



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 01:52 AM GMT

PDB ID : 3NTT
Title : Structural insights of Adeno-Associated virus 5. A gene therapy Vector for Cystic Fibrosis
Authors : Govindasamy, L.; DiMattia, M.; Chiorini, J.A.; McKenna, R.; Muzyczka, N.; Agbandje-McKenna, M.
Deposited on : 2010-07-05
Resolution : 3.45 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>

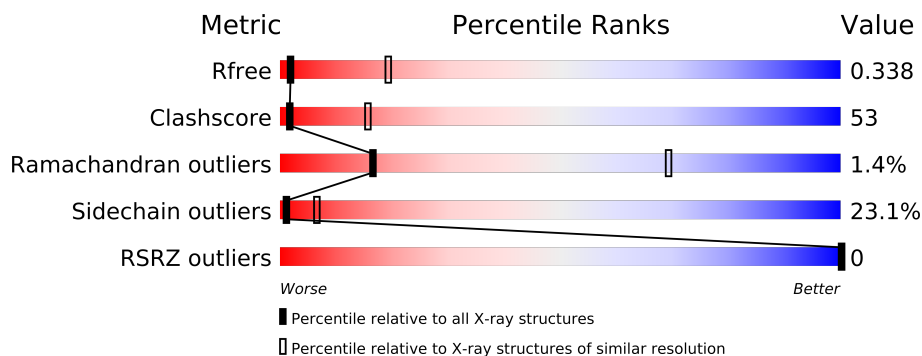
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.45 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	1149 (3.62-3.30)
Clashscore	79885	1012 (3.60-3.32)
Ramachandran outliers	78287	1401 (3.62-3.30)
Sidechain outliers	78261	1401 (3.62-3.30)
RSRZ outliers	66119	1149 (3.62-3.30)

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	724	

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 4120 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 Capsid protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	516	Total	C	N	O	S	0	0	0
			4111	2600	705	790	16			

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

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

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

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	264.70Å 447.90Å 629.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.96 – 3.45 49.96 – 3.45	Depositor EDS
% Data completeness (in resolution range)	78.6 (49.96-3.45) 78.6 (49.96-3.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.16	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.48 (at 3.48Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.252 , 0.252 0.349 , 0.338	Depositor DCC
R_{free} test set	2000 reflections (0.26%)	DCC
Wilson B-factor (Å ²)	46.9	Xtriage
Anisotropy	0.301	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 6.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	2 of 762206 reflections (0.000%)	Xtriage
F_o, F_c correlation	0.67	EDS
Total number of atoms	4120	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.85% 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: GOL, NA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.31	0/4239	0.55	1/5793 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	505	PRO	C-N-CD	-6.00	107.40	120.60

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	4111	0	3858	421	0
2	A	6	0	8	1	0
3	A	3	0	0	0	0
All	All	4120	0	3866	421	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 53.

All (421) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:480:GLY:O	1:A:481:VAL:HG23	1.31	1.30
1:A:472:THR:HG22	1:A:493:ASN:ND2	1.44	1.28
1:A:477:LEU:HD12	1:A:521:TYR:CD2	1.71	1.25
1:A:553:SER:O	1:A:556:GLN:HG2	1.41	1.17
1:A:477:LEU:HD12	1:A:521:TYR:CE2	1.79	1.16
1:A:477:LEU:CD1	1:A:521:TYR:CD2	2.29	1.15
1:A:550:THR:HG21	1:A:602:TYR:CZ	1.83	1.12
1:A:316:VAL:HG22	1:A:321:THR:HA	1.21	1.11
1:A:316:VAL:HG22	1:A:321:THR:CA	1.83	1.08
1:A:480:GLY:O	1:A:481:VAL:CG2	2.05	1.03
1:A:646:ASN:C	1:A:647:ILE:HD12	1.83	0.99
1:A:647:ILE:N	1:A:647:ILE:HD12	1.76	0.96
1:A:468:PRO:HG3	1:A:590:ILE:HD13	1.49	0.95
1:A:332:GLN:HE21	1:A:641:THR:HG22	1.29	0.94
1:A:489:PHE:HD2	1:A:489:PHE:O	1.49	0.94
1:A:647:ILE:N	1:A:647:ILE:CD1	2.30	0.93
1:A:375:ASN:HD22	1:A:375:ASN:N	1.68	0.92
1:A:406:TYR:CD1	1:A:407:ASN:N	2.37	0.92
1:A:531:SER:HA	1:A:548:LEU:HD11	1.52	0.92
1:A:505:PRO:CB	1:A:506:PRO:HD2	1.98	0.90
1:A:515:LEU:HD11	1:A:561:VAL:CG1	2.03	0.89
1:A:370:THR:HG22	1:A:371:LEU:H	1.37	0.89
1:A:325:ASN:HD22	1:A:325:ASN:H	1.19	0.89
1:A:505:PRO:HB3	1:A:506:PRO:HD2	1.53	0.88
1:A:481:VAL:HG12	1:A:481:VAL:O	1.70	0.88
1:A:515:LEU:HD11	1:A:561:VAL:HG12	1.54	0.88
1:A:289:ARG:HH11	1:A:289:ARG:HG2	1.38	0.88
1:A:550:THR:HG21	1:A:602:TYR:CE2	2.09	0.88
1:A:451:LYS:O	1:A:453:LEU:HD12	1.73	0.87
1:A:215:SER:HB2	1:A:308:ASN:H	1.40	0.87
1:A:477:LEU:HD11	1:A:521:TYR:CD2	2.10	0.87
1:A:519:ASN:O	1:A:521:TYR:CD2	2.27	0.86
1:A:232:LYS:HG2	1:A:670:GLU:HG3	1.57	0.85
1:A:489:PHE:CE2	1:A:494:ARG:NH2	2.44	0.85
1:A:679:ASN:C	1:A:679:ASN:HD22	1.80	0.84
1:A:591:VAL:HG13	1:A:592:PRO:HD2	1.59	0.84
1:A:509:ASN:N	1:A:509:ASN:HD22	1.75	0.84
1:A:513:ASN:HB3	1:A:522:ALA:HB3	1.60	0.83
1:A:515:LEU:O	1:A:516:GLN:HB2	1.76	0.83
1:A:516:GLN:HG2	1:A:553:SER:HB2	1.60	0.83
1:A:234:THR:OG1	1:A:668:THR:HB	1.79	0.82
1:A:546:ASN:ND2	1:A:546:ASN:H	1.73	0.81
1:A:604:GLN:OE1	1:A:714:PRO:HA	1.81	0.81

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:610:LYS:HB2	1:A:632:PRO:HG3	1.62	0.81
1:A:468:PRO:HG3	1:A:590:ILE:CD1	2.11	0.80
1:A:289:ARG:HH11	1:A:289:ARG:CG	1.94	0.80
1:A:476:ASN:HB3	1:A:480:GLY:HA2	1.64	0.80
1:A:531:SER:CA	1:A:548:LEU:HD11	2.13	0.80
1:A:509:ASN:H	1:A:509:ASN:ND2	1.81	0.79
1:A:489:PHE:O	1:A:489:PHE:CD2	2.36	0.79
1:A:460:THR:O	1:A:462:LYS:HD2	1.83	0.79
1:A:472:THR:HG22	1:A:493:ASN:HD22	1.48	0.78
1:A:519:ASN:O	1:A:521:TYR:HD2	1.63	0.78
1:A:481:VAL:O	1:A:481:VAL:CG1	2.30	0.78
1:A:509:ASN:HD22	1:A:509:ASN:H	1.31	0.78
1:A:477:LEU:CD1	1:A:521:TYR:CE2	2.57	0.77
1:A:550:THR:CG2	1:A:602:TYR:CZ	2.65	0.77
1:A:351:GLY:HA3	1:A:364:PRO:HG3	1.64	0.77
1:A:476:ASN:HD22	1:A:476:ASN:N	1.79	0.77
1:A:375:ASN:OD1	1:A:500:ALA:HB2	1.85	0.77
1:A:646:ASN:HD22	1:A:646:ASN:C	1.88	0.77
1:A:689:TYR:HB2	1:A:719:TYR:CE2	2.20	0.77
1:A:471:ARG:HH12	1:A:565:VAL:CG1	1.98	0.76
1:A:550:THR:CG2	1:A:602:TYR:CE2	2.68	0.76
1:A:428:ASN:HD21	1:A:431:VAL:CG2	1.99	0.76
1:A:489:PHE:HD2	1:A:489:PHE:C	1.89	0.76
1:A:316:VAL:CG2	1:A:321:THR:HA	2.08	0.76
1:A:513:ASN:HB2	1:A:522:ALA:H	1.50	0.76
1:A:292:ASN:HD22	1:A:688:GLN:HB3	1.51	0.76
1:A:471:ARG:HH12	1:A:565:VAL:HG12	1.50	0.75
1:A:370:THR:HG22	1:A:371:LEU:N	2.01	0.75
1:A:403:GLU:CD	1:A:403:GLU:H	1.91	0.74
1:A:472:THR:HB	1:A:524:GLU:HG3	1.68	0.74
1:A:281:HIS:CE1	1:A:669:VAL:HG11	2.23	0.74
1:A:553:SER:O	1:A:556:GLN:CG	2.30	0.74
1:A:302:LEU:HD21	1:A:304:VAL:HG23	1.69	0.74
1:A:472:THR:HG22	1:A:493:ASN:HD21	1.49	0.74
1:A:406:TYR:HD1	1:A:407:ASN:N	1.83	0.73
1:A:472:THR:CG2	1:A:493:ASN:ND2	2.39	0.73
1:A:334:PHE:HB3	1:A:393:SER:HB3	1.70	0.73
1:A:215:SER:HB2	1:A:307:PHE:HB2	1.70	0.72
1:A:423:LEU:O	1:A:426:LEU:HG	1.87	0.72
1:A:698:PHE:HD2	1:A:698:PHE:O	1.70	0.72
1:A:489:PHE:C	1:A:489:PHE:CD2	2.62	0.72
1:A:523:LEU:O	1:A:526:THR:HG22	1.89	0.72

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:278:PHE:CE1	1:A:607:ILE:HA	2.25	0.71
1:A:259:ASN:HB2	1:A:375:ASN:HB3	1.70	0.71
1:A:406:TYR:CD1	1:A:406:TYR:C	2.64	0.71
1:A:391:PHE:H	1:A:391:PHE:HD1	1.39	0.71
1:A:307:PHE:HE1	1:A:668:THR:CG2	2.03	0.71
1:A:307:PHE:HE1	1:A:668:THR:HG22	1.55	0.71
1:A:247:TYR:CE2	1:A:268:THR:HG22	2.25	0.70
1:A:317:GLN:O	1:A:320:THR:HG23	1.92	0.70
1:A:307:PHE:CE1	1:A:668:THR:HG22	2.27	0.70
1:A:693:TYR:HE2	1:A:713:ARG:CZ	2.04	0.70
1:A:480:GLY:O	1:A:481:VAL:CB	2.39	0.70
1:A:591:VAL:HG13	1:A:592:PRO:CD	2.23	0.69
1:A:332:GLN:NE2	1:A:641:THR:HG22	2.04	0.69
1:A:312:LYS:O	1:A:661:GLN:HB2	1.93	0.69
1:A:645:GLY:O	1:A:647:ILE:CD1	2.41	0.69
1:A:682:ARG:NH1	1:A:686:GLU:HG3	2.08	0.69
1:A:294:TYR:CE1	1:A:675:LEU:HD23	2.28	0.69
1:A:489:PHE:HE2	1:A:494:ARG:CZ	2.06	0.68
1:A:326:ASN:HD21	1:A:329:SER:HB2	1.58	0.68
1:A:370:THR:HG21	1:A:383:SER:HB2	1.74	0.68
1:A:356:PHE:CD2	1:A:358:PRO:HG2	2.29	0.68
1:A:489:PHE:HE2	1:A:494:ARG:NH2	1.92	0.68
1:A:316:VAL:HG22	1:A:321:THR:CB	2.23	0.68
1:A:650:PHE:CD2	1:A:651:SER:N	2.62	0.68
1:A:292:ASN:HD22	1:A:688:GLN:CB	2.07	0.67
1:A:468:PRO:CG	1:A:590:ILE:CD1	2.73	0.67
1:A:437:ARG:O	1:A:449:PHE:HB3	1.95	0.66
1:A:270:TRP:CE2	1:A:639:LYS:HD3	2.30	0.66
1:A:527:MET:CE	1:A:624:MET:HA	2.25	0.66
1:A:325:ASN:ND2	1:A:325:ASN:H	1.93	0.66
1:A:371:LEU:H	1:A:371:LEU:HD22	1.59	0.66
1:A:279:HIS:HB3	1:A:603:LEU:O	1.95	0.66
1:A:312:LYS:HG3	1:A:325:ASN:HB3	1.78	0.65
1:A:510:GLY:C	1:A:559:ASN:ND2	2.49	0.65
1:A:424:PHE:HD1	1:A:462:LYS:HZ3	1.45	0.65
1:A:403:GLU:N	1:A:403:GLU:OE1	2.30	0.65
1:A:533:PRO:O	1:A:534:ALA:HB3	1.97	0.65
1:A:469:MET:CE	1:A:566:GLY:HA3	2.26	0.65
1:A:400:ASN:OD1	1:A:400:ASN:N	2.30	0.65
1:A:332:GLN:O	1:A:638:ILE:HA	1.95	0.65
1:A:693:TYR:HE1	1:A:700:ASP:HB2	1.62	0.65
1:A:504:VAL:O	1:A:507:GLN:NE2	2.30	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:700:ASP:OD2	1:A:712:THR:HB	1.97	0.64
1:A:513:ASN:O	1:A:514:ASN:CB	2.45	0.64
1:A:292:ASN:ND2	1:A:688:GLN:HB3	2.12	0.64
1:A:493:ASN:O	1:A:494:ARG:HG2	1.97	0.64
1:A:320:THR:O	1:A:321:THR:HG22	1.98	0.64
1:A:646:ASN:HD22	1:A:647:ILE:N	1.96	0.64
1:A:645:GLY:O	1:A:647:ILE:HD13	1.98	0.64
1:A:281:HIS:HE1	1:A:669:VAL:HG11	1.63	0.64
1:A:546:ASN:HD22	1:A:546:ASN:H	1.42	0.64
1:A:370:THR:HG22	1:A:371:LEU:CD2	2.28	0.63
1:A:292:ASN:HD21	1:A:689:TYR:N	1.95	0.63
1:A:468:PRO:CG	1:A:590:ILE:HD13	2.27	0.63
1:A:287:TRP:O	1:A:291:ILE:HG23	1.98	0.63
1:A:587:LEU:HD13	1:A:587:LEU:O	1.98	0.63
1:A:406:TYR:CE1	1:A:407:ASN:C	2.72	0.63
1:A:311:VAL:HG23	1:A:663:SER:HB3	1.79	0.63
1:A:619:HIS:ND1	1:A:619:HIS:O	2.30	0.63
1:A:406:TYR:HD1	1:A:406:TYR:C	2.00	0.63
1:A:428:ASN:HD21	1:A:431:VAL:HG23	1.62	0.63
1:A:419:PRO:HD3	1:A:597:MET:HE1	1.81	0.63
1:A:272:TYR:CE2	1:A:364:PRO:HB2	2.34	0.62
1:A:320:THR:O	1:A:321:THR:CG2	2.47	0.62
1:A:489:PHE:CD2	1:A:494:ARG:NH2	2.67	0.61
1:A:477:LEU:O	1:A:519:ASN:ND2	2.33	0.61
1:A:371:LEU:CD2	1:A:371:LEU:H	2.13	0.61
1:A:370:THR:CG2	1:A:371:LEU:H	2.11	0.61
1:A:302:LEU:HD23	1:A:303:ARG:N	2.15	0.61
1:A:600:ASP:OD2	1:A:601:VAL:N	2.34	0.61
1:A:530:ASN:HD22	1:A:531:SER:H	1.46	0.61
1:A:558:VAL:CG1	1:A:596:TRP:HA	2.30	0.61
1:A:419:PRO:HB3	1:A:724:LEU:HD21	1.83	0.61
1:A:391:PHE:CD1	1:A:391:PHE:N	2.68	0.61
1:A:406:TYR:C	1:A:407:ASN:HD22	2.05	0.60
1:A:523:LEU:CD2	1:A:523:LEU:N	2.65	0.60
1:A:370:THR:HG22	1:A:371:LEU:HD22	1.82	0.60
1:A:521:TYR:O	1:A:523:LEU:HD23	2.01	0.60
1:A:453:LEU:O	1:A:456:ARG:HG2	2.02	0.60
1:A:356:PHE:O	1:A:359:GLN:HG2	2.01	0.60
1:A:476:ASN:CB	1:A:480:GLY:HA2	2.30	0.60
1:A:554:GLU:HG3	1:A:718:ARG:HG3	1.84	0.60
1:A:476:ASN:HD22	1:A:476:ASN:H	1.48	0.60
1:A:528:ILE:CG2	1:A:547:MET:HG3	2.31	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:375:ASN:ND2	1:A:375:ASN:N	2.40	0.60
1:A:548:LEU:HD12	1:A:548:LEU:N	2.16	0.60
1:A:332:GLN:HE21	1:A:641:THR:CG2	2.11	0.59
1:A:678:GLU:HG3	1:A:720:LEU:HD13	1.84	0.59
1:A:243:ASN:O	1:A:246:GLN:HG2	2.03	0.59
1:A:334:PHE:HB3	1:A:393:SER:CB	2.32	0.59
1:A:511:MET:N	1:A:559:ASN:HD22	2.01	0.59
1:A:325:ASN:N	1:A:325:ASN:HD22	1.88	0.59
1:A:433:GLN:NE2	1:A:460:THR:HB	2.17	0.59
1:A:403:GLU:CD	1:A:403:GLU:N	2.56	0.58
1:A:515:LEU:O	1:A:516:GLN:CB	2.47	0.58
1:A:556:GLN:HG3	1:A:557:PRO:HD3	1.84	0.58
1:A:345:VAL:HG23	1:A:635:MET:SD	2.44	0.58
1:A:451:LYS:O	1:A:453:LEU:CD1	2.51	0.58
1:A:320:THR:C	1:A:321:THR:HG22	2.24	0.58
1:A:302:LEU:C	1:A:302:LEU:HD23	2.24	0.58
1:A:469:MET:HE1	1:A:566:GLY:HA3	1.86	0.57
1:A:394:LYS:HE3	1:A:396:LEU:HD21	1.87	0.57
1:A:572:ASN:OD1	1:A:572:ASN:C	2.42	0.57
1:A:311:VAL:HG11	1:A:329:SER:HB3	1.85	0.57
1:A:406:TYR:HE1	1:A:408:PHE:HA	1.69	0.57
1:A:650:PHE:CE2	1:A:651:SER:O	2.57	0.57
1:A:618:PHE:O	1:A:619:HIS:C	2.41	0.57
1:A:698:PHE:CE1	1:A:710:ARG:NH1	2.73	0.57
1:A:436:TYR:CD1	1:A:436:TYR:N	2.72	0.57
1:A:476:ASN:N	1:A:476:ASN:ND2	2.51	0.56
1:A:292:ASN:HD21	1:A:689:TYR:H	1.51	0.56
1:A:698:PHE:CD2	1:A:698:PHE:C	2.79	0.56
1:A:531:SER:HA	1:A:548:LEU:CD1	2.32	0.56
1:A:695:ASP:N	1:A:696:PRO:HD3	2.21	0.56
1:A:471:ARG:NH1	1:A:565:VAL:HG12	2.20	0.56
1:A:289:ARG:O	1:A:293:ASN:ND2	2.39	0.56
1:A:504:VAL:HG23	1:A:504:VAL:O	2.05	0.56
1:A:293:ASN:N	1:A:293:ASN:ND2	2.54	0.56
1:A:317:GLN:HA	1:A:317:GLN:OE1	2.05	0.56
1:A:513:ASN:O	1:A:514:ASN:HB3	2.06	0.55
1:A:436:TYR:N	1:A:436:TYR:HD1	2.04	0.55
1:A:505:PRO:CB	1:A:506:PRO:CD	2.81	0.55
1:A:420:SER:HB3	1:A:721:THR:HG23	1.88	0.55
1:A:548:LEU:CD1	1:A:548:LEU:N	2.68	0.55
1:A:252:SER:O	1:A:262:ALA:HA	2.06	0.55
1:A:525:ASN:OD1	1:A:525:ASN:C	2.45	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:354:PRO:HD3	1:A:361:PHE:CD2	2.41	0.55
1:A:532:GLN:HB2	1:A:533:PRO:HD2	1.88	0.55
1:A:292:ASN:ND2	1:A:689:TYR:H	2.05	0.55
1:A:370:THR:CG2	1:A:371:LEU:N	2.71	0.54
1:A:215:SER:CB	1:A:308:ASN:H	2.18	0.54
1:A:691:ASN:C	1:A:691:ASN:HD22	2.11	0.54
1:A:300:ARG:HG3	1:A:300:ARG:HH11	1.73	0.54
1:A:276:ASN:ND2	1:A:608:TRP:O	2.36	0.53
1:A:510:GLY:C	1:A:559:ASN:HD22	2.10	0.53
1:A:304:VAL:HG22	1:A:669:VAL:HG22	1.88	0.53
1:A:698:PHE:CD1	1:A:710:ARG:NH1	2.77	0.53
1:A:693:TYR:CE1	1:A:700:ASP:HB2	2.42	0.53
1:A:523:LEU:N	1:A:523:LEU:HD22	2.24	0.53
1:A:247:TYR:HE2	1:A:268:THR:HG22	1.72	0.53
1:A:698:PHE:HD2	1:A:698:PHE:C	2.12	0.53
1:A:432:ASP:HA	1:A:454:ALA:H	1.74	0.53
1:A:679:ASN:C	1:A:679:ASN:ND2	2.52	0.52
1:A:599:ARG:HD2	1:A:623:ALA:O	2.10	0.52
1:A:435:LEU:C	1:A:436:TYR:HD1	2.13	0.52
1:A:270:TRP:CZ2	1:A:639:LYS:HD3	2.45	0.52
1:A:289:ARG:CG	1:A:289:ARG:NH1	2.63	0.52
1:A:528:ILE:HG22	1:A:547:MET:HG3	1.92	0.52
1:A:488:ALA:O	1:A:492:THR:HG23	2.10	0.52
1:A:530:ASN:HD22	1:A:531:SER:N	2.08	0.52
1:A:435:LEU:C	1:A:436:TYR:CD1	2.83	0.52
1:A:318:ASP:O	1:A:319:SER:HB2	2.10	0.52
1:A:514:ASN:C	1:A:515:LEU:HD12	2.30	0.51
1:A:519:ASN:N	1:A:519:ASN:OD1	2.43	0.51
1:A:693:TYR:HB2	1:A:696:PRO:HG3	1.92	0.51
1:A:444:THR:O	1:A:446:GLY:N	2.38	0.51
1:A:403:GLU:CD	1:A:403:GLU:O	2.48	0.51
1:A:432:ASP:N	1:A:432:ASP:OD2	2.42	0.51
1:A:425:LYS:HB3	1:A:457:TYR:CG	2.45	0.51
1:A:556:GLN:CG	1:A:557:PRO:HD3	2.39	0.51
1:A:684:ASN:HB2	1:A:685:PRO:HD2	1.92	0.51
1:A:262:ALA:O	1:A:372:ASN:ND2	2.43	0.51
1:A:651:SER:OG	1:A:653:VAL:HG12	2.11	0.51
1:A:519:ASN:O	1:A:521:TYR:CE2	2.62	0.50
1:A:371:LEU:HD21	1:A:383:SER:HA	1.93	0.50
1:A:285:ARG:O	1:A:288:GLN:HB3	2.10	0.50
1:A:241:SER:OG	1:A:661:GLN:O	2.27	0.50
1:A:437:ARG:CD	1:A:459:ASN:HB2	2.41	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:619:HIS:ND1	1:A:619:HIS:C	2.64	0.50
1:A:249:GLU:HA	1:A:266:TYR:CD2	2.47	0.50
1:A:522:ALA:O	1:A:525:ASN:O	2.30	0.50
1:A:441:THR:HA	1:A:446:GLY:O	2.12	0.50
1:A:513:ASN:CB	1:A:522:ALA:HB3	2.39	0.50
1:A:298:ARG:HG2	1:A:413:PHE:CE2	2.47	0.50
1:A:535:ASN:HB3	1:A:536:PRO:HD2	1.93	0.50
1:A:276:ASN:OD1	1:A:276:ASN:O	2.30	0.49
1:A:477:LEU:HD11	1:A:521:TYR:CG	2.48	0.49
1:A:525:ASN:O	1:A:525:ASN:OD1	2.30	0.49
1:A:406:TYR:HE1	1:A:407:ASN:C	2.15	0.49
1:A:370:THR:CG2	1:A:383:SER:HB2	2.43	0.49
1:A:279:HIS:ND1	1:A:355:ALA:HB2	2.28	0.49
1:A:302:LEU:CD2	1:A:304:VAL:HG23	2.41	0.49
1:A:295:TRP:CH2	1:A:679:ASN:O	2.65	0.49
1:A:548:LEU:HB3	1:A:714:PRO:HD3	1.93	0.49
1:A:403:GLU:O	1:A:403:GLU:OE2	2.30	0.48
1:A:292:ASN:ND2	1:A:689:TYR:N	2.59	0.48
1:A:357:PRO:N	1:A:358:PRO:HD2	2.29	0.48
1:A:613:GLU:OE2	1:A:613:GLU:HA	2.12	0.48
1:A:273:PHE:CE1	1:A:638:ILE:HG21	2.49	0.48
1:A:370:THR:CG2	1:A:371:LEU:HD22	2.43	0.48
1:A:527:MET:HE3	1:A:624:MET:HB3	1.94	0.48
1:A:471:ARG:HH12	1:A:565:VAL:HG13	1.77	0.48
1:A:437:ARG:NE	1:A:459:ASN:HB2	2.28	0.48
1:A:422:ASN:HB3	1:A:425:LYS:HG2	1.95	0.48
1:A:308:ASN:HB2	1:A:666:GLN:HG2	1.95	0.47
1:A:492:THR:HG21	1:A:503:GLN:NE2	2.29	0.47
1:A:621:SER:O	1:A:622:PRO:C	2.51	0.47
1:A:460:THR:O	1:A:462:LYS:CD	2.58	0.47
1:A:574:GLN:OE1	1:A:575:SER:N	2.47	0.47
1:A:591:VAL:CG1	1:A:592:PRO:N	2.75	0.47
1:A:674:GLU:C	1:A:675:LEU:HD12	2.34	0.47
1:A:414:HIS:CE1	1:A:601:VAL:HG22	2.50	0.47
1:A:239:LEU:HD12	1:A:638:ILE:HG12	1.95	0.47
1:A:428:ASN:OD1	1:A:431:VAL:HG22	2.14	0.47
1:A:600:ASP:OD1	1:A:717:THR:N	2.36	0.47
1:A:426:LEU:HD21	1:A:724:LEU:HD12	1.96	0.47
1:A:236:THR:HG23	1:A:666:GLN:NE2	2.30	0.47
1:A:279:HIS:CG	1:A:355:ALA:HB2	2.50	0.47
1:A:469:MET:HE3	1:A:588:GLN:H	1.80	0.47
1:A:533:PRO:O	1:A:534:ALA:CB	2.63	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:414:HIS:CD2	1:A:414:HIS:C	2.87	0.47
1:A:406:TYR:HE1	1:A:408:PHE:N	2.13	0.47
1:A:276:ASN:OD1	1:A:276:ASN:C	2.54	0.47
1:A:275:PHE:CD2	1:A:669:VAL:HG21	2.50	0.46
1:A:435:LEU:HD13	1:A:461:TYR:CD1	2.50	0.46
1:A:511:MET:N	1:A:559:ASN:ND2	2.62	0.46
1:A:293:ASN:HA	1:A:720:LEU:HD11	1.97	0.46
1:A:211:VAL:HG23	1:A:398:THR:HG21	1.96	0.46
1:A:264:PHE:HB2	1:A:377:GLU:O	2.15	0.46
1:A:514:ASN:O	1:A:515:LEU:HD12	2.15	0.46
1:A:550:THR:CG2	1:A:602:TYR:OH	2.64	0.46
1:A:587:LEU:N	1:A:587:LEU:HD12	2.30	0.46
1:A:646:ASN:ND2	1:A:646:ASN:C	2.58	0.46
1:A:468:PRO:CG	1:A:590:ILE:HD11	2.44	0.46
1:A:572:ASN:ND2	1:A:581:ALA:N	2.63	0.46
1:A:507:GLN:O	1:A:508:PRO:C	2.54	0.46
1:A:543:LEU:H	1:A:543:LEU:HG	1.43	0.46
1:A:354:PRO:CB	1:A:359:GLN:HG3	2.46	0.46
1:A:521:TYR:O	1:A:523:LEU:CD2	2.64	0.46
1:A:468:PRO:HG2	1:A:590:ILE:HD11	1.97	0.46
1:A:512:THR:HG22	1:A:560:ARG:O	2.16	0.46
1:A:513:ASN:ND2	1:A:526:THR:HB	2.31	0.46
1:A:406:TYR:HE1	1:A:408:PHE:CA	2.29	0.46
1:A:277:ARG:HE	1:A:279:HIS:CE1	2.34	0.46
1:A:270:TRP:CE3	1:A:637:LEU:HB3	2.50	0.46
1:A:374:ASP:C	1:A:375:ASN:HD22	2.19	0.45
1:A:211:VAL:HG21	1:A:327:LEU:HD23	1.97	0.45
1:A:598:GLU:HG2	1:A:598:GLU:H	1.51	0.45
1:A:513:ASN:HD22	1:A:526:THR:HB	1.81	0.45
1:A:295:TRP:CZ2	1:A:722:ARG:HG2	2.52	0.45
1:A:428:ASN:ND2	1:A:431:VAL:CG2	2.76	0.45
1:A:334:PHE:C	1:A:334:PHE:CD1	2.90	0.45
1:A:645:GLY:C	1:A:647:ILE:CD1	2.84	0.45
1:A:395:MET:HE3	1:A:641:THR:HG21	1.99	0.45
1:A:325:ASN:ND2	1:A:325:ASN:N	2.58	0.45
1:A:530:ASN:O	2:A:725:GOL:H32	2.17	0.45
1:A:531:SER:CB	1:A:548:LEU:HD11	2.47	0.45
1:A:437:ARG:HD3	1:A:459:ASN:HB2	1.99	0.45
1:A:264:PHE:CE2	1:A:379:PRO:HB3	2.52	0.45
1:A:423:LEU:O	1:A:423:LEU:HD23	2.17	0.45
1:A:422:ASN:HB3	1:A:425:LYS:CG	2.46	0.45
1:A:472:THR:HB	1:A:524:GLU:CG	2.44	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:316:VAL:HG13	1:A:321:THR:H	1.80	0.45
1:A:276:ASN:OD1	1:A:607:ILE:N	2.38	0.45
1:A:442:ASN:O	1:A:444:THR:O	2.35	0.45
1:A:521:TYR:HB2	1:A:523:LEU:HD21	1.98	0.45
1:A:530:ASN:ND2	1:A:531:SER:H	2.13	0.45
1:A:297:PHE:HA	1:A:674:GLU:O	2.17	0.45
1:A:531:SER:CA	1:A:548:LEU:CD1	2.90	0.44
1:A:695:ASP:CG	1:A:695:ASP:O	2.55	0.44
1:A:436:TYR:CZ	1:A:451:LYS:HD2	2.53	0.44
1:A:370:THR:HG22	1:A:371:LEU:HD23	1.99	0.44
1:A:527:MET:CE	1:A:624:MET:CA	2.94	0.44
1:A:469:MET:HE2	1:A:566:GLY:HA3	1.98	0.44
1:A:613:GLU:C	1:A:614:THR:HG23	2.38	0.44
1:A:556:GLN:HG3	1:A:557:PRO:CD	2.46	0.44
1:A:449:PHE:N	1:A:449:PHE:CD2	2.86	0.44
1:A:417:PHE:CD1	1:A:417:PHE:C	2.90	0.44
1:A:506:PRO:O	1:A:507:GLN:C	2.55	0.44
1:A:304:VAL:O	1:A:404:PHE:N	2.33	0.43
1:A:371:LEU:CD2	1:A:383:SER:HA	2.48	0.43
1:A:307:PHE:CE2	1:A:666:GLN:HG3	2.53	0.43
1:A:692:ASN:O	1:A:693:TYR:HD2	2.01	0.43
1:A:404:PHE:CE1	1:A:406:TYR:HB2	2.53	0.43
1:A:304:VAL:HG22	1:A:669:VAL:CG2	2.49	0.43
1:A:394:LYS:HE3	1:A:394:LYS:HB3	1.61	0.43
1:A:512:THR:CG2	1:A:560:ARG:O	2.66	0.43
1:A:245:HIS:CG	1:A:642:PRO:HB3	2.53	0.43
1:A:494:ARG:HB3	1:A:502:TYR:O	2.18	0.43
1:A:423:LEU:HD23	1:A:423:LEU:C	2.39	0.43
1:A:547:MET:C	1:A:548:LEU:HD12	2.39	0.43
1:A:254:SER:HB2	1:A:258:SER:C	2.38	0.42
1:A:469:MET:HG2	1:A:511:MET:SD	2.60	0.42
1:A:237:TRP:HD1	1:A:667:VAL:HG12	1.84	0.42
1:A:371:LEU:HD23	1:A:383:SER:HB3	2.00	0.42
1:A:332:GLN:HG3	1:A:641:THR:HG23	2.01	0.42
1:A:522:ALA:O	1:A:525:ASN:C	2.58	0.42
1:A:406:TYR:CE2	1:A:634:PRO:HD3	2.54	0.42
1:A:465:PHE:HA	1:A:466:PRO:HD3	1.91	0.42
1:A:604:GLN:HE21	1:A:604:GLN:HB3	1.55	0.42
1:A:302:LEU:CD2	1:A:302:LEU:C	2.88	0.42
1:A:406:TYR:CD1	1:A:407:ASN:C	2.93	0.42
1:A:289:ARG:NH1	1:A:289:ARG:HG2	2.18	0.42
1:A:693:TYR:HE2	1:A:713:ARG:NH2	2.17	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:252:SER:HB3	1:A:263:TYR:CE2	2.55	0.42
1:A:242:TYR:HB3	1:A:365:GLN:OE1	2.19	0.42
1:A:473:GLN:HG2	1:A:474:GLY:N	2.34	0.42
1:A:320:THR:C	1:A:321:THR:CG2	2.87	0.42
1:A:227:ASP:O	1:A:675:LEU:HB2	2.20	0.42
1:A:354:PRO:HB3	1:A:359:GLN:HG3	2.00	0.42
1:A:530:ASN:ND2	1:A:531:SER:N	2.68	0.41
1:A:326:ASN:O	1:A:326:ASN:OD1	2.38	0.41
1:A:420:SER:CB	1:A:721:THR:HG23	2.48	0.41
1:A:546:ASN:N	1:A:546:ASN:HD22	2.14	0.41
1:A:395:MET:CE	1:A:641:THR:HG21	2.51	0.41
1:A:424:PHE:HB3	1:A:462:LYS:NZ	2.35	0.41
1:A:403:GLU:O	1:A:403:GLU:CG	2.68	0.41
1:A:235:ARG:HD3	1:A:357:PRO:HA	2.03	0.41
1:A:442:ASN:OD1	1:A:444:THR:N	2.53	0.41
1:A:590:ILE:CG2	1:A:591:VAL:N	2.81	0.41
1:A:302:LEU:HD21	1:A:304:VAL:CG2	2.45	0.41
1:A:531:SER:HB3	1:A:548:LEU:HD11	2.02	0.41
1:A:370:THR:HG21	1:A:383:SER:CB	2.49	0.41
1:A:691:ASN:C	1:A:691:ASN:ND2	2.74	0.41
1:A:480:GLY:O	1:A:481:VAL:HB	2.18	0.41
1:A:291:ILE:HG13	1:A:719:TYR:HD2	1.85	0.41
1:A:493:ASN:O	1:A:494:ARG:CG	2.68	0.41
1:A:513:ASN:ND2	1:A:526:THR:CB	2.83	0.41
1:A:239:LEU:HD22	1:A:240:PRO:O	2.20	0.41
1:A:304:VAL:HB	1:A:404:PHE:HB3	2.02	0.41
1:A:633:PRO:HA	1:A:634:PRO:HD3	1.87	0.41
1:A:666:GLN:H	1:A:666:GLN:HG2	1.61	0.41
1:A:287:TRP:CG	1:A:603:LEU:HD13	2.56	0.41
1:A:587:LEU:HD12	1:A:587:LEU:H	1.86	0.41
1:A:300:ARG:O	1:A:408:PHE:HB2	2.20	0.41
1:A:428:ASN:HD22	1:A:428:ASN:N	2.19	0.41
1:A:357:PRO:HB2	1:A:358:PRO:CD	2.51	0.41
1:A:318:ASP:O	1:A:318:ASP:OD1	2.38	0.41
1:A:607:ILE:HB	1:A:608:TRP:CE3	2.56	0.40
1:A:254:SER:HB3	1:A:259:ASN:HA	2.03	0.40
1:A:718:ARG:O	1:A:719:TYR:CD1	2.74	0.40
1:A:341:LEU:HG	1:A:391:PHE:CZ	2.55	0.40
1:A:574:GLN:OE1	1:A:574:GLN:C	2.60	0.40
1:A:290:LEU:HD11	1:A:297:PHE:CD2	2.56	0.40
1:A:543:LEU:O	1:A:546:ASN:ND2	2.55	0.40
1:A:211:VAL:HG13	1:A:212:GLY:N	2.37	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	514/724 (71%)	488 (95%)	19 (4%)	7 (1%)	16 69

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	481	VAL
1	A	506	PRO
1	A	445	GLY
1	A	620	PRO
1	A	466	PRO
1	A	514	ASN
1	A	534	ALA

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	451/613 (74%)	347 (77%)	104 (23%)	1 6

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	220	CYS
1	A	225	MET
1	A	229	VAL
1	A	231	THR

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Mol	Chain	Res	Type
1	A	236	THR
1	A	238	VAL
1	A	239	LEU
1	A	241	SER
1	A	251	LYS
1	A	275	PHE
1	A	277	ARG
1	A	279	HIS
1	A	285	ARG
1	A	289	ARG
1	A	291	ILE
1	A	293	ASN
1	A	302	LEU
1	A	303	ARG
1	A	309	ILE
1	A	311	VAL
1	A	312	LYS
1	A	314	VAL
1	A	315	THR
1	A	325	ASN
1	A	328	THR
1	A	330	THR
1	A	331	VAL
1	A	335	THR
1	A	337	ASP
1	A	344	VAL
1	A	349	THR
1	A	362	THR
1	A	371	LEU
1	A	375	ASN
1	A	380	THR
1	A	391	PHE
1	A	400	ASN
1	A	403	GLU
1	A	406	TYR
1	A	420	SER
1	A	428	ASN
1	A	432	ASP
1	A	435	LEU
1	A	436	TYR
1	A	439	VAL
1	A	441	THR

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Mol	Chain	Res	Type
1	A	448	GLN
1	A	449	PHE
1	A	459	ASN
1	A	462	LYS
1	A	469	MET
1	A	476	ASN
1	A	483	ARG
1	A	489	PHE
1	A	491	THR
1	A	501	SER
1	A	509	ASN
1	A	512	THR
1	A	519	ASN
1	A	523	LEU
1	A	530	ASN
1	A	543	LEU
1	A	546	ASN
1	A	547	MET
1	A	548	LEU
1	A	550	THR
1	A	552	GLU
1	A	554	GLU
1	A	561	VAL
1	A	572	ASN
1	A	574	GLN
1	A	587	LEU
1	A	589	GLU
1	A	594	SER
1	A	595	VAL
1	A	598	GLU
1	A	604	GLN
1	A	619	HIS
1	A	630	LYS
1	A	637	LEU
1	A	639	LYS
1	A	646	ASN
1	A	647	ILE
1	A	657	SER
1	A	660	THR
1	A	664	THR
1	A	666	GLN
1	A	668	THR

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Mol	Chain	Res	Type
1	A	677	LYS
1	A	678	GLU
1	A	679	ASN
1	A	680	SER
1	A	686	GLU
1	A	687	ILE
1	A	691	ASN
1	A	692	ASN
1	A	698	PHE
1	A	699	VAL
1	A	705	SER
1	A	706	THR
1	A	708	GLU
1	A	711	THR
1	A	721	THR
1	A	722	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	245	HIS
1	A	292	ASN
1	A	293	ASN
1	A	310	GLN
1	A	325	ASN
1	A	326	ASN
1	A	332	GLN
1	A	340	GLN
1	A	375	ASN
1	A	407	ASN
1	A	414	HIS
1	A	428	ASN
1	A	448	GLN
1	A	476	ASN
1	A	509	ASN
1	A	514	ASN
1	A	530	ASN
1	A	546	ASN
1	A	617	HIS
1	A	646	ASN
1	A	661	GLN
1	A	666	GLN

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Mol	Chain	Res	Type
1	A	679	ASN
1	A	692	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 ⓘ

Of 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 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	GOL	A	725	-	5,5,5	0.32	0	5,5,5	0.24	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	GOL	A	725	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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	516/724 (71%)	-0.10	0 100 100	25, 54, 77, 122	0

There are no RSRZ outliers to report.

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	GOL	A	725	6/6	0.20	0.71	34,43,61,76	0
3	NA	A	726	1/1	0.20	0.16	20,20,20,20	0
3	NA	A	727	1/1	0.16	-2.03	8,8,8,8	0
3	NA	A	728	1/1	0.19	-3.10	7,7,7,7	0

6.5 Other polymers ⓘ

There are no such residues in this entry.