (3%)	48	78
1	C	334/408 (82%)	323 (97%)	11 (3%)	45	75
1	D	334/408 (82%)	317 (95%)	17 (5%)	29	57
All	All	1336/1632 (82%)	1290 (97%)	46 (3%)	44	74

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	83	VAL
1	A	163	ILE
1	A	229	SER
1	A	231	CYS
1	A	267	VAL
1	A	297	HIS
1	A	415	LEU
1	A	455	TRP
1	B	117	ILE
1	B	127	LEU
1	B	168	SER
1	B	200	ASN
1	B	229	SER
1	B	231	CYS
1	B	268	GLU
1	B	297	HIS
1	B	417	CYS
1	B	455	TRP
1	C	83	VAL
1	C	89	SER
1	C	90	SER
1	C	176	SER
1	C	280	SER
1	C	297	HIS
1	C	340	SER
1	C	410	PRO
1	C	452	THR
1	C	455	TRP
1	C	469	LYS
1	D	89	SER
1	D	92	CYS
1	D	123	SER
1	D	149	ILE

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Mol	Chain	Res	Type
1	D	253	TYR
1	D	297	HIS
1	D	299	SER
1	D	305	SER
1	D	334	SER
1	D	344	ASN
1	D	368	ARG
1	D	390	LYS
1	D	416	ASP
1	D	430	ARG
1	D	441	SER
1	D	455	TRP
1	D	466	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	275	HIS

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 17 ligands modelled in this entry, 5 are monoatomic - leaving 12 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$
2	NAG	A	511	1	14,14,15	0.52	0	15,19,21	2.03	2 (13%)
3	ZMR	A	601	-	15,23,23	5.35	7 (46%)	18,32,32	4.26	5 (27%)
2	NAG	B	501	1	14,14,15	0.51	0	15,19,21	1.43	1 (6%)
2	NAG	B	511	1	14,14,15	0.49	0	15,19,21	0.68	0
3	ZMR	B	601	-	15,23,23	5.37	7 (46%)	18,32,32	4.31	5 (27%)
2	NAG	C	501	1	14,14,15	0.58	0	15,19,21	1.31	2 (13%)
2	NAG	C	511	1	14,14,15	0.49	0	15,19,21	1.62	1 (6%)
2	NAG	C	521	1	14,14,15	0.47	0	15,19,21	1.78	1 (6%)
3	ZMR	C	601	-	15,23,23	5.26	7 (46%)	18,32,32	4.53	5 (27%)
2	NAG	D	501	1	14,14,15	0.39	0	15,19,21	1.32	2 (13%)
2	NAG	D	511	1	14,14,15	0.52	0	15,19,21	2.64	1 (6%)
3	ZMR	D	601	-	15,23,23	5.23	7 (46%)	18,32,32	4.46	6 (33%)

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	511	1	-	0/6/23/26	0/1/1/1
3	ZMR	A	601	-	-	0/14/38/38	0/1/1/1
2	NAG	B	501	1	-	0/6/23/26	0/1/1/1
2	NAG	B	511	1	-	0/6/23/26	0/1/1/1
3	ZMR	B	601	-	-	0/14/38/38	0/1/1/1
2	NAG	C	501	1	-	0/6/23/26	0/1/1/1
2	NAG	C	511	1	-	0/6/23/26	0/1/1/1
2	NAG	C	521	1	-	0/6/23/26	0/1/1/1
3	ZMR	C	601	-	-	0/14/38/38	0/1/1/1
2	NAG	D	501	1	-	0/6/23/26	0/1/1/1
2	NAG	D	511	1	-	0/6/23/26	0/1/1/1
3	ZMR	D	601	-	-	0/14/38/38	0/1/1/1

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	601	ZMR	C6-C5	-4.58	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	ZMR	C6-C5	-4.37	1.45	1.53
3	B	601	ZMR	C6-C5	-4.07	1.46	1.53
3	D	601	ZMR	C6-C5	-4.01	1.46	1.53
3	A	601	ZMR	O8-C8	-2.35	1.38	1.43
3	C	601	ZMR	O8-C8	-2.32	1.38	1.43
3	B	601	ZMR	O8-C8	-2.19	1.38	1.43
3	D	601	ZMR	O8-C8	-2.04	1.38	1.43
3	C	601	ZMR	C10-N5	2.45	1.43	1.34
3	D	601	ZMR	C10-N5	2.68	1.44	1.34
3	A	601	ZMR	C10-N5	2.83	1.45	1.34
3	B	601	ZMR	C10-N5	2.86	1.45	1.34
3	D	601	ZMR	C5-N5	5.17	1.54	1.45
3	C	601	ZMR	C5-N5	5.39	1.54	1.45
3	B	601	ZMR	C5-N5	5.68	1.55	1.45
3	C	601	ZMR	O6-C2	5.75	1.49	1.37
3	B	601	ZMR	O6-C2	5.98	1.49	1.37
3	D	601	ZMR	O6-C2	6.03	1.49	1.37
3	A	601	ZMR	C5-N5	6.07	1.55	1.45
3	A	601	ZMR	O6-C2	6.19	1.49	1.37
3	B	601	ZMR	C4-NE	7.14	1.54	1.46
3	A	601	ZMR	C4-NE	7.64	1.55	1.46
3	C	601	ZMR	C4-NE	7.95	1.55	1.46
3	D	601	ZMR	C4-NE	8.07	1.55	1.46
3	C	601	ZMR	C3-C2	15.74	1.54	1.32
3	D	601	ZMR	C3-C2	15.82	1.54	1.32
3	A	601	ZMR	C3-C2	16.10	1.54	1.32
3	B	601	ZMR	C3-C2	16.73	1.55	1.32

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	601	ZMR	C4-C3-C2	-13.72	109.58	122.76
3	C	601	ZMR	C4-C3-C2	-12.97	110.30	122.76
3	B	601	ZMR	C4-C3-C2	-12.54	110.71	122.76
3	C	601	ZMR	O6-C2-C3	-12.28	106.33	124.12
3	A	601	ZMR	O6-C2-C3	-12.10	106.59	124.12
3	A	601	ZMR	C4-C3-C2	-12.08	111.16	122.76
3	D	601	ZMR	O6-C2-C3	-11.52	107.43	124.12
3	B	601	ZMR	O6-C2-C3	-11.31	107.73	124.12
3	C	601	ZMR	C6-O6-C2	-4.60	107.67	114.79
3	B	601	ZMR	C6-O6-C2	-4.32	108.11	114.79
3	A	601	ZMR	C7-C6-C5	-3.06	109.68	114.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	601	ZMR	C6-C5-N5	-2.49	106.73	111.07
3	D	601	ZMR	C8-C7-C6	-2.49	108.01	113.01
2	D	501	NAG	C4-C3-C2	-2.36	107.55	111.23
3	D	601	ZMR	C4-C5-N5	-2.24	108.91	110.89
2	A	511	NAG	C2-N2-C7	-2.09	120.36	123.04
3	A	601	ZMR	C11-C10-N5	2.08	120.08	116.11
3	B	601	ZMR	O9-C9-C8	2.10	115.65	111.10
3	C	601	ZMR	O9-C9-C8	2.11	115.68	111.10
3	C	601	ZMR	C11-C10-N5	2.14	120.20	116.11
3	B	601	ZMR	C11-C10-N5	2.60	121.08	116.11
2	C	501	NAG	C1-O5-C5	2.91	115.94	112.25
2	C	501	NAG	C4-C3-C2	2.99	115.88	111.23
3	A	601	ZMR	O9-C9-C8	3.31	118.30	111.10
3	D	601	ZMR	O9-C9-C8	3.33	118.34	111.10
2	D	501	NAG	C1-O5-C5	3.84	117.12	112.25
2	B	501	NAG	C1-O5-C5	4.25	117.64	112.25
2	C	511	NAG	C1-O5-C5	5.50	119.23	112.25
2	C	521	NAG	C1-O5-C5	6.39	120.36	112.25
2	A	511	NAG	C1-O5-C5	6.41	120.38	112.25
2	D	511	NAG	C1-O5-C5	9.66	124.51	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	511	NAG	1	0
3	D	601	ZMR	1	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 ⓘ

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, 95th 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	387/469 (82%)	0.41	34 (8%) 12 10	21, 35, 52, 74	0
1	B	387/469 (82%)	-0.11	0 100 100	20, 31, 44, 62	0
1	C	387/469 (82%)	-0.25	0 100 100	19, 29, 44, 57	0
1	D	387/469 (82%)	0.14	15 (3%) 43 43	18, 33, 49, 66	0
All	All	1548/1876 (82%)	0.05	49 (3%) 51 52	18, 32, 48, 74	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	321	ILE	6.7
1	A	323	GLY	4.6
1	A	330	ASP	4.3
1	A	322	PHE	4.2
1	A	338	VAL	4.0
1	A	317	ILE	3.8
1	A	359	ILE	3.8
1	A	274	TYR	3.3
1	D	310	LEU	3.2
1	A	387	PHE	3.2
1	A	319	SER	3.1
1	A	357	VAL	3.1
1	D	274	TYR	3.1
1	A	335	CYS	3.0
1	A	331	LYS	3.0
1	A	363	LYS	3.0
1	D	267	VAL	3.0
1	D	270	ASN	2.9
1	A	367	SER	2.8
1	A	392	ASP	2.7
1	A	380	TRP	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	300	ASN	2.6
1	A	374	ILE	2.6
1	A	289	THR	2.6
1	A	394	VAL	2.6
1	D	256	PHE	2.6
1	A	276	TYR	2.5
1	A	385	ASN	2.5
1	A	366	SER	2.4
1	A	328	PRO	2.3
1	A	383	THR	2.3
1	D	257	ARG	2.3
1	A	458	PRO	2.3
1	D	275	HIS	2.3
1	D	271	ALA	2.3
1	D	312	TYR	2.3
1	A	299	SER	2.2
1	D	273	ASN	2.2
1	D	269	MET	2.2
1	D	172	SER	2.2
1	A	353	TYR	2.1
1	A	372	GLU	2.1
1	A	86	ALA	2.1
1	A	369	ASN	2.1
1	A	291	VAL	2.0
1	D	334	SER	2.0
1	D	255	ILE	2.0
1	D	328	PRO	2.0
1	A	395	GLY	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 [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
3	ZMR	B	601	23/23	0.95	0.17	-0.15	5,31,38,39	0
3	ZMR	C	601	23/23	0.97	0.15	-0.42	3,21,35,38	0
4	CA	C	701	1/1	0.98	0.13	-0.50	26,26,26,26	0
3	ZMR	A	601	23/23	0.96	0.14	-0.59	12,30,37,39	0
3	ZMR	D	601	23/23	0.95	0.13	-1.05	23,29,39,44	0
4	CA	A	702	1/1	0.93	0.14	-1.52	77,77,77,77	0
4	CA	D	701	1/1	0.97	0.08	-1.92	41,41,41,41	0
4	CA	A	701	1/1	0.97	0.05	-2.75	42,42,42,42	0
4	CA	B	701	1/1	0.99	0.06	-5.80	20,20,20,20	0
2	NAG	B	501	14/15	0.75	0.26	-	63,79,101,105	0
2	NAG	D	511	14/15	0.89	0.14	-	46,59,68,70	0
2	NAG	A	511	14/15	0.90	0.18	-	35,43,51,55	0
2	NAG	B	511	14/15	0.90	0.20	-	50,67,76,80	0
2	NAG	C	511	14/15	0.92	0.19	-	25,54,63,63	0
2	NAG	C	501	14/15	0.90	0.26	-	40,58,65,66	0
2	NAG	D	501	14/15	0.84	0.31	-	67,71,76,77	0
2	NAG	C	521	14/15	0.82	0.27	-	57,74,87,89	0

6.5 Other polymers

There are no such residues in this entry.