



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 07:20 AM GMT

PDB ID : 2HTQ
Title : N8 neuraminidase in complex with zanamivir
Authors : Russell, R.J.; Haire, L.F.; Stevens, D.J.; Collins, P.J.; Lin, Y.P.; Blackburn, G.M.; Hay, A.J.; Gamblin, S.J.; Skehel, J.J.
Deposited on : 2006-07-26
Resolution : 2.20 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

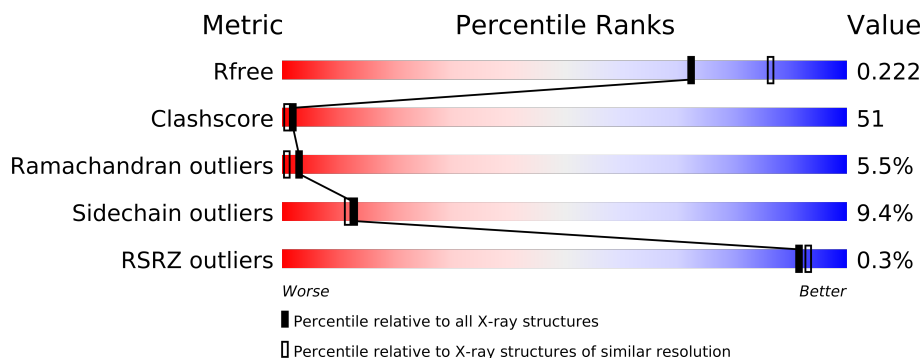
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

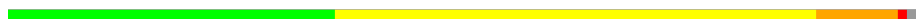
The reported resolution of this entry is 2.20 Å.

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}	66092	2938 (2.20-2.20)
Clashscore	79885	3751 (2.20-2.20)
Ramachandran outliers	78287	3681 (2.20-2.20)
Sidechain outliers	78261	3682 (2.20-2.20)
RSRZ outliers	66119	2939 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	390	

2 Entry composition i

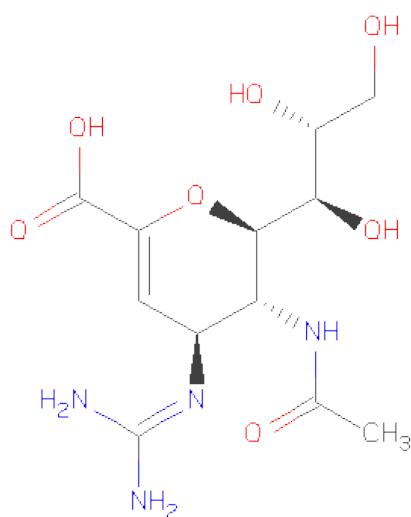
There are 3 unique types of molecules in this entry. The entry contains 3124 atoms, of which 0 are hydrogen and 0 are deuterium.

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
			Total	C	N	O	S			
1	A	387	2998	1878	524	572	24	0	0	0

- Molecule 2 is ZANAMIVIR (three-letter code: ZMR) (formula: C₁₂H₂₀N₄O₇).



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

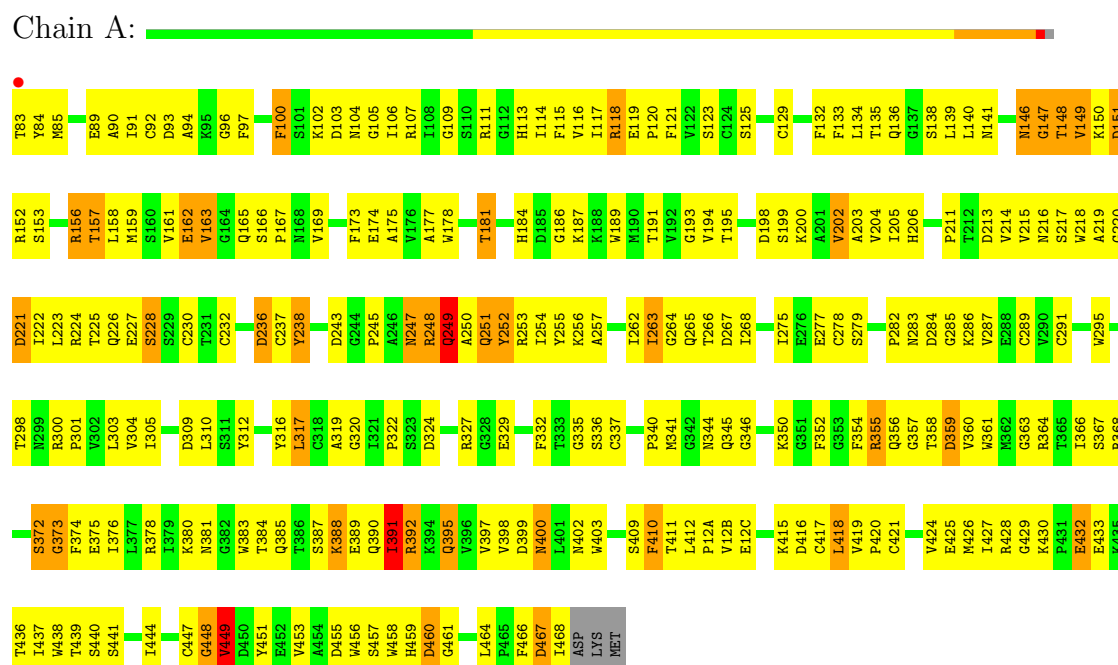
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	103	Total 103 O 103	0	0

3 Residue-property plots

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: Neuraminidase



4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α , β , γ	90.40Å 90.40Å 109.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.20 19.85 – 2.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.20) 91.0 (19.85-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.32 (at 2.21Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.271 , 0.334 0.215 , 0.222	Depositor DCC
R_{free} test set	1034 reflections (5.37%)	DCC
Wilson B-factor (Å ²)	24.8	Xtriage
Anisotropy	1.159	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 18.7	EDS
Estimated twinning fraction	0.467 for -h,k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$	Xtriage
Outliers	0 of 20254 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	3124	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.04% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZMR

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	0.43	0/3073	0.75	2/4171 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	337	CYS	CA-CB-SG	5.47	123.85	114.00
1	A	116	VAL	N-CA-C	-5.29	96.71	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2998	0	2861	299	0
2	A	23	0	17	2	0
3	A	103	0	0	33	0
All	All	3124	0	2878	299	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 51.

All (299) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:466:PHE:C	1:A:468:ILE:H	1.67	0.95
1:A:109:GLY:HA3	1:A:140:LEU:HD12	1.50	0.94
1:A:358:THR:HB	1:A:384:THR:OG1	1.71	0.88
1:A:355:ARG:HD3	1:A:357:GLY:O	1.74	0.87
1:A:426:MET:CE	1:A:459:HIS:HA	2.09	0.82
1:A:150:LYS:O	1:A:151:ASP:HB2	1.80	0.81
1:A:264:GLY:HA3	3:A:486:HOH:O	1.80	0.81
1:A:448:GLY:O	1:A:449:VAL:HB	1.80	0.80
1:A:424:VAL:HB	1:A:444:ILE:CG2	2.11	0.80
1:A:372:SER:HB2	1:A:400:ASN:ND2	1.97	0.79
1:A:257:ALA:HA	1:A:263:ILE:HG12	1.63	0.79
1:A:135:THR:HG21	1:A:159:MET:CE	2.12	0.78
1:A:100:PHE:HB2	3:A:557:HOH:O	1.83	0.78
1:A:254:ILE:O	1:A:265:GLN:HB2	1.84	0.77
1:A:135:THR:HG21	1:A:159:MET:HE3	1.66	0.77
1:A:83:THR:HG22	1:A:84:TYR:N	2.01	0.76
1:A:312:TYR:HB3	3:A:498:HOH:O	1.85	0.76
1:A:411:THR:HG21	1:A:418:LEU:HB3	1.65	0.76
1:A:466:PHE:O	1:A:468:ILE:N	2.19	0.75
1:A:387:SER:HB3	3:A:532:HOH:O	1.85	0.75
1:A:117:ILE:HG22	1:A:135:THR:HA	1.67	0.75
1:A:113:HIS:C	1:A:114:ILE:HD13	2.08	0.75
1:A:236:ASP:OD1	1:A:263:ILE:HD11	1.86	0.75
1:A:132:PHE:HD1	3:A:517:HOH:O	1.70	0.73
1:A:390:GLN:C	1:A:391:ILE:HG12	2.08	0.73
1:A:324:ASP:HB2	3:A:508:HOH:O	1.87	0.73
1:A:148:THR:O	1:A:439:THR:HB	1.88	0.73
1:A:118:ARG:HH11	1:A:427:ILE:HD11	1.53	0.72
1:A:367:SER:HB2	1:A:400:ASN:HD21	1.52	0.72
1:A:228:SER:HB2	1:A:350:LYS:NZ	2.05	0.71
1:A:344:ASN:HB3	3:A:539:HOH:O	1.91	0.71
1:A:251:GLN:HB2	3:A:477:HOH:O	1.89	0.71
1:A:427:ILE:O	1:A:428:ARG:HD2	1.91	0.71
1:A:426:MET:HE1	1:A:459:HIS:HA	1.72	0.70
1:A:329:GLU:HG2	1:A:368:ARG:HH11	1.56	0.70
1:A:118:ARG:HB3	1:A:156:ARG:HH12	1.57	0.70
1:A:118:ARG:HB3	1:A:156:ARG:NH1	2.06	0.69
1:A:150:LYS:HE3	1:A:153:SER:HB3	1.75	0.69
1:A:158:LEU:O	1:A:174:GLU:HB2	1.93	0.68
1:A:224:ARG:HD2	3:A:479:HOH:O	1.94	0.67
1:A:360:VAL:HB	3:A:474:HOH:O	1.94	0.67
1:A:356:GLN:O	1:A:359:ASP:HB2	1.94	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:372:SER:HB2	1:A:400:ASN:HD21	1.58	0.67
1:A:468:ILE:HG23	1:A:468:ILE:O	1.94	0.67
1:A:249:GLN:HG2	1:A:295:TRP:CZ3	2.29	0.67
1:A:105:GLY:HA3	3:A:536:HOH:O	1.93	0.66
1:A:149:VAL:HG22	1:A:439:THR:OG1	1.96	0.66
1:A:424:VAL:HB	1:A:444:ILE:HG23	1.77	0.66
1:A:466:PHE:C	1:A:468:ILE:N	2.42	0.65
1:A:355:ARG:C	1:A:355:ARG:HH11	2.00	0.65
1:A:447:CYS:O	1:A:448:GLY:O	2.15	0.65
1:A:332:PHE:HB3	3:A:559:HOH:O	1.96	0.65
1:A:107:ARG:HD2	1:A:461:GLY:HA3	1.79	0.64
1:A:238:TYR:HA	1:A:255:TYR:O	1.97	0.64
1:A:83:THR:HG22	1:A:84:TYR:H	1.62	0.64
1:A:194:VAL:HG11	1:A:223:LEU:O	1.98	0.63
1:A:178:TRP:CE2	1:A:195:THR:HA	2.34	0.63
1:A:206:HIS:HA	1:A:211:PRO:HA	1.81	0.63
1:A:301:PRO:HA	1:A:316:TYR:HA	1.80	0.62
1:A:399:ASP:OD1	1:A:402:ASN:ND2	2.33	0.62
1:A:173:PHE:CE2	1:A:175:ALA:HA	2.34	0.61
1:A:12(B):VAL:HG13	1:A:415:LYS:O	2.00	0.61
1:A:329:GLU:HG2	1:A:368:ARG:NH1	2.14	0.61
1:A:175:ALA:HB2	1:A:206:HIS:CD2	2.35	0.61
1:A:249:GLN:HG2	1:A:295:TRP:HZ3	1.63	0.61
1:A:438:TRP:HZ2	1:A:464:LEU:HD22	1.65	0.61
1:A:395:GLN:NE2	1:A:453:VAL:HB	2.16	0.60
1:A:157:THR:HG22	1:A:159:MET:HE2	1.83	0.60
1:A:373:GLY:HA2	1:A:398:VAL:HG12	1.83	0.60
1:A:118:ARG:NH1	1:A:427:ILE:HD11	2.17	0.60
1:A:316:TYR:CZ	1:A:340:PRO:HB3	2.37	0.60
1:A:395:GLN:HG3	1:A:395:GLN:O	2.00	0.60
1:A:191:THR:OG1	1:A:206:HIS:HB2	2.01	0.59
1:A:217:SER:HA	1:A:223:LEU:HD22	1.85	0.59
1:A:448:GLY:O	1:A:449:VAL:CB	2.51	0.59
1:A:356:GLN:O	1:A:359:ASP:N	2.34	0.59
1:A:385:GLN:HB2	3:A:532:HOH:O	2.02	0.59
1:A:147:GLY:O	1:A:149:VAL:N	2.35	0.58
1:A:12(C):GLU:OE1	1:A:12(C):GLU:N	2.33	0.58
1:A:409:SER:O	1:A:410:PHE:HB3	2.02	0.58
1:A:428:ARG:HG3	1:A:460:ASP:OD1	2.03	0.58
1:A:355:ARG:HD2	1:A:356:GLN:N	2.18	0.58
1:A:94:ALA:HB1	1:A:449:VAL:O	2.04	0.58
1:A:202:VAL:HG23	1:A:216:ASN:HA	1.86	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:411:THR:HG22	1:A:412:LEU:N	2.18	0.58
1:A:83:THR:CG2	1:A:84:TYR:N	2.66	0.57
1:A:150:LYS:O	1:A:151:ASP:CB	2.52	0.57
1:A:390:GLN:O	1:A:391:ILE:HG12	2.03	0.57
1:A:97:PHE:HA	1:A:448:GLY:O	2.04	0.57
1:A:157:THR:CG2	1:A:159:MET:HE2	2.35	0.57
1:A:236:ASP:OD2	1:A:256:LYS:HE2	2.05	0.57
1:A:238:TYR:N	1:A:238:TYR:CD1	2.72	0.57
1:A:395:GLN:HE22	1:A:453:VAL:HB	1.68	0.57
1:A:83:THR:CG2	1:A:84:TYR:H	2.18	0.56
1:A:214:VAL:CG1	1:A:215:VAL:N	2.67	0.56
1:A:283:ASN:HD21	1:A:355:ARG:NH1	2.03	0.56
1:A:253:ARG:HA	1:A:266:THR:O	2.04	0.56
1:A:114:ILE:HD13	1:A:114:ILE:N	2.21	0.56
1:A:361:TRP:HE3	1:A:376:ILE:HG12	1.71	0.56
1:A:114:ILE:HG22	1:A:167:PRO:HG2	1.87	0.56
1:A:205:ILE:HB	1:A:213:ASP:O	2.05	0.56
1:A:298:THR:HG22	1:A:345:GLN:HB2	1.88	0.56
1:A:254:ILE:CG2	1:A:305:ILE:HD13	2.35	0.56
1:A:109:GLY:HA2	1:A:114:ILE:HG12	1.87	0.56
1:A:133:PHE:O	1:A:134:LEU:HD23	2.05	0.56
1:A:355:ARG:O	1:A:355:ARG:NH1	2.39	0.55
1:A:115:PHE:CE1	1:A:169:VAL:HG22	2.41	0.55
1:A:133:PHE:HE2	1:A:161:VAL:HG22	1.71	0.55
1:A:361:TRP:CE3	1:A:376:ILE:HG12	2.42	0.55
1:A:156:ARG:HG2	1:A:156:ARG:HH21	1.69	0.55
1:A:118:ARG:HH11	1:A:427:ILE:CD1	2.17	0.55
1:A:436:THR:HB	1:A:438:TRP:CD1	2.42	0.55
1:A:367:SER:HB2	1:A:400:ASN:ND2	2.21	0.55
1:A:336:SER:HB2	1:A:341:MET:SD	2.47	0.55
1:A:391:ILE:O	1:A:392:ARG:HB2	2.07	0.55
1:A:219:ALA:HB3	1:A:243:ASP:CG	2.27	0.55
1:A:444:ILE:HD12	1:A:458:TRP:HB2	1.88	0.55
1:A:352:PHE:HZ	1:A:376:ILE:HD12	1.70	0.55
1:A:380:LYS:HB3	1:A:389:GLU:HG2	1.89	0.55
1:A:223:LEU:HG	1:A:223:LEU:O	2.06	0.55
1:A:447:CYS:HB2	3:A:557:HOH:O	2.06	0.54
1:A:133:PHE:O	1:A:158:LEU:HD12	2.07	0.54
1:A:135:THR:HG21	1:A:159:MET:HE2	1.88	0.54
1:A:282:PRO:HG2	1:A:418:LEU:HD13	1.90	0.54
1:A:199:SER:O	1:A:200:LYS:HG2	2.07	0.54
1:A:403:TRP:HA	1:A:403:TRP:CE3	2.43	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:437:ILE:H	1:A:468:ILE:HD11	1.72	0.54
1:A:278:CYS:HB3	1:A:289:CYS:HB3	1.90	0.54
1:A:252:TYR:HB2	1:A:268:ILE:HB	1.89	0.53
1:A:411:THR:HG23	1:A:419:VAL:O	2.08	0.53
1:A:295:TRP:O	1:A:346:GLY:HA2	2.08	0.53
1:A:132:PHE:CD1	3:A:517:HOH:O	2.51	0.53
1:A:118:ARG:HG2	1:A:118:ARG:HH21	1.73	0.53
1:A:265:GLN:OE1	1:A:265:GLN:N	2.42	0.53
1:A:102:LYS:HD3	1:A:104:ASN:HD21	1.73	0.52
1:A:178:TRP:CH2	1:A:194:VAL:HG12	2.44	0.52
1:A:228:SER:HB2	1:A:350:LYS:HZ3	1.75	0.52
1:A:427:ILE:HA	1:A:441:SER:HB3	1.91	0.52
1:A:85:MET:HE3	1:A:12(C):GLU:OE1	2.10	0.52
1:A:178:TRP:NE1	1:A:195:THR:HA	2.25	0.51
1:A:125:SER:O	1:A:12(A):PRO:HG3	2.11	0.51
1:A:194:VAL:HG22	1:A:203:ALA:HB2	1.93	0.51
1:A:205:ILE:O	1:A:211:PRO:HA	2.10	0.51
1:A:177:ALA:HB2	1:A:193:GLY:CA	2.40	0.51
1:A:118:ARG:HG3	1:A:119:GLU:H	1.76	0.51
1:A:360:VAL:CB	3:A:474:HOH:O	2.56	0.51
1:A:138:SER:O	1:A:139:LEU:HD23	2.10	0.51
1:A:312:TYR:CD1	1:A:312:TYR:C	2.84	0.50
1:A:316:TYR:O	1:A:317:LEU:C	2.50	0.50
1:A:254:ILE:HD13	1:A:305:ILE:HG12	1.94	0.50
1:A:120:PRO:HD2	1:A:425:GLU:OE2	2.11	0.50
1:A:320:GLY:HA2	1:A:335:GLY:CA	2.42	0.50
1:A:303:LEU:HD12	1:A:303:LEU:O	2.11	0.50
1:A:257:ALA:HB2	1:A:262:ILE:HA	1.94	0.50
1:A:303:LEU:HD12	1:A:305:ILE:HG13	1.93	0.50
1:A:152:ARG:HD3	2:A:472:ZMR:H111	1.93	0.49
1:A:118:ARG:NH1	1:A:427:ILE:CD1	2.74	0.49
1:A:388:LYS:HB3	1:A:388:LYS:NZ	2.28	0.49
1:A:146:ASN:ND2	1:A:437:ILE:HB	2.27	0.49
1:A:106:ILE:HD12	1:A:460:ASP:OD1	2.12	0.49
1:A:115:PHE:CZ	1:A:169:VAL:HG22	2.48	0.49
1:A:363:GLY:HA2	1:A:376:ILE:HA	1.95	0.49
1:A:118:ARG:HH21	1:A:118:ARG:CG	2.26	0.49
1:A:254:ILE:HG23	1:A:305:ILE:HD13	1.95	0.49
1:A:367:SER:CB	1:A:400:ASN:HD21	2.24	0.49
1:A:366:ILE:HG12	1:A:375:GLU:OE1	2.13	0.49
1:A:283:ASN:HD21	1:A:355:ARG:CZ	2.26	0.49
1:A:133:PHE:CE1	1:A:159:MET:HB2	2.48	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:254:ILE:HG22	1:A:255:TYR:N	2.28	0.48
1:A:146:ASN:O	1:A:437:ILE:O	2.31	0.48
1:A:238:TYR:N	1:A:238:TYR:HD1	2.12	0.48
1:A:220:GLY:O	1:A:221:ASP:HB2	2.13	0.48
1:A:430:LYS:HB2	1:A:439:THR:OG1	2.13	0.48
1:A:248:ARG:HA	1:A:295:TRP:CE2	2.49	0.48
1:A:202:VAL:HG23	1:A:216:ASN:OD1	2.14	0.48
1:A:327:ARG:NH1	1:A:366:ILE:O	2.47	0.48
1:A:165:GLN:HG3	3:A:525:HOH:O	2.12	0.48
1:A:283:ASN:HD21	1:A:355:ARG:NH2	2.12	0.48
1:A:303:LEU:CD1	1:A:305:ILE:HG13	2.44	0.47
1:A:397:VAL:HG13	1:A:458:TRP:HE3	1.78	0.47
1:A:429:GLY:HA2	1:A:433:GLU:HB2	1.95	0.47
1:A:156:ARG:HG2	1:A:178:TRP:HA	1.96	0.47
1:A:428:ARG:NH1	1:A:464:LEU:HG	2.30	0.47
1:A:103:ASP:OD1	1:A:105:GLY:N	2.42	0.47
1:A:252:TYR:O	1:A:253:ARG:HG3	2.14	0.47
1:A:232:CYS:HA	1:A:237:CYS:HA	1.97	0.47
1:A:121:PHE:CE1	1:A:132:PHE:HB2	2.49	0.47
1:A:395:GLN:HA	1:A:455:ASP:OD1	2.14	0.47
1:A:146:ASN:HD22	1:A:437:ILE:HB	1.80	0.47
1:A:275:ILE:HG23	1:A:291:CYS:HB2	1.97	0.47
1:A:158:LEU:N	1:A:175:ALA:O	2.47	0.46
1:A:90:ALA:HA	1:A:283:ASN:OD1	2.16	0.46
1:A:226:GLN:O	1:A:227:GLU:HB2	2.14	0.46
1:A:85:MET:HG3	1:A:186:GLY:CA	2.45	0.46
1:A:411:THR:CG2	1:A:412:LEU:N	2.78	0.46
1:A:354:PHE:O	1:A:360:VAL:HG23	2.16	0.46
1:A:247:ASN:O	1:A:248:ARG:O	2.34	0.46
1:A:317:LEU:CD2	3:A:474:HOH:O	2.64	0.46
1:A:136:GLN:NE2	1:A:156:ARG:NE	2.63	0.46
1:A:430:LYS:HG3	1:A:436:THR:O	2.16	0.46
1:A:283:ASN:HD21	1:A:355:ARG:HH12	1.63	0.46
1:A:381:ASN:HB3	1:A:385:GLN:NE2	2.31	0.46
1:A:309:ASP:O	1:A:310:LEU:HB2	2.15	0.46
1:A:397:VAL:HG13	1:A:458:TRP:CE3	2.50	0.46
1:A:304:VAL:HG12	3:A:551:HOH:O	2.16	0.46
1:A:287:VAL:HB	1:A:305:ILE:HB	1.98	0.46
1:A:117:ILE:HD13	1:A:167:PRO:HG3	1.97	0.46
1:A:213:ASP:OD1	1:A:214:VAL:N	2.47	0.46
1:A:96:GLY:O	1:A:448:GLY:O	2.34	0.46
1:A:133:PHE:C	1:A:134:LEU:HD23	2.36	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:161:VAL:O	1:A:162:GLU:C	2.52	0.46
1:A:345:GLN:HA	1:A:345:GLN:OE1	2.16	0.46
1:A:447:CYS:O	1:A:448:GLY:C	2.55	0.45
1:A:300:ARG:NH2	1:A:300:ARG:HG2	2.30	0.45
1:A:426:MET:SD	1:A:459:HIS:HA	2.55	0.45
1:A:460:ASP:HB2	3:A:560:HOH:O	2.17	0.45
1:A:102:LYS:HE2	1:A:458:TRP:O	2.16	0.45
1:A:289:CYS:HB2	1:A:303:LEU:HG	1.99	0.45
1:A:89:GLU:O	1:A:418:LEU:HD12	2.17	0.45
1:A:341:MET:HE3	3:A:553:HOH:O	2.16	0.45
1:A:310:LEU:HA	1:A:310:LEU:HD13	1.75	0.45
1:A:403:TRP:CZ2	1:A:432:GLU:HG3	2.52	0.45
1:A:427:ILE:O	1:A:428:ARG:CD	2.63	0.45
1:A:388:LYS:HZ2	1:A:388:LYS:CB	2.29	0.45
1:A:286:LYS:HD3	3:A:551:HOH:O	2.16	0.45
1:A:118:ARG:HB3	1:A:119:GLU:OE1	2.16	0.45
1:A:256:LYS:HE3	3:A:566:HOH:O	2.16	0.45
1:A:254:ILE:HG21	1:A:305:ILE:HD13	1.99	0.45
1:A:85:MET:HG3	1:A:186:GLY:HA2	1.99	0.45
1:A:363:GLY:O	1:A:364:ARG:HB3	2.16	0.45
1:A:83:THR:HA	1:A:187:LYS:HE3	1.98	0.44
1:A:354:PHE:CE2	1:A:420:PRO:HB2	2.52	0.44
1:A:380:LYS:CB	1:A:389:GLU:HG2	2.46	0.44
1:A:374:PHE:N	1:A:398:VAL:HB	2.32	0.44
1:A:411:THR:HG21	1:A:418:LEU:HD22	1.99	0.44
1:A:285:GLY:HA3	3:A:519:HOH:O	2.16	0.44
1:A:399:ASP:OD2	1:A:457:SER:HB2	2.18	0.44
1:A:118:ARG:NH2	1:A:118:ARG:CG	2.80	0.44
1:A:411:THR:HG21	1:A:418:LEU:CB	2.43	0.44
1:A:344:ASN:ND2	3:A:562:HOH:O	2.49	0.44
1:A:266:THR:HG22	1:A:267:ASP:N	2.33	0.43
1:A:436:THR:HB	1:A:438:TRP:NE1	2.33	0.43
1:A:84:TYR:CE2	1:A:187:LYS:HD2	2.53	0.43
1:A:152:ARG:NE	1:A:198:ASP:OD2	2.48	0.43
1:A:225:THR:OG1	1:A:226:GLN:N	2.49	0.43
1:A:410:PHE:CZ	1:A:421:CYS:HB2	2.53	0.43
1:A:230:CYS:HA	3:A:499:HOH:O	2.19	0.43
1:A:123:SER:OG	1:A:189:TRP:HZ3	2.01	0.43
1:A:115:PHE:HA	1:A:139:LEU:HD23	2.00	0.43
1:A:360:VAL:O	1:A:378:ARG:HA	2.18	0.43
1:A:106:ILE:HD12	1:A:460:ASP:CG	2.39	0.43
1:A:129:CYS:O	1:A:163:VAL:HG22	2.19	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:175:ALA:HB1	3:A:482:HOH:O	2.18	0.43
1:A:279:SER:O	1:A:409:SER:OG	2.35	0.43
1:A:438:TRP:HZ2	1:A:464:LEU:CD2	2.31	0.43
1:A:372:SER:HG	1:A:403:TRP:HZ3	1.66	0.43
1:A:381:ASN:C	3:A:532:HOH:O	2.56	0.43
1:A:447:CYS:N	3:A:557:HOH:O	2.51	0.42
1:A:84:TYR:N	1:A:187:LYS:HE3	2.34	0.42
1:A:262:ILE:HG22	1:A:263:ILE:N	2.34	0.42
1:A:184:HIS:HD2	1:A:186:GLY:H	1.67	0.42
1:A:249:GLN:OE1	1:A:250:ALA:O	2.36	0.42
1:A:355:ARG:C	1:A:355:ARG:HD2	2.39	0.42
1:A:218:TRP:CD1	1:A:253:ARG:CZ	3.02	0.42
1:A:184:HIS:HD2	1:A:186:GLY:N	2.16	0.42
1:A:298:THR:HG21	3:A:510:HOH:O	2.19	0.42
1:A:322:PRO:HG2	1:A:327:ARG:HD2	2.01	0.42
1:A:181:THR:HB	1:A:226:GLN:HB2	2.01	0.42
1:A:204:VAL:HA	1:A:214:VAL:HG22	2.00	0.42
1:A:214:VAL:HG13	1:A:215:VAL:N	2.32	0.42
1:A:291:CYS:SG	1:A:303:LEU:HD23	2.60	0.42
1:A:184:HIS:NE2	1:A:187:LYS:C	2.73	0.42
1:A:141:ASN:OD1	1:A:467:ASP:HB2	2.19	0.42
1:A:117:ILE:O	1:A:440:SER:HA	2.19	0.42
1:A:300:ARG:HG3	3:A:508:HOH:O	2.20	0.42
1:A:146:ASN:O	1:A:148:THR:N	2.52	0.42
1:A:83:THR:HA	1:A:187:LYS:CE	2.50	0.42
1:A:92:CYS:SG	1:A:417:CYS:O	2.78	0.42
1:A:156:ARG:NH2	1:A:156:ARG:HG2	2.34	0.41
1:A:279:SER:HB3	1:A:409:SER:H	1.84	0.41
1:A:91:ILE:HG22	1:A:92:CYS:O	2.20	0.41
1:A:427:ILE:HG22	1:A:428:ARG:N	2.35	0.41
1:A:215:VAL:HG22	1:A:262:ILE:CD1	2.49	0.41
1:A:372:SER:O	1:A:373:GLY:O	2.37	0.41
1:A:228:SER:HB2	1:A:350:LYS:HZ1	1.80	0.41
1:A:267:ASP:HB3	3:A:571:HOH:O	2.19	0.41
1:A:449:VAL:HG13	1:A:451:TYR:H	1.86	0.41
1:A:114:ILE:O	1:A:139:LEU:HA	2.20	0.41
1:A:184:HIS:HB2	1:A:189:TRP:CE3	2.56	0.41
1:A:152:ARG:NH2	2:A:472:ZMR:O10	2.46	0.41
1:A:388:LYS:CB	1:A:388:LYS:NZ	2.83	0.41
1:A:227:GLU:HA	1:A:227:GLU:OE1	2.21	0.41
1:A:444:ILE:CD1	1:A:458:TRP:HB2	2.51	0.40
1:A:300:ARG:HH21	1:A:300:ARG:HG2	1.86	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:245:PRO:HG2	1:A:248:ARG:O	2.21	0.40
1:A:184:HIS:CD2	1:A:186:GLY:H	2.39	0.40
1:A:320:GLY:HA2	1:A:335:GLY:HA3	2.03	0.40
1:A:251:GLN:HB3	3:A:572:HOH:O	2.20	0.40
1:A:383:TRP:CD1	1:A:383:TRP:O	2.75	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	385/390 (99%)	314 (82%)	50 (13%)	21 (6%)	3 1

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	146	ASN
1	A	148	THR
1	A	151	ASP
1	A	221	ASP
1	A	248	ARG
1	A	319	ALA
1	A	391	ILE
1	A	392	ARG
1	A	448	GLY
1	A	449	VAL
1	A	467	ASP
1	A	222	ILE
1	A	373	GLY
1	A	410	PHE
1	A	147	GLY
1	A	460	ASP
1	A	249	GLN
1	A	277	GLU

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Mol	Chain	Res	Type
1	A	418	LEU
1	A	263	ILE
1	A	149	VAL

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	329/332 (99%)	298 (91%)	31 (9%)	13	11

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	93	ASP
1	A	100	PHE
1	A	111	ARG
1	A	118	ARG
1	A	156	ARG
1	A	157	THR
1	A	162	GLU
1	A	163	VAL
1	A	166	SER
1	A	181	THR
1	A	202	VAL
1	A	228	SER
1	A	236	ASP
1	A	238	TYR
1	A	247	ASN
1	A	249	GLN
1	A	251	GLN
1	A	252	TYR
1	A	284	ASP
1	A	317	LEU
1	A	355	ARG
1	A	359	ASP
1	A	372	SER
1	A	388	LYS
1	A	391	ILE

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Mol	Chain	Res	Type
1	A	395	GLN
1	A	400	ASN
1	A	416	ASP
1	A	432	GLU
1	A	449	VAL
1	A	456	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	86	ASN
1	A	104	ASN
1	A	136	GLN
1	A	146	ASN
1	A	249	GLN
1	A	330(B)	GLN
1	A	344	ASN
1	A	381	ASN
1	A	385	GLN
1	A	395	GLN
1	A	400	ASN
1	A	402	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

1 ligand is 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	ZMR	A	472	-	23,23,23	3.27	7 (30%)	32,32,32	2.59	9 (28%)

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	ZMR	A	472	-	-	0/21/38/38	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	472	ZMR	O7-C7	-13.17	1.11	1.43
2	A	472	ZMR	C8-C7	-4.11	1.44	1.53
2	A	472	ZMR	CZ-NE	3.75	1.36	1.29
2	A	472	ZMR	C7-C6	3.50	1.57	1.52
2	A	472	ZMR	C6-C5	3.34	1.58	1.53
2	A	472	ZMR	C4-C5	-2.64	1.50	1.54
2	A	472	ZMR	C3-C2	2.29	1.37	1.33

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	472	ZMR	O7-C7-C6	-9.71	88.45	109.45
2	A	472	ZMR	C4-C3-C2	-5.06	118.95	122.77
2	A	472	ZMR	O7-C7-C8	4.84	120.97	108.74
2	A	472	ZMR	C6-O6-C2	4.11	120.87	114.72
2	A	472	ZMR	C7-C6-C5	3.37	119.22	114.24
2	A	472	ZMR	O6-C6-C5	-2.86	106.70	110.29
2	A	472	ZMR	C3-C4-NE	2.59	114.89	109.17
2	A	472	ZMR	O8-C8-C7	-2.53	102.75	109.05
2	A	472	ZMR	O6-C2-C1	2.28	116.37	111.88

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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	387/390 (99%)	-0.33	1 (0%) 91 93	9, 22, 32, 40	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	83	THR	2.0

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

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

6.3 Carbohydrates ⓘ

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, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	ZMR	A	472	23/23	0.10	-	14,19,22,23	0

6.5 Other polymers ⓘ

There are no such residues in this entry.