



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:29 PM UTC

PDB ID : 3NTT / pdb_00003ntt
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 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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

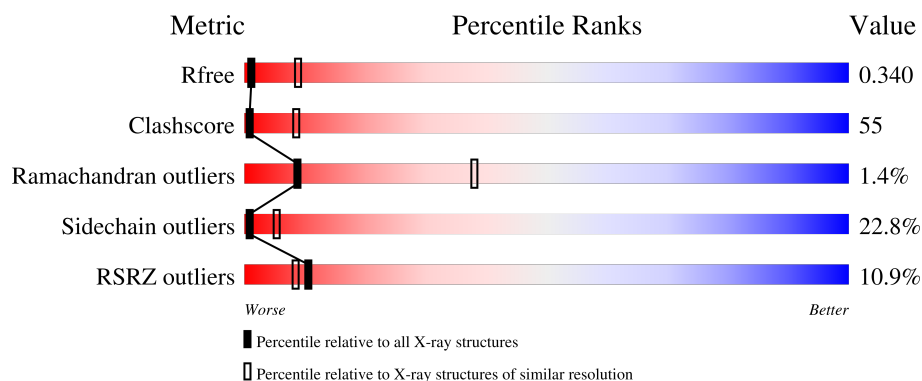
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1070 (3.50-3.42)
Clashscore	190562	1128 (3.50-3.42)
Ramachandran outliers	187476	1101 (3.50-3.42)
Sidechain outliers	187428	1102 (3.50-3.42)
RSRZ outliers	180081	1070 (3.50-3.42)

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 $\leq 5\%$. 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	724	8% 26% 35% 10% 29%

2 Entry composition [i](#)

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

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

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 1: Capsid protein





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) 78.5 (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 0.348 , 0.340	Depositor DCC
R_{free} test set	2000 reflections (0.26%)	wwPDB-VP
Wilson B-factor (Å ²)	46.9	Xtriage
Anisotropy	0.301	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 70.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.09	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.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: NA, GOL

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	0.39	0/4239	0.89	13/5793 (0.2%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	467	GLY	CA-C-N	7.08	127.12	119.90
1	A	467	GLY	C-N-CA	7.08	127.12	119.90
1	A	321	THR	N-CA-C	6.67	120.59	111.39
1	A	618	PHE	N-CA-C	-5.88	102.76	110.53
1	A	347	ASN	N-CA-C	5.67	118.98	112.57
1	A	398	THR	N-CA-C	5.59	118.09	111.33
1	A	400	ASN	N-CA-C	5.50	117.63	110.53
1	A	431	VAL	N-CA-C	5.47	115.83	108.17
1	A	454	ALA	CB-CA-C	-5.45	110.27	116.54
1	A	631	HIS	CA-C-N	5.38	125.92	120.38
1	A	631	HIS	C-N-CA	5.38	125.92	120.38
1	A	619	HIS	N-CA-C	-5.16	103.23	109.57
1	A	516	GLN	N-CA-C	-5.13	99.86	110.80

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	4111	0	3858	440	0
2	A	6	0	8	1	0
3	A	3	0	0	0	0
All	All	4120	0	3866	440	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 55.

All (440) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A: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:646:ASN:C	1:A:647:ILE:HD12	1.83	1.03
1:A:480:GLY:O	1:A:481:VAL:CG2	2.05	1.03
1:A:468:PRO:HG3	1:A:590:ILE:HD13	1.49	0.95
1:A:647:ILE:HD12	1:A:647:ILE:N	1.76	0.94
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:679:ASN:HD22	1:A:679:ASN:C	1.80	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:HG2	1:A:289:ARG:HH11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:646:ASN:C	1:A:646:ASN:HD22	1.88	0.82
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
1:A:610:LYS:HB2	1:A:632:PRO:HG3	1.62	0.81
1:A:489:PHE:HD2	1:A:489:PHE:C	1.89	0.80
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:403:GLU:CD	1:A:403:GLU:H	1.91	0.79
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:N	1:A:476:ASN:HD22	1.79	0.77
1:A:375:ASN:OD1	1:A:500:ALA:HB2	1.85	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:428:ASN:HD21	1:A:431:VAL:CG2	1.99	0.76
1:A:550:THR:CG2	1:A:602:TYR:CE2	2.68	0.76
1:A:316:VAL:CG2	1:A:321:THR:HA	2.08	0.76
1:A:406:TYR:CD1	1:A:406:TYR:C	2.64	0.76
1:A:292:ASN:HD22	1:A:688:GLN:HB3	1.51	0.76
1:A:513:ASN:HB2	1:A:522:ALA:H	1.50	0.76
1:A:471:ARG:HH12	1:A:565:VAL:HG12	1.50	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:THR:HG22	1:A:371:LEU:N	2.01	0.75
1:A:281:HIS:CE1	1:A:669:VAL:HG11	2.23	0.74
1:A:472:THR:HB	1:A:524:GLU:HG3	1.68	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:334:PHE:HB3	1:A:393:SER:HB3	1.70	0.73
1:A:472:THR:CG2	1:A:493:ASN:ND2	2.39	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
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:391:PHE:HD1	1:A:391:PHE:H	1.39	0.71
1:A:307:PHE:HE1	1:A:668:THR:CG2	2.03	0.71
1:A:469:MET:HE2	1:A:566:GLY:HA3	1.70	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:510:GLY:C	1:A:559:ASN:ND2	2.49	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:294:TYR:CE1	1:A:675:LEU:HD23	2.28	0.69
1:A:682:ARG:NH1	1:A:686:GLU:HG3	2.08	0.69
1:A:326:ASN:HD21	1:A:329:SER:HB2	1.58	0.68
1:A:489:PHE:HE2	1:A:494:ARG:CZ	2.06	0.68
1:A:419:PRO:HD3	1:A:597:MET:HE1	1.75	0.68
1:A:356:PHE:CD2	1:A:358:PRO:HG2	2.29	0.68
1:A:370:THR:HG21	1:A:383:SER:HB2	1.74	0.68
1:A:316:VAL:HG22	1:A:321:THR:CB	2.23	0.68
1:A:489:PHE:HE2	1:A:494:ARG:NH2	1.92	0.68
1:A:406:TYR:CE1	1:A:407:ASN:C	2.72	0.68
1:A:650:PHE:CD2	1:A:651:SER:N	2.62	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:TYR:C	1:A:406:TYR:HD1	2.00	0.67
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:270:TRP:CE2	1:A:639:LYS:HD3	2.30	0.66
1:A:437:ARG:O	1:A:449:PHE:HB3	1.95	0.66
1:A:527:MET:CE	1:A:624:MET:HA	2.25	0.66
1:A:325:ASN:H	1:A:325:ASN:ND2	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:406:TYR:C	1:A:407:ASN:HD22	2.05	0.65
1:A:424:PHE:HD1	1:A:462:LYS:HZ3	1.45	0.65
1:A:403:GLU:OE1	1:A:403:GLU:N	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:N	1:A:400:ASN:OD1	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
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:645:GLY:O	1:A:647:ILE:HD13	1.98	0.64
1:A:646:ASN:HD22	1:A:647:ILE:N	1.96	0.64
1:A:281:HIS:HE1	1:A:669:VAL:HG11	1.63	0.64
1:A:546:ASN:H	1:A:546:ASN:HD22	1.42	0.64
1:A:292:ASN:HD21	1:A:689:TYR:N	1.95	0.63
1:A:370:THR:HG22	1:A:371:LEU:CD2	2.28	0.63
1:A:468:PRO:CG	1:A:590:ILE:HD13	2.27	0.63
1:A:403:GLU:CD	1:A:403:GLU:N	2.56	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:311:VAL:HG23	1:A:663:SER:HB3	1.79	0.63
1:A:619:HIS:O	1:A:619:HIS:ND1	2.30	0.63
1:A:428:ASN:HD21	1:A:431:VAL:HG23	1.62	0.63
1:A:320:THR:C	1:A:321:THR:HG22	2.24	0.62
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:572:ASN:OD1	1:A:572:ASN:C	2.42	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:LEU:C	1:A:302:LEU:HD23	2.24	0.62
1:A:370:THR:CG2	1:A:371:LEU:H	2.11	0.61
1:A:371:LEU:H	1:A:371:LEU:CD2	2.13	0.61
1:A:477:LEU:O	1:A:519:ASN:ND2	2.33	0.61
1:A:489:PHE:CD2	1:A:494:ARG:NH2	2.67	0.61
1:A:618:PHE:O	1:A:619:HIS:C	2.41	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:391:PHE:N	1:A:391:PHE:CD1	2.68	0.61
1:A:419:PRO:HB3	1:A:724:LEU:HD21	1.83	0.61
1:A:698:PHE:C	1:A:698:PHE:CD2	2.79	0.61
1:A:370:THR:HG22	1:A:371:LEU:HD22	1.82	0.60
1:A:523:LEU:N	1:A:523:LEU:CD2	2.65	0.60
1:A:356:PHE:O	1:A:359:GLN:HG2	2.01	0.60
1:A:453:LEU:O	1:A:456:ARG:HG2	2.02	0.60
1:A:521:TYR:O	1:A:523:LEU:HD23	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
1:A:375:ASN:N	1:A:375:ASN:ND2	2.40	0.60
1:A:548:LEU:HD12	1:A:548:LEU:N	2.16	0.60
1:A:525:ASN:OD1	1:A:525:ASN:C	2.45	0.59
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:480:GLY:C	1:A:481:VAL:HG23	2.23	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:HD22	1:A:325:ASN:N	1.88	0.59
1:A:433:GLN:NE2	1:A:460:THR:HB	2.17	0.59
1:A:691:ASN:HD22	1:A:691:ASN:C	2.11	0.59
1:A:395:MET:HE3	1:A:641:THR:HG21	1.83	0.59
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:510:GLY:C	1:A:559:ASN:HD22	2.10	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:394:LYS:HE3	1:A:396:LEU:HD21	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:698:PHE:HD2	1:A:698:PHE:C	2.12	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:435:LEU:C	1:A:436:TYR:HD1	2.13	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:292:ASN:HD21	1:A:689:TYR:H	1.51	0.56
1:A:531:SER:HA	1:A:548:LEU:CD1	2.32	0.56
1:A:679:ASN:C	1:A:679:ASN:ND2	2.52	0.56
1:A:435:LEU:C	1:A:436:TYR:CD1	2.83	0.56
1:A:514:ASN:C	1:A:515:LEU:HD12	2.30	0.56
1:A:695:ASP:N	1:A:696:PRO:HD3	2.21	0.56
1:A:403:GLU:CD	1:A:403:GLU:O	2.48	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:O	1:A:504:VAL:HG23	2.05	0.56
1:A:293:ASN:ND2	1:A:293:ASN:N	2.54	0.56
1:A:317:GLN:HA	1:A:317:GLN:OE1	2.05	0.55
1:A:436:TYR:HD1	1:A:436:TYR:N	2.04	0.55
1:A:513:ASN:O	1:A:514:ASN:HB3	2.06	0.55
1:A:420:SER:HB3	1:A:721:THR:HG23	1.88	0.55
1:A:505:PRO:CB	1:A:506:PRO:CD	2.81	0.55
1:A:548:LEU:N	1:A:548:LEU:CD1	2.68	0.55
1:A:252:SER:O	1:A:262:ALA:HA	2.06	0.55
1:A:619:HIS:ND1	1:A:619:HIS:C	2.64	0.55
1:A:354:PRO:HD3	1:A:361:PHE:CD2	2.41	0.55
1:A:406:TYR:HE1	1:A:407:ASN:C	2.15	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: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: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:247:TYR:HE2	1:A:268:THR:HG22	1.72	0.53
1:A:523:LEU:N	1:A:523:LEU:HD22	2.24	0.53
1:A:432:ASP:HA	1:A:454:ALA:H	1.74	0.53
1:A:599:ARG:HD2	1:A:623:ALA:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:621:SER:O	1:A:622:PRO:C	2.51	0.52
1:A:674:GLU:C	1:A:675:LEU:HD12	2.34	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:488:ALA:O	1:A:492:THR:HG23	2.10	0.52
1:A:528:ILE:HG22	1:A:547:MET:HG3	1.92	0.52
1:A:646:ASN:C	1:A:646:ASN:ND2	2.58	0.52
1:A:318:ASP:O	1:A:319:SER:HB2	2.10	0.52
1:A:530:ASN:HD22	1:A:531:SER:N	2.08	0.52
1:A:414:HIS:C	1:A:414:HIS:CD2	2.87	0.51
1:A:444:THR:O	1:A:446:GLY:N	2.38	0.51
1:A:519:ASN:OD1	1:A:519:ASN:N	2.43	0.51
1:A:693:TYR:HB2	1:A:696:PRO:HG3	1.92	0.51
1:A:276:ASN:OD1	1:A:276:ASN:C	2.54	0.51
1:A:425:LYS:HB3	1:A:457:TYR:CG	2.45	0.51
1:A:432:ASP:OD2	1:A:432:ASP:N	2.42	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:507:GLN:O	1:A:508:PRO:C	2.54	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:285:ARG:O	1:A:288:GLN:HB3	2.10	0.50
1:A:371:LEU:HD21	1:A:383:SER:HA	1.93	0.50
1:A:241:SER:OG	1:A:661:GLN:O	2.27	0.50
1:A:249:GLU:HA	1:A:266:TYR:CD2	2.47	0.50
1:A:374:ASP:C	1:A:375:ASN:HD22	2.19	0.50
1:A:437:ARG:CD	1:A:459:ASN:HB2	2.41	0.50
1:A:334:PHE:CD1	1:A:334:PHE:C	2.90	0.50
1:A:441:THR:HA	1:A:446:GLY:O	2.12	0.50
1:A:522:ALA:O	1:A:525:ASN:O	2.30	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:645:GLY:C	1:A:647:ILE:CD1	2.84	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:223:THR:HG21	1:A:225:MET:HE2	1.93	0.49
1:A:370:THR:CG2	1:A:383:SER:HB2	2.43	0.49
1:A:477:LEU:HD11	1:A:521:TYR:CG	2.48	0.49
1:A:525:ASN:OD1	1:A:525:ASN:O	2.30	0.49
1:A:695:ASP:CG	1:A:695:ASP:O	2.55	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:HIS:ND1	1:A:355:ALA:HB2	2.28	0.49
1:A:295:TRP:CH2	1:A:679:ASN:O	2.65	0.49
1:A:302:LEU:CD2	1:A:304:VAL:HG23	2.41	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:417:PHE:CD1	1:A:417:PHE:C	2.90	0.48
1:A:613:GLU:C	1:A:614:THR:HG23	2.38	0.48
1:A:292:ASN:ND2	1:A:689:TYR:N	2.59	0.48
1:A:506:PRO:O	1:A:507:GLN:C	2.55	0.48
1:A:357:PRO:N	1:A:358:PRO:HD2	2.29	0.48
1:A:613:GLU:HA	1:A:613:GLU:OE2	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:321:THR:O	1:A:321:THR:OG1	2.30	0.48
1:A:437:ARG:NE	1:A:459:ASN:HB2	2.28	0.48
1:A:471:ARG:HH12	1:A:565:VAL:HG13	1.77	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:423:LEU:HD23	1:A:423:LEU:C	2.39	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:636:MET:HE3	1:A:636:MET:HB2	1.64	0.47
1:A:547:MET:C	1:A:548:LEU:HD12	2.39	0.47
1:A:591:VAL:CG1	1:A:592:PRO:N	2.75	0.47
1:A:406:TYR:CD1	1:A:407:ASN:C	2.93	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:254:SER:HB2	1:A:258:SER:C	2.38	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:522:ALA:O	1:A:525:ASN:C	2.58	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:533:PRO:O	1:A:534:ALA:CB	2.63	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:ASN:HA	1:A:720:LEU:HD11	1.97	0.46
1:A:320:THR:C	1:A:321:THR:CG2	2.87	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: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: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:406:TYR:HE1	1:A:408:PHE:N	2.13	0.46
1:A:302:LEU:C	1:A:302:LEU:CD2	2.88	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:521:TYR:O	1:A:523:LEU:CD2	2.64	0.46
1:A:527:MET:HE1	1:A:624:MET:CB	2.45	0.46
1:A:277:ARG:HE	1:A:279:HIS:CE1	2.34	0.46
1:A:406:TYR:HE1	1:A:408:PHE:CA	2.29	0.46
1:A:513:ASN:ND2	1:A:526:THR:HB	2.31	0.46
1:A:270:TRP:CE3	1:A:637:LEU:HB3	2.50	0.46
1:A:211:VAL:HG21	1:A:327:LEU:HD23	1.97	0.45
1:A:598:GLU:H	1:A:598:GLU:HG2	1.51	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:513:ASN:HD22	1:A:526:THR:HB	1.81	0.45
1:A:325:ASN:ND2	1:A:325:ASN:N	2.58	0.45
1:A:574:GLN:OE1	1:A:574:GLN:C	2.60	0.45
1:A:264:PHE:CE2	1:A:379:PRO:HB3	2.52	0.45
1:A:437:ARG:HD3	1:A:459:ASN:HB2	1.99	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:408:PHE:HE1	1:A:671:MET:HE3	1.82	0.45
1:A:422:ASN:HB3	1:A:425:LYS:CG	2.46	0.45
1:A:423:LEU:O	1:A:423:LEU:HD23	2.17	0.45
1:A:276:ASN:OD1	1:A:607:ILE:N	2.38	0.45
1:A:316:VAL:HG13	1:A:321:THR:H	1.80	0.45
1:A:442:ASN:O	1:A:444:THR:O	2.35	0.45
1:A:472:THR:HB	1:A:524:GLU:CG	2.44	0.45
1:A:297:PHE:HA	1:A:674:GLU:O	2.17	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:531:SER:CA	1:A:548:LEU:CD1	2.90	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:ARG:O	1:A:376:THR:OG1	2.31	0.44
1:A:436:TYR:CZ	1:A:451:LYS:HD2	2.53	0.44
1:A:493:ASN:C	1:A:494:ARG:CG	2.90	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:449:PHE:CD2	1:A:449:PHE:N	2.86	0.44
1:A:556:GLN:HG3	1:A:557:PRO:CD	2.46	0.44
1:A:574:GLN:C	1:A:574:GLN:CD	2.85	0.43
1:A:304:VAL:O	1:A:404:PHE:N	2.33	0.43
1:A:307:PHE:CE2	1:A:666:GLN:HG3	2.53	0.43
1:A:371:LEU:CD2	1:A:383:SER:HA	2.48	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:225:MET:HE3	1:A:230:VAL:HG13	1.99	0.43
1:A:304:VAL:HG22	1:A:669:VAL:CG2	2.49	0.43
1:A:326:ASN:OD1	1:A:326:ASN:C	2.61	0.43
1:A:394:LYS:HE3	1:A:394:LYS:HB3	1.61	0.43
1:A:419:PRO:CD	1:A:597:MET:HE1	2.45	0.43
1:A:512:THR:CG2	1:A:560:ARG:O	2.66	0.43
1:A:691:ASN:C	1:A:691:ASN:ND2	2.74	0.43
1:A:245:HIS:CG	1:A:642:PRO:HB3	2.53	0.43
1:A:505:PRO:O	1:A:506:PRO:C	2.60	0.43
1:A:494:ARG:HB3	1:A:502:TYR:O	2.18	0.43
1:A:650:PHE:CD2	1:A:650:PHE:C	2.94	0.42
1:A:237:TRP:HD1	1:A:667:VAL:HG12	1.84	0.42
1:A:469:MET:HG2	1:A:511:MET:SD	2.60	0.42
1:A:692:ASN:O	1:A:692:ASN:CG	2.61	0.42
1:A:371:LEU:HD23	1:A:383:SER:HB3	2.00	0.42
1:A:469:MET:HB3	1:A:469:MET:HE3	1.64	0.42
1:A:671:MET:HE2	1:A:671:MET:HB3	1.97	0.42
1:A:332:GLN:HG3	1:A:641:THR:HG23	2.01	0.42
1:A:608:TRP:CD1	1:A:608:TRP:C	2.96	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:218:TRP:CD1	1:A:218:TRP:C	2.97	0.42
1:A:242:TYR:HB3	1:A:365:GLN:OE1	2.19	0.42
1:A:252:SER:HB3	1:A:263:TYR:CE2	2.55	0.42
1:A:289:ARG:HG2	1:A:289:ARG:NH1	2.18	0.42
1:A:473:GLN:HG2	1:A:474:GLY:N	2.34	0.42
1:A:693:TYR:HE2	1:A:713:ARG:NH2	2.17	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:279:HIS:CD2	1:A:279:HIS:C	2.98	0.42
1:A:694:ASN:O	1:A:695:ASP:C	2.62	0.42
1:A:326:ASN:OD1	1:A:326:ASN:O	2.38	0.41
1:A:420:SER:CB	1:A:721:THR:HG23	2.48	0.41
1:A:530:ASN:ND2	1:A:531:SER:N	2.68	0.41
1:A:546:ASN:HD22	1:A:546:ASN:N	2.14	0.41
1:A:235:ARG:HD3	1:A:357:PRO:HA	2.03	0.41
1:A:403:GLU:O	1:A:403:GLU:CG	2.68	0.41
1:A:424:PHE:HB3	1:A:462:LYS:NZ	2.35	0.41
1:A:442:ASN:OD1	1:A:444:THR:N	2.53	0.41
1:A:234:THR:C	1:A:235:ARG:HG2	2.45	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:370:THR:HG21	1:A:383:SER:CB	2.49	0.41
1:A:531:SER:HB3	1:A:548:LEU:HD11	2.02	0.41
1:A:291:ILE:HG13	1:A:719:TYR:HD2	1.85	0.41
1:A:480:GLY:O	1:A:481:VAL:HB	2.18	0.41
1:A:239:LEU:HD22	1:A:240:PRO:O	2.20	0.41
1:A:287:TRP:CG	1:A:603:LEU:HD13	2.56	0.41
1:A:304:VAL:HB	1:A:404:PHE:HB3	2.02	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:587:LEU:HD12	1:A:587:LEU:H	1.86	0.41
1:A:633:PRO:HA	1:A:634:PRO:HD3	1.87	0.41
1:A:666:GLN:HG2	1:A:666:GLN:H	1.61	0.41
1:A:300:ARG:O	1:A:408:PHE:HB2	2.20	0.41
1:A:318:ASP:O	1:A:318:ASP:OD1	2.38	0.41
1:A:357:PRO:HB2	1:A:358:PRO:CD	2.51	0.41
1:A:428:ASN:HD22	1:A:428:ASN:N	2.19	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:341:LEU:HG	1:A:391:PHE:CZ	2.55	0.40
1:A:476:ASN:N	1:A:476:ASN:ND2	2.51	0.40
1:A:718:ARG:O	1:A:719:TYR:CD1	2.74	0.40
1:A:516:GLN:O	1:A:517:GLY:C	2.63	0.40
1:A:290:LEU:HD11	1:A:297:PHE:CD2	2.56	0.40
1:A:211:VAL:HG13	1:A:212:GLY:N	2.37	0.40
1:A:543:LEU:O	1:A:546:ASN:ND2	2.55	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	514/724 (71%)	488 (95%)	19 (4%)	7 (1%)	9	38

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 [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	451/613 (74%)	348 (77%)	103 (23%)	1	5

All (103) 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	230	VAL

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Mol	Chain	Res	Type
1	A	231	THR
1	A	236	THR
1	A	238	VAL
1	A	239	LEU
1	A	241	SER
1	A	255	VAL
1	A	277	ARG
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	394	LYS
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	450	ASN
1	A	459	ASN
1	A	476	ASN
1	A	483	ARG
1	A	489	PHE
1	A	491	THR
1	A	497	LEU
1	A	509	ASN
1	A	512	THR
1	A	519	ASN
1	A	523	LEU
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	558	VAL
1	A	561	VAL
1	A	572	ASN
1	A	587	LEU
1	A	589	GLU
1	A	591	VAL
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	646	ASN
1	A	647	ILE
1	A	653	VAL
1	A	656	SER
1	A	660	THR
1	A	664	THR
1	A	666	GLN
1	A	668	THR
1	A	669	VAL
1	A	676	LYS

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Mol	Chain	Res	Type
1	A	677	LYS
1	A	678	GLU
1	A	679	ASN
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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	245	HIS
1	A	288	GLN
1	A	292	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	421	GLN
1	A	428	ASN
1	A	476	ASN
1	A	503	GLN
1	A	509	ASN
1	A	514	ASN
1	A	530	ASN
1	A	546	ASN
1	A	604	GLN
1	A	617	HIS
1	A	646	ASN
1	A	661	GLN

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Mol	Chain	Res	Type
1	A	666	GLN
1	A	679	ASN
1	A	692	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	0.36	0	5,5,5	0.34	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	-

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	725	GOL	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	1.06	56 (10%) 10 8	25, 54, 77, 122	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	533	PRO	5.2
1	A	518	SER	4.3
1	A	318	ASP	4.1
1	A	546	ASN	4.0
1	A	319	SER	4.0
1	A	543	LEU	3.5
1	A	340	GLN	3.2
1	A	498	GLU	3.2
1	A	623	ALA	3.2
1	A	530	ASN	3.2
1	A	445	GLY	3.2
1	A	390	TYR	3.1
1	A	455	GLY	3.1
1	A	571	THR	3.0
1	A	695	ASP	3.0
1	A	531	SER	2.9
1	A	317	GLN	2.8
1	A	370	THR	2.8
1	A	391	PHE	2.7
1	A	716	GLY	2.7
1	A	490	ALA	2.7
1	A	499	GLY	2.6
1	A	481	VAL	2.6
1	A	346	GLY	2.6
1	A	545	GLY	2.6
1	A	263	TYR	2.5
1	A	625	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	677	LYS	2.5
1	A	692	ASN	2.5
1	A	283	SER	2.4
1	A	211	VAL	2.3
1	A	553	SER	2.3
1	A	381	GLU	2.3
1	A	670	GLU	2.3
1	A	422	ASN	2.3
1	A	458	ALA	2.3
1	A	539	THR	2.3
1	A	694	ASN	2.2
1	A	374	ASP	2.2
1	A	715	ILE	2.2
1	A	256	ASP	2.2
1	A	353	LEU	2.2
1	A	280	SER	2.1
1	A	470	GLY	2.1
1	A	679	ASN	2.1
1	A	474	GLY	2.1
1	A	657	SER	2.1
1	A	259	ASN	2.1
1	A	506	PRO	2.1
1	A	510	GLY	2.1
1	A	663	SER	2.1
1	A	538	THR	2.1
1	A	439	VAL	2.1
1	A	424	PHE	2.0
1	A	303	ARG	2.0
1	A	617	HIS	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 oligosaccharides 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. 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	B-factors(Å ²)	Q<0.9
3	NA	A	727	1/1	0.89	0.23	8,8,8,8	0
2	GOL	A	725	6/6	0.91	0.20	34,43,61,76	0
3	NA	A	728	1/1	0.95	0.12	7,7,7,7	0
3	NA	A	726	1/1	0.97	0.06	20,20,20,20	0

6.5 Other polymers [i](#)

There are no such residues in this entry.