Full wwPDB X-ray Structure Validation Report (i)

Aug 4, 2016 – 09:14 PM EDT

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 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

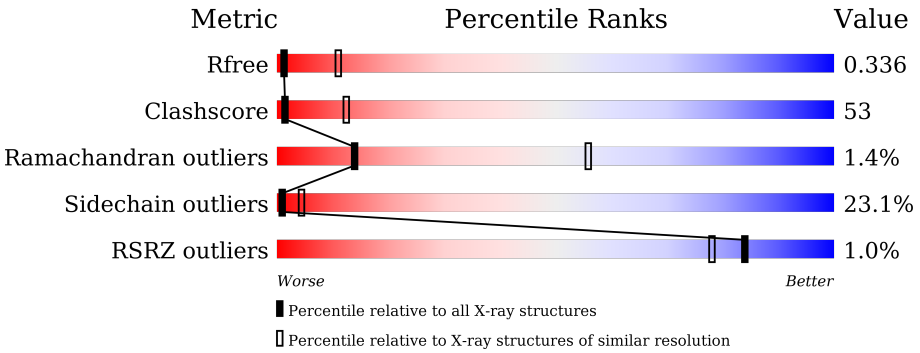
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 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}	91344	1000 (3.56-3.36)
Clashscore	102246	1090 (3.56-3.36)
Ramachandran outliers	100387	1057 (3.56-3.36)
Sidechain outliers	100360	1058 (3.56-3.36)
RSRZ outliers	91569	1005 (3.56-3.36)

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 <=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	% 28% 34% 10% 29%

2 Entry composition

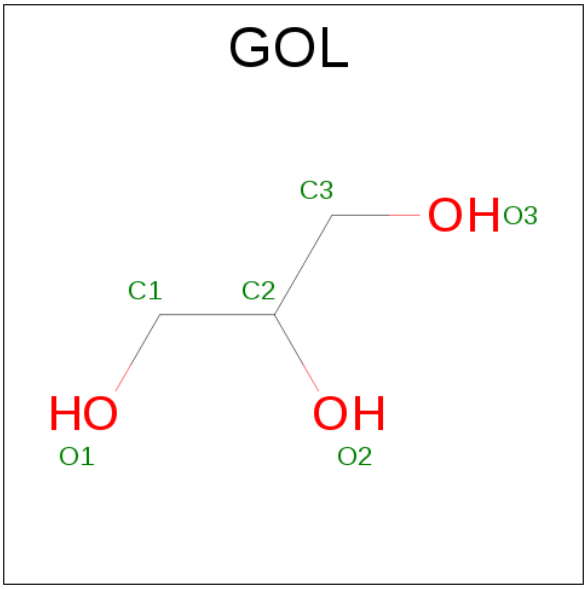
There are 3 unique types of molecules in this entry. The entry contains 4120 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (three-letter code: 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 (three-letter code: NA) (formula: Na).

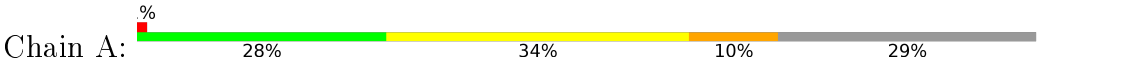
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
3	A	3	3	3	0	0

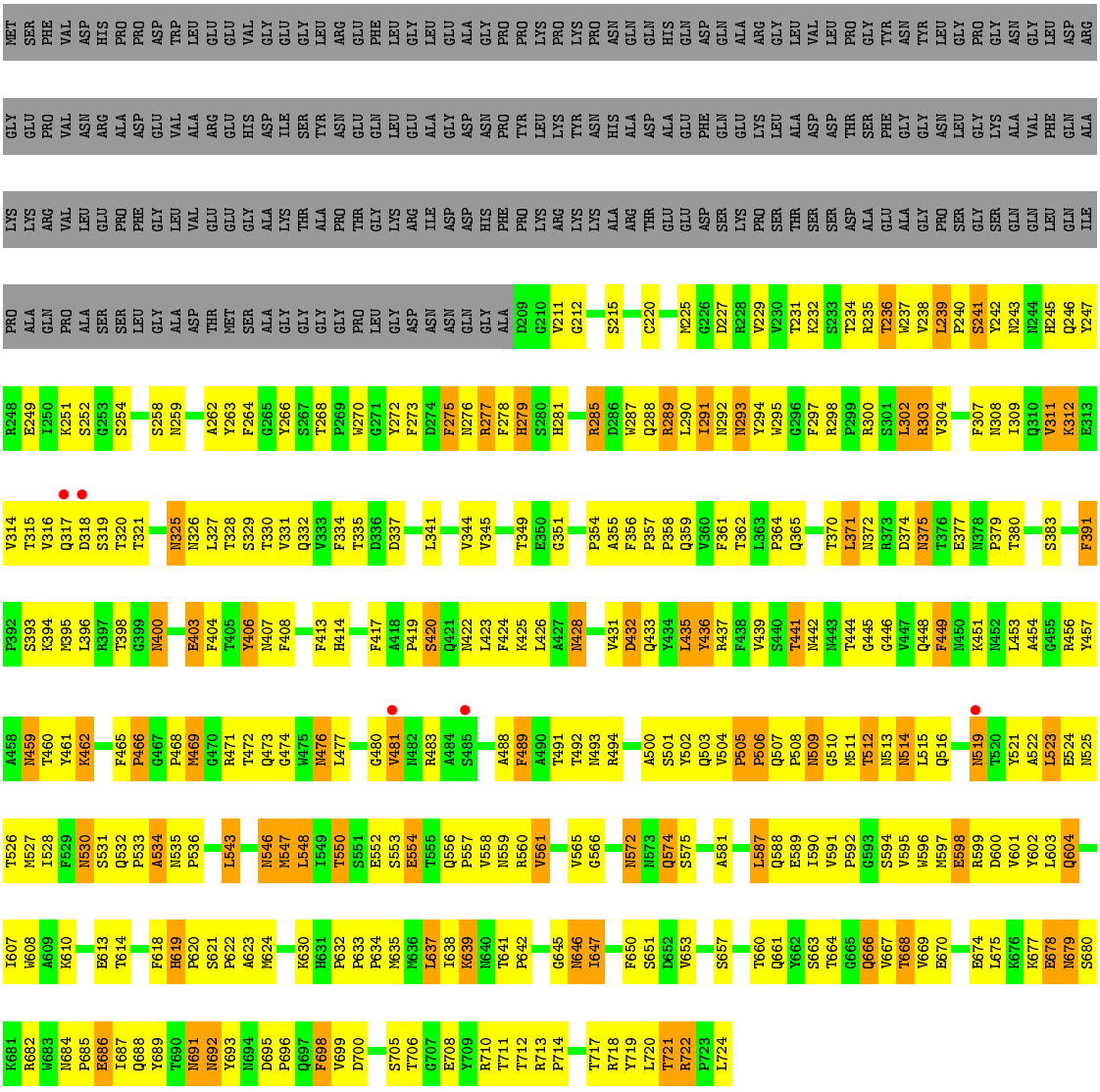
3 Residue-property plots (i)

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: Capsid protein

Chain A:





4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	3.48 (at 3.48Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.252 , 0.252 0.349 , 0.336	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)	0.31 , 45.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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(^{o})	Ideal(^{o})
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 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	421	0
2	A	6	0	8	1	0
3	A	3	0	0	0	0
All	All	4120	0	3866	421	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 53.

All (421) 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: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:O	1:A:481:VAL:HG12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:489:PHE:HD2	1:A:489:PHE:C	1.89	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H	1:A:391:PHE:HD1	1.39	0.71
1:A:406:TYR:CD1	1:A:406:TYR:C	2.64	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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:619:HIS:ND1	1:A:619:HIS:O	2.30	0.63
1:A:311:VAL:HG23	1:A:663:SER:HB3	1.79	0.63
1:A:406:TYR:HD1	1:A:406:TYR:C	2.00	0.63
1:A:419:PRO:HD3	1:A:597:MET:HE1	1.81	0.63
1:A:428:ASN:HD21	1:A:431:VAL:HG23	1.62	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: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: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: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:CD1	1:A:391:PHE:N	2.68	0.61
1:A:419:PRO:HB3	1:A:724:LEU:HD21	1.83	0.61
1:A:406:TYR:C	1:A:407:ASN:HD22	2.05	0.60
1:A:370:THR:HG22	1:A:371:LEU:HD22	1.82	0.60
1:A:523:LEU:CD2	1:A:523:LEU:N	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:302:LEU:C	1:A:302:LEU:HD23	2.24	0.58
1:A:320:THR:C	1:A:321:THR:HG22	2.24	0.58
1:A:394:LYS:HE3	1:A:396:LEU:HD21	1.87	0.57
1:A:469:MET:HE1	1:A:566:GLY:HA3	1.86	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:618:PHE:O	1:A:619:HIS:C	2.41	0.57
1:A:650:PHE:CE2	1:A:651:SER:O	2.57	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:436:TYR:N	1:A:436:TYR:HD1	2.04	0.55
1:A:513:ASN:O	1:A:514:ASN:HB3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:354:PRO:HD3	1:A:361:PHE:CD2	2.41	0.55
1:A:525:ASN:OD1	1:A:525:ASN:C	2.45	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:510:GLY:C	1:A:559:ASN:HD22	2.10	0.53
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:698:PHE:HD2	1:A:698:PHE:C	2.12	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: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:318:ASP:O	1:A:319:SER:HB2	2.10	0.52
1:A:435:LEU:C	1:A:436:TYR:CD1	2.83	0.52
1:A:530:ASN:HD22	1:A:531:SER:N	2.08	0.52
1:A:444:THR:O	1:A:446:GLY:N	2.38	0.51
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:403:GLU:CD	1:A:403:GLU:O	2.48	0.51
1:A:425:LYS:HB3	1:A:457:TYR:CG	2.45	0.51
1:A:432:ASP:N	1:A:432:ASP:OD2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:437:ARG:CD	1:A:459:ASN:HB2	2.41	0.50
1:A:619:HIS:ND1	1:A:619:HIS:C	2.64	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: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:370:THR:CG2	1:A:383:SER:HB2	2.43	0.49
1:A:406:TYR:HE1	1:A:407:ASN:C	2.15	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: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: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: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:273:PHE:CE1	1:A:638:ILE:HG21	2.49	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:279:HIS:CG	1:A:355:ALA:HB2	2.50	0.47
1:A:414:HIS:CD2	1:A:414:HIS:C	2.87	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
1:A:236:THR:HG23	1:A:666:GLN:NE2	2.30	0.47
1:A:276:ASN:OD1	1:A:276:ASN:C	2.54	0.47
1:A:406:TYR:HE1	1:A:408:PHE:N	2.13	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:264:PHE:HB2	1:A:377:GLU:O	2.15	0.46
1:A:211:VAL:HG23	1:A:398:THR:HG21	1.96	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:646:ASN:ND2	1:A:646:ASN:C	2.58	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:468:PRO:HG2	1:A:590:ILE:HD11	1.97	0.46
1:A:521:TYR:O	1:A:523:LEU:CD2	2.64	0.46
1:A:512:THR:HG22	1:A:560:ARG:O	2.16	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:374:ASP:C	1:A:375:ASN:HD22	2.19	0.45
1:A:598:GLU:HG2	1:A:598:GLU:H	1.51	0.45
1:A:295:TRP:CZ2	1:A:722:ARG:HG2	2.52	0.45
1:A:334:PHE:C	1:A:334:PHE:CD1	2.90	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:395:MET:HE3	1:A:641:THR:HG21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:645:GLY:C	1:A:647:ILE:CD1	2.84	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: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: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
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:417:PHE:CD1	1:A:417:PHE:C	2.90	0.44
1:A:449:PHE:N	1:A:449:PHE:CD2	2.86	0.44
1:A:556:GLN:HG3	1:A:557:PRO:CD	2.46	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:GLN:HG3	1:A:641:THR:HG23	2.01	0.42
1:A:465:PHE:HA	1:A:466:PRO:HD3	1.91	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:604:GLN:HB3	1:A:604:GLN:HE21	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: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:NH1	1:A:289:ARG:HG2	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
1:A:320:THR:C	1:A:321:THR:CG2	2.87	0.42
1:A:354:PRO:HB3	1:A:359:GLN:HG3	2.00	0.42
1:A:227:ASP:O	1:A:675:LEU:HB2	2.20	0.42
1:A:326:ASN:O	1:A:326:ASN:OD1	2.38	0.41
1:A:530:ASN:ND2	1:A:531:SER:N	2.68	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: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:395:MET:CE	1:A:641:THR:HG21	2.51	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: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: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:H	1:A:666:GLN:HG2	1.61	0.41
1:A:300:ARG:O	1:A:408:PHE:HB2	2.20	0.41
1:A:318:ASP:OD1	1:A:318:ASP:O	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:574:GLN:C	1:A:574:GLN:OE1	2.60	0.40
1:A:718:ARG:O	1:A:719:TYR:CD1	2.74	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%)	14 56

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%)	347 (77%)	104 (23%)	1 4

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no 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	0.34	0	5,5,5	0.22	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.

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, 95^{th} 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%)	-0.05	5 (0%)	84	78	25, 54, 77, 122	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	519	ASN	2.9
1	A	318	ASP	2.5
1	A	317	GLN	2.5
1	A	481	VAL	2.5
1	A	485	SER	2.5

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, 95^{th} 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
2	GOL	A	725	6/6	0.92	0.22	1.83	34,43,61,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	NA	A	726	1/1	0.93	0.18	-	20,20,20,20	0
3	NA	A	728	1/1	0.90	0.16	-	7,7,7,7	0
3	NA	A	727	1/1	0.95	0.16	-	8,8,8,8	0

6.5 Other polymers (i)

There are no such residues in this entry.