



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:22 PM GMT

PDB ID : 1AIV
Title : APO OVOTRANSFERRIN
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Deposited on : 1997-04-28
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

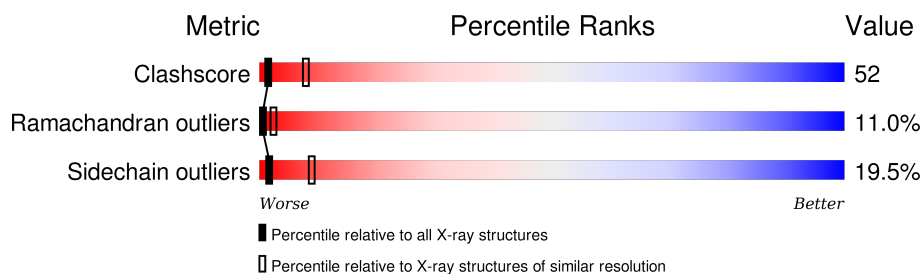
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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))
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	686	<div> <div></div> <div>26%</div> <div>56%</div> <div>16%</div> <div>.</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5340 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 OVOTRANSFERRIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	686	Total	C	N	O	S	0	0	0
			5312	3321	922	1028	41			

- Molecule 2 is a polymer of unknown type called SUGAR (2-MER).

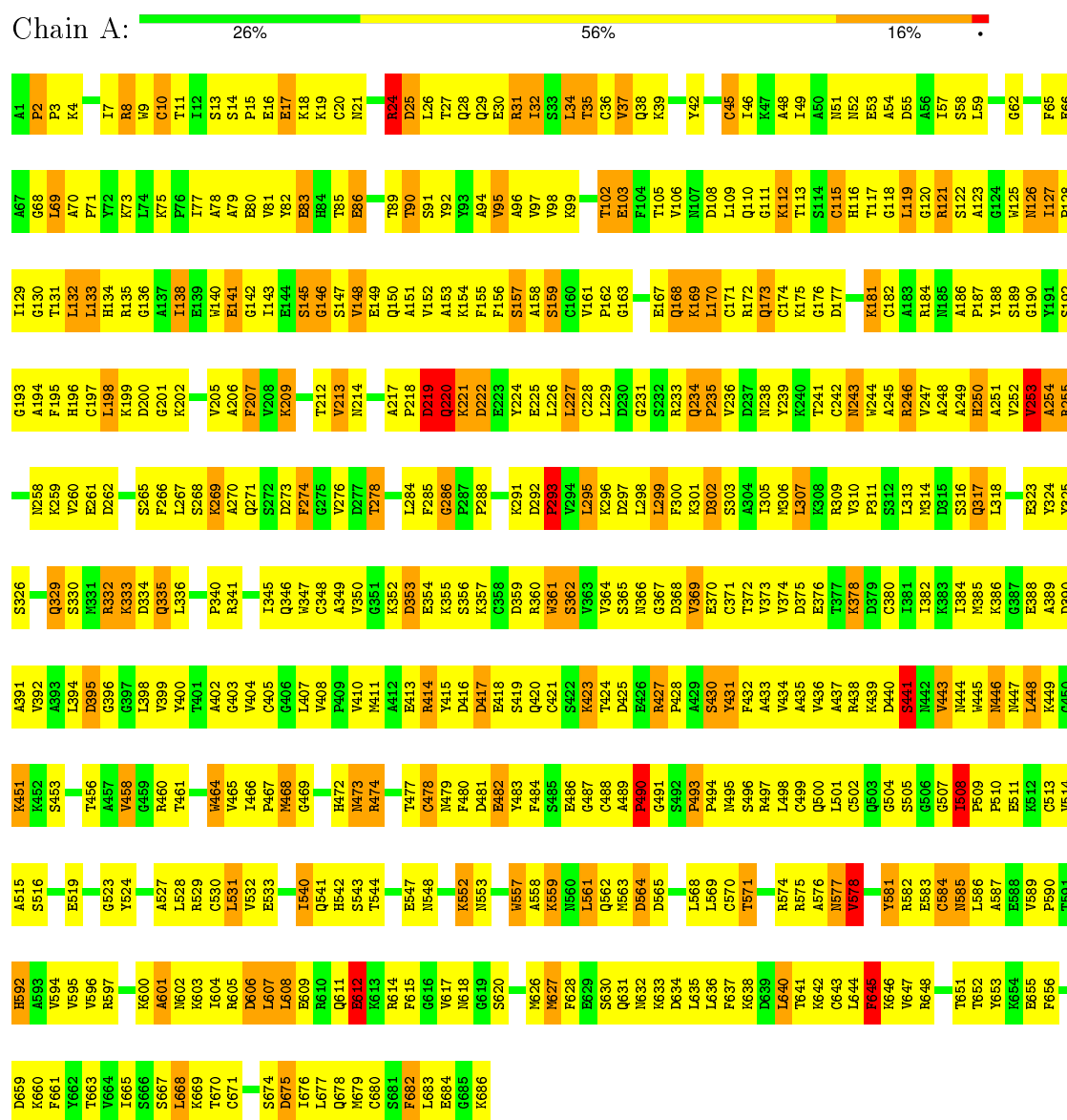
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	2	Total	C	N	O	0	0
			28	16	2	10		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

• Molecule 1: OVOTRANSFERRIN



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	92.26 Å 92.26 Å 178.19 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00	Depositor
% Data completeness (in resolution range)	74.9 (20.00-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.231 , 0.265	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5340	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.51	0/5418	0.79	1/7315 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	430	SER	N-CA-C	6.72	129.14	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	431	TYR	Sidechain

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5312	0	5188	546	0
2	A	28	0	25	6	0
All	All	5340	0	5213	547	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 52.

All (547) 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:508:ILE:HB	1:A:509:PRO:HD3	1.27	1.16
1:A:32:ILE:HB	1:A:266:PHE:HD1	1.29	0.98
1:A:19:LYS:HD3	1:A:299:LEU:HB2	1.46	0.95
1:A:117:THR:HA	1:A:189:SER:HB2	1.46	0.95
1:A:548:ASN:HD22	1:A:553:ASN:HD22	1.10	0.94
1:A:97:VAL:HB	1:A:226:LEU:HD23	1.50	0.93
1:A:135:ARG:HH21	1:A:229:LEU:HD22	1.30	0.93
1:A:99:LYS:HG3	1:A:198:LEU:HD12	1.52	0.92
1:A:82:TYR:HA	1:A:305:ILE:HD13	1.52	0.92
1:A:95:VAL:HG22	1:A:96:ALA:H	1.36	0.90
1:A:153:ALA:HA	1:A:169:LYS:HD2	1.54	0.89
1:A:181:LYS:HE3	1:A:182:CYS:SG	2.13	0.89
1:A:8:ARG:HG3	1:A:35:THR:HB	1.56	0.88
1:A:411:MET:SD	1:A:605:ARG:HA	2.14	0.88
1:A:524:TYR:HD1	1:A:540:ILE:HG22	1.38	0.88
1:A:143:ILE:HG23	1:A:147:SER:HB2	1.57	0.87
1:A:46:ILE:HD11	1:A:59:LEU:HD11	1.54	0.86
1:A:508:ILE:HB	1:A:509:PRO:CD	2.03	0.85
1:A:83:GLU:HG3	1:A:305:ILE:HD11	1.59	0.85
1:A:32:ILE:HB	1:A:266:PHE:CD1	2.11	0.85
1:A:134:HIS:HE1	1:A:329:GLN:HB3	1.40	0.85
1:A:119:LEU:HD13	1:A:184:ARG:HE	1.40	0.85
1:A:313:LEU:HD22	1:A:675:ASP:HB2	1.59	0.84
1:A:34:LEU:HD23	1:A:35:THR:H	1.41	0.84
1:A:132:LEU:HD12	1:A:135:ARG:HD2	1.56	0.84
1:A:581:TYR:H	1:A:581:TYR:HD1	1.22	0.84
1:A:147:SER:N	1:A:150:GLN:HB2	1.94	0.83
1:A:630:SER:HB2	1:A:635:LEU:HD12	1.60	0.83
1:A:174:CYS:HB2	1:A:181:LYS:HG3	1.61	0.82
1:A:493:PRO:HB2	1:A:496:SER:HB2	1.61	0.82
1:A:365:SER:HB2	1:A:369:VAL:HG23	1.62	0.82
1:A:667:SER:CB	2:A:688:NAG:H62	2.09	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:651:THR:HG22	1:A:652:THR:H	1.44	0.82
1:A:3:PRO:HB2	1:A:31:ARG:HH22	1.44	0.82
1:A:548:ASN:ND2	1:A:553:ASN:HD22	1.76	0.81
1:A:127:ILE:HB	1:A:128:PRO:HD3	1.61	0.80
1:A:152:VAL:HG11	1:A:170:LEU:HB3	1.61	0.80
1:A:118:GLY:HA2	1:A:162:PRO:HD2	1.64	0.80
1:A:488:CYS:SG	1:A:490:PRO:HD3	2.21	0.80
1:A:314:MET:SD	1:A:682:PHE:CZ	2.75	0.80
1:A:617:VAL:HG21	1:A:642:LYS:HA	1.62	0.79
1:A:135:ARG:NH2	1:A:229:LEU:HD22	1.96	0.79
1:A:558:ALA:HA	1:A:561:LEU:HD22	1.63	0.79
1:A:140:TRP:HE1	1:A:142:GLY:C	1.86	0.78
1:A:427:ARG:HB3	1:A:428:PRO:HD3	1.65	0.78
1:A:441:SER:HB3	1:A:575:ARG:NH2	1.97	0.78
1:A:133:LEU:HB3	1:A:330:SER:HB3	1.65	0.76
1:A:361:TRP:CZ3	1:A:369:VAL:HG11	2.20	0.76
1:A:131:THR:O	1:A:135:ARG:HG2	1.85	0.76
1:A:158:ALA:HA	1:A:172:ARG:HG3	1.66	0.76
1:A:234:GLN:HB3	1:A:235:PRO:HD2	1.67	0.76
1:A:21:ASN:O	1:A:24:ARG:HB3	1.84	0.76
1:A:663:THR:HG23	2:A:689:NDG:C5	2.17	0.74
1:A:405:CYS:HA	1:A:680:CYS:HB3	1.70	0.74
1:A:663:THR:HG23	2:A:689:NDG:H5	1.70	0.74
1:A:314:MET:SD	1:A:682:PHE:CE1	2.81	0.73
1:A:161:VAL:HG12	1:A:163:GLY:H	1.52	0.73
1:A:260:VAL:HG23	1:A:261:GLU:H	1.51	0.73
1:A:32:ILE:HD12	1:A:32:ILE:H	1.53	0.73
1:A:355:LYS:HB2	1:A:373:VAL:HB	1.69	0.73
1:A:110:GLN:HE21	1:A:155:PHE:HA	1.51	0.73
1:A:376:GLU:HB3	1:A:378:LYS:HG3	1.71	0.73
1:A:392:VAL:O	1:A:594:VAL:HA	1.89	0.73
1:A:347:TRP:HE1	1:A:392:VAL:HA	1.53	0.72
1:A:543:SER:O	1:A:547:GLU:HG3	1.89	0.72
1:A:149:GLU:HB3	1:A:167:GLU:HB2	1.70	0.72
1:A:16:GLU:CD	1:A:299:LEU:H	1.93	0.72
1:A:615:PHE:O	1:A:627:MET:SD	2.48	0.72
1:A:11:THR:OG1	1:A:38:GLN:HA	1.90	0.71
1:A:143:ILE:HD11	1:A:332:ARG:HH11	1.56	0.71
1:A:444:ASN:HA	1:A:569:LEU:HD11	1.72	0.71
1:A:540:ILE:HG13	1:A:544:THR:HG21	1.73	0.71
1:A:143:ILE:HG23	1:A:147:SER:CB	2.22	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:345:ILE:HG22	1:A:368:ASP:O	1.92	0.70
1:A:105:THR:HG21	1:A:231:GLY:HA2	1.73	0.70
1:A:19:LYS:HD2	1:A:298:LEU:HD12	1.73	0.70
1:A:196:HIS:HA	1:A:199:LYS:HB3	1.74	0.69
1:A:301:LYS:HE3	1:A:303:SER:OG	1.92	0.69
1:A:626:MET:SD	1:A:627:MET:N	2.65	0.69
1:A:451:LYS:O	1:A:484:PHE:HB3	1.93	0.69
1:A:458:VAL:HA	1:A:464:TRP:CE3	2.28	0.69
1:A:473:ASN:O	1:A:474:ARG:HG2	1.93	0.68
1:A:514:VAL:HG23	1:A:519:GLU:HB2	1.73	0.68
1:A:235:PRO:HG2	1:A:238:ASN:HB2	1.75	0.68
1:A:385:MET:HB3	1:A:407:LEU:HD11	1.76	0.68
1:A:134:HIS:CE1	1:A:329:GLN:HB3	2.27	0.67
1:A:147:SER:H	1:A:150:GLN:HB2	1.59	0.67
1:A:501:LEU:HD23	1:A:530:CYS:SG	2.35	0.67
1:A:335:GLN:HG3	1:A:336:LEU:H	1.60	0.67
1:A:26:LEU:HD12	1:A:26:LEU:H	1.60	0.67
1:A:14:SER:HB2	1:A:15:PRO:HD3	1.77	0.67
1:A:667:SER:HB2	2:A:688:NAG:H62	1.75	0.66
1:A:143:ILE:HG12	1:A:147:SER:HA	1.77	0.66
1:A:2:PRO:HB3	1:A:3:PRO:HD2	1.77	0.66
1:A:98:VAL:HG22	1:A:99:LYS:H	1.61	0.65
1:A:527:ALA:O	1:A:530:CYS:HB3	1.96	0.65
1:A:128:PRO:HG2	1:A:207:PHE:CD1	2.30	0.65
1:A:352:LYS:HB3	1:A:352:LYS:NZ	2.11	0.65
1:A:157:SER:HA	1:A:169:LYS:HD3	1.78	0.64
2:A:688:NAG:H5	2:A:689:NDG:O	1.96	0.64
1:A:314:MET:SD	1:A:682:PHE:HZ	2.19	0.64
1:A:113:THR:O	1:A:205:VAL:HG22	1.98	0.64
1:A:116:HIS:CE1	1:A:129:ILE:HD11	2.33	0.64
1:A:9:TRP:HH2	1:A:58:SER:HB2	1.62	0.64
1:A:298:LEU:HD23	1:A:298:LEU:H	1.61	0.64
1:A:229:LEU:HD21	1:A:244:TRP:CZ3	2.33	0.63
1:A:541:GLN:HG2	1:A:542:HIS:H	1.61	0.63
1:A:581:TYR:N	1:A:581:TYR:CD1	2.65	0.63
1:A:34:LEU:CD2	1:A:35:THR:H	2.10	0.63
1:A:478:CYS:N	1:A:671:CYS:SG	2.72	0.63
1:A:267:LEU:O	1:A:271:GLN:HG3	1.98	0.63
1:A:32:ILE:HG21	1:A:266:PHE:HB2	1.80	0.63
1:A:615:PHE:C	1:A:627:MET:SD	2.77	0.63
1:A:133:LEU:HD21	1:A:140:TRP:HB3	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:THR:HB	1:A:686:LYS:HD3	1.79	0.63
1:A:274:PHE:HA	1:A:278:THR:OG1	1.99	0.63
1:A:141:GLU:O	1:A:335:GLN:HB2	1.97	0.63
1:A:24:ARG:HD2	1:A:25:ASP:N	2.14	0.63
1:A:438:ARG:HB2	1:A:441:SER:HB2	1.81	0.62
1:A:561:LEU:H	1:A:561:LEU:HD12	1.63	0.62
1:A:158:ALA:HB1	1:A:173:GLN:OE1	1.99	0.62
1:A:146:GLY:O	1:A:151:ALA:HB2	2.00	0.62
1:A:98:VAL:HG22	1:A:99:LYS:N	2.15	0.62
1:A:188:TYR:OH	1:A:197:CYS:HA	2.00	0.62
1:A:292:ASP:HB3	1:A:295:LEU:HD21	1.81	0.61
1:A:576:ALA:HB3	1:A:584:CYS:SG	2.40	0.61
1:A:651:THR:HG22	1:A:652:THR:N	2.12	0.61
1:A:42:TYR:O	1:A:46:ILE:HG12	2.01	0.61
1:A:432:PHE:HD1	1:A:585:ASN:OD1	1.83	0.61
1:A:561:LEU:H	1:A:561:LEU:CD1	2.12	0.61
1:A:132:LEU:HA	1:A:135:ARG:HG2	1.81	0.61
1:A:161:VAL:O	1:A:171:CYS:SG	2.59	0.61
1:A:418:GLU:C	1:A:420:GLN:H	2.04	0.61
1:A:38:GLN:O	1:A:39:LYS:HD3	2.01	0.61
1:A:441:SER:HB3	1:A:575:ARG:HH22	1.65	0.61
1:A:199:LYS:HA	1:A:224:TYR:OH	2.00	0.61
1:A:132:LEU:HA	1:A:135:ARG:CG	2.30	0.61
1:A:541:GLN:HG2	1:A:542:HIS:N	2.16	0.61
1:A:317:GLN:HA	1:A:325:TYR:CD2	2.35	0.61
1:A:628:PHE:CD1	1:A:641:THR:HB	2.35	0.61
1:A:119:LEU:HD13	1:A:184:ARG:NE	2.13	0.61
1:A:175:LYS:HG2	1:A:202:LYS:NZ	2.16	0.61
1:A:403:GLY:HA2	1:A:407:LEU:O	2.01	0.61
1:A:356:SER:HA	1:A:359:ASP:HB2	1.82	0.61
1:A:77:ILE:HG13	1:A:252:VAL:O	2.00	0.60
1:A:117:THR:CA	1:A:189:SER:HB2	2.28	0.60
1:A:435:ALA:HB2	1:A:586:LEU:HD21	1.83	0.60
1:A:92:TYR:O	1:A:247:VAL:HB	2.01	0.60
1:A:445:TRP:O	1:A:448:LEU:HD22	2.02	0.60
1:A:323:GLU:H	1:A:323:GLU:CD	2.04	0.60
1:A:552:LYS:HB2	1:A:552:LYS:NZ	2.16	0.60
1:A:395:ASP:OD1	1:A:398:LEU:HD12	2.02	0.59
1:A:116:HIS:HE1	1:A:129:ILE:HD11	1.66	0.59
1:A:493:PRO:O	1:A:499:CYS:SG	2.60	0.59
1:A:349:ALA:HB3	1:A:373:VAL:HA	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:421:CYS:SG	1:A:645:PHE:HB3	2.42	0.59
1:A:310:VAL:HG13	1:A:314:MET:SD	2.43	0.59
1:A:181:LYS:HG2	1:A:182:CYS:N	2.17	0.59
1:A:152:VAL:HG13	1:A:156:PHE:CD1	2.37	0.59
1:A:347:TRP:NE1	1:A:636:LEU:HD21	2.18	0.59
1:A:175:LYS:HD3	1:A:176:GLY:H	1.68	0.59
1:A:469:GLY:HA2	1:A:668:LEU:HD13	1.84	0.58
1:A:414:ARG:HB3	1:A:643:CYS:HB3	1.86	0.58
1:A:80:GLU:HG3	1:A:250:HIS:O	2.03	0.58
1:A:407:LEU:N	1:A:407:LEU:HD12	2.19	0.58
1:A:314:MET:HE1	1:A:679:MET:HG2	1.84	0.58
1:A:384:ILE:HA	1:A:389:ALA:O	2.03	0.58
1:A:414:ARG:HB2	1:A:414:ARG:HH11	1.68	0.58
1:A:49:ILE:HG22	1:A:54:ALA:HB3	1.86	0.58
1:A:347:TRP:CD1	1:A:348:CYS:N	2.72	0.58
1:A:347:TRP:CD1	1:A:636:LEU:HD21	2.38	0.58
1:A:391:ALA:HA	1:A:596:VAL:HG12	1.85	0.57
1:A:427:ARG:CB	1:A:428:PRO:HD3	2.33	0.57
1:A:274:PHE:HA	1:A:278:THR:CB	2.34	0.57
1:A:453:SER:HB3	1:A:484:PHE:CD1	2.39	0.57
1:A:416:ASP:O	1:A:417:ASP:HB2	2.04	0.57
1:A:159:SER:OG	1:A:170:LEU:HA	2.04	0.57
1:A:432:PHE:HB2	1:A:542:HIS:HB3	1.86	0.57
1:A:439:LYS:HB3	1:A:439:LYS:HZ3	1.69	0.57
1:A:335:GLN:OE1	1:A:336:LEU:HB2	2.04	0.57
1:A:481:ASP:HB2	1:A:498:LEU:HD12	1.86	0.57
1:A:581:TYR:O	1:A:585:ASN:HB3	2.05	0.56
1:A:271:GLN:HE22	1:A:307:LEU:HB2	1.70	0.56
1:A:3:PRO:HB2	1:A:31:ARG:NH2	2.19	0.56
1:A:25:ASP:O	1:A:29:GLN:HG2	2.06	0.56
1:A:540:ILE:CG1	1:A:544:THR:HG21	2.35	0.56
1:A:34:LEU:HD22	1:A:36:CYS:SG	2.46	0.55
1:A:400:TYR:O	1:A:404:VAL:HG23	2.06	0.55
1:A:611:GLN:HA	1:A:614:ARG:HB2	1.88	0.55
1:A:473:ASN:C	1:A:474:ARG:HG2	2.26	0.55
1:A:563:MET:C	1:A:565:ASP:H	2.09	0.55
1:A:346:GLN:HB2	1:A:370:GLU:HB2	1.88	0.55
1:A:314:MET:HE1	1:A:682:PHE:HE1	1.72	0.55
1:A:350:VAL:HG22	1:A:374:VAL:CG2	2.36	0.55
1:A:253:VAL:O	1:A:254:ALA:HB2	2.07	0.55
1:A:562:GLN:C	1:A:564:ASP:H	2.08	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:VAL:HG13	1:A:96:ALA:N	2.20	0.55
1:A:385:MET:HA	1:A:597:ARG:HE	1.72	0.55
1:A:395:ASP:O	1:A:399:VAL:HG23	2.06	0.55
1:A:652:THR:HG22	1:A:655:GLU:CG	2.38	0.55
1:A:355:LYS:HB2	1:A:373:VAL:CB	2.35	0.54
1:A:448:LEU:H	1:A:448:LEU:CD2	2.19	0.54
1:A:346:GLN:HE21	1:A:372:THR:N	2.06	0.54
1:A:414:ARG:CB	1:A:643:CYS:HB3	2.37	0.54
1:A:384:ILE:N	1:A:389:ALA:HB3	2.21	0.54
1:A:487:GLY:C	1:A:501:LEU:HB2	2.27	0.54
1:A:75:LYS:O	1:A:253:VAL:HA	2.08	0.54
1:A:345:ILE:HG12	1:A:346:GLN:N	2.22	0.54
1:A:94:ALA:HB3	1:A:245:ALA:HB3	1.89	0.54
1:A:194:ALA:O	1:A:197:CYS:HB2	2.08	0.54
1:A:175:LYS:HD3	1:A:176:GLY:N	2.23	0.54
1:A:473:ASN:ND2	2:A:688:NAG:O6	2.41	0.54
1:A:570:CYS:SG	1:A:574:ARG:O	2.66	0.54
1:A:643:CYS:SG	1:A:644:LEU:N	2.81	0.54
1:A:600:LYS:O	1:A:604:ILE:HB	2.08	0.54
1:A:119:LEU:HD22	1:A:184:ARG:HH21	1.74	0.54
1:A:79:ALA:O	1:A:307:LEU:HD23	2.08	0.54
1:A:350:VAL:HG13	1:A:374:VAL:HG23	1.91	0.53
1:A:10:CYS:HB3	1:A:57:ILE:HB	1.89	0.53
1:A:604:ILE:O	1:A:608:LEU:HD22	2.09	0.53
1:A:221:LYS:HG3	1:A:222:ASP:H	1.73	0.53
1:A:48:ALA:O	1:A:53:GLU:HB2	2.08	0.53
1:A:153:ALA:CA	1:A:169:LYS:HD2	2.33	0.53
1:A:345:ILE:HG13	1:A:604:ILE:HD11	1.90	0.53
1:A:91:SER:HB2	1:A:247:VAL:O	2.09	0.53
1:A:347:TRP:HD1	1:A:348:CYS:N	2.06	0.53
1:A:675:ASP:OD1	1:A:676:ILE:HG22	2.09	0.53
1:A:350:VAL:HG22	1:A:374:VAL:HG22	1.91	0.53
1:A:16:GLU:O	1:A:19:LYS:HG2	2.08	0.53
1:A:174:CYS:HB2	1:A:181:LYS:CG	2.34	0.53
1:A:314:MET:SD	1:A:682:PHE:HE1	2.31	0.53
1:A:188:TYR:OH	1:A:202:LYS:HB3	2.09	0.53
1:A:200:ASP:O	1:A:202:LYS:N	2.41	0.53
1:A:414:ARG:CB	1:A:414:ARG:HH11	2.22	0.53
1:A:128:PRO:HA	1:A:131:THR:OG1	2.09	0.53
1:A:347:TRP:NE1	1:A:392:VAL:HA	2.22	0.53
1:A:410:VAL:HG22	1:A:605:ARG:HE	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:603:LYS:O	1:A:607:LEU:HD12	2.08	0.53
1:A:528:LEU:O	1:A:532:VAL:HG23	2.09	0.53
1:A:608:LEU:O	1:A:612:GLU:HB2	2.09	0.53
1:A:472:HIS:CD2	1:A:671:CYS:HB2	2.44	0.52
1:A:478:CYS:HB3	1:A:480:PHE:CZ	2.44	0.52
1:A:410:VAL:CG2	1:A:605:ARG:HE	2.22	0.52
1:A:25:ASP:O	1:A:28:GLN:HB2	2.09	0.52
1:A:373:VAL:HG22	1:A:374:VAL:N	2.24	0.52
1:A:24:ARG:HD2	1:A:25:ASP:H	1.74	0.52
1:A:612:GLU:HA	1:A:627:MET:HE1	1.91	0.52
1:A:487:GLY:HA2	1:A:501:LEU:HD13	1.92	0.52
1:A:674:SER:O	1:A:678:GLN:HG3	2.10	0.52
1:A:138:ILE:HG23	1:A:155:PHE:HB2	1.92	0.52
1:A:464:TRP:HZ3	1:A:489:ALA:CB	2.22	0.52
1:A:292:ASP:HB3	1:A:295:LEU:CD2	2.39	0.52
1:A:466:ILE:HG21	1:A:587:ALA:HB2	1.92	0.52
1:A:335:GLN:O	1:A:336:LEU:HG	2.09	0.52
1:A:353:ASP:O	1:A:635:LEU:HD13	2.10	0.52
1:A:444:ASN:HA	1:A:569:LEU:CD1	2.38	0.52
1:A:228:CYS:N	1:A:242:CYS:SG	2.83	0.51
1:A:269:LYS:C	1:A:271:GLN:H	2.12	0.51
1:A:95:VAL:HG22	1:A:96:ALA:N	2.17	0.51
1:A:674:SER:O	1:A:678:GLN:N	2.44	0.51
1:A:94:ALA:O	1:A:244:TRP:N	2.43	0.51
1:A:468:MET:HG3	1:A:480:PHE:CG	2.46	0.51
1:A:37:VAL:HG12	1:A:38:GLN:H	1.75	0.51
1:A:110:GLN:NE2	1:A:155:PHE:HA	2.23	0.51
1:A:270:ALA:HA	1:A:274:PHE:HD2	1.75	0.51
1:A:346:GLN:NE2	1:A:372:THR:HB	2.26	0.51
1:A:140:TRP:HZ2	1:A:143:ILE:HG13	1.76	0.51
1:A:435:ALA:HB3	1:A:569:LEU:HB3	1.92	0.51
1:A:447:ASN:O	1:A:451:LYS:HD3	2.11	0.51
1:A:128:PRO:HA	1:A:131:THR:HG1	1.76	0.51
1:A:96:ALA:HA	1:A:207:PHE:HA	1.93	0.51
1:A:464:TRP:CZ3	1:A:489:ALA:HB1	2.45	0.51
1:A:260:VAL:HG23	1:A:261:GLU:N	2.24	0.50
1:A:464:TRP:HZ3	1:A:489:ALA:HB1	1.76	0.50
1:A:131:THR:OG1	1:A:244:TRP:HZ3	1.94	0.50
1:A:349:ALA:O	1:A:374:VAL:HG22	2.10	0.50
1:A:444:ASN:OD1	1:A:447:ASN:N	2.44	0.50
1:A:219:ASP:HB2	1:A:220:GLN:OE1	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:MET:HA	1:A:597:ARG:NE	2.27	0.50
1:A:361:TRP:HZ3	1:A:369:VAL:HG11	1.72	0.50
1:A:159:SER:CB	1:A:170:LEU:HA	2.42	0.50
1:A:542:HIS:CG	1:A:543:SER:N	2.80	0.50
1:A:212:THR:C	1:A:214:ASN:H	2.15	0.50
1:A:293:PRO:HA	1:A:296:LYS:CG	2.41	0.50
1:A:437:ALA:HB1	1:A:575:ARG:NH2	2.26	0.50
1:A:341:ARG:HG2	1:A:341:ARG:O	2.12	0.50
1:A:83:GLU:HG3	1:A:305:ILE:CD1	2.38	0.50
1:A:601:ALA:O	1:A:604:ILE:HG22	2.10	0.50
1:A:564:ASP:OD1	1:A:564:ASP:N	2.43	0.50
1:A:103:GLU:CD	1:A:103:GLU:H	2.14	0.50
1:A:410:VAL:HG12	1:A:594:VAL:O	2.11	0.49
1:A:461:THR:O	1:A:466:ILE:HG12	2.12	0.49
1:A:449:LYS:HD3	1:A:483:TYR:O	2.11	0.49
1:A:13:SER:HA	1:A:38:GLN:HE22	1.77	0.49
1:A:113:THR:HB	1:A:158:ALA:HB3	1.94	0.49
1:A:138:ILE:HG12	1:A:155:PHE:CE2	2.47	0.49
1:A:490:PRO:HB3	1:A:514:VAL:O	2.12	0.49
1:A:175:LYS:HA	1:A:202:LYS:HZ3	1.77	0.49
1:A:464:TRP:O	1:A:467:PRO:HD2	2.12	0.49
1:A:408:VAL:O	1:A:595:VAL:HA	2.12	0.49
1:A:213:VAL:HG23	1:A:236:VAL:HG13	1.94	0.49
1:A:305:ILE:HD12	1:A:305:ILE:N	2.27	0.49
1:A:82:TYR:CA	1:A:305:ILE:HD13	2.34	0.49
1:A:174:CYS:SG	1:A:181:LYS:NZ	2.82	0.49
1:A:410:VAL:HG22	1:A:605:ARG:HG2	1.93	0.49
1:A:147:SER:H	1:A:150:GLN:HE21	1.61	0.49
1:A:92:TYR:HB3	1:A:209:LYS:HZ2	1.78	0.49
1:A:626:MET:CE	1:A:628:PHE:HB2	2.43	0.49
1:A:198:LEU:HD23	1:A:206:ALA:HB3	1.93	0.49
1:A:676:ILE:HG23	1:A:677:LEU:H	1.77	0.49
1:A:345:ILE:HB	1:A:607:LEU:HD22	1.95	0.48
1:A:458:VAL:O	1:A:458:VAL:HG22	2.13	0.48
1:A:562:GLN:C	1:A:564:ASP:N	2.66	0.48
1:A:175:LYS:HG2	1:A:202:LYS:HZ3	1.76	0.48
1:A:568:LEU:HG	1:A:578:VAL:HA	1.95	0.48
1:A:570:CYS:SG	1:A:576:ALA:HB2	2.53	0.48
1:A:333:LYS:HD3	1:A:333:LYS:O	2.13	0.48
1:A:262:ASP:HA	1:A:265:SER:OG	2.12	0.48
1:A:615:PHE:CB	1:A:627:MET:SD	3.02	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:439:LYS:HD3	1:A:564:ASP:O	2.13	0.48
1:A:461:THR:HA	1:A:465:VAL:CG2	2.44	0.48
1:A:239:TYR:C	1:A:241:THR:H	2.16	0.48
1:A:27:THR:CG2	1:A:266:PHE:HZ	2.27	0.48
1:A:628:PHE:CE1	1:A:641:THR:HB	2.48	0.48
1:A:317:GLN:HB3	1:A:386:LYS:NZ	2.28	0.48
1:A:66:GLU:HA	1:A:69:LEU:HD22	1.94	0.48
1:A:456:THR:HG23	1:A:523:GLY:CA	2.43	0.48
1:A:234:GLN:HB3	1:A:238:ASN:CG	2.34	0.48
1:A:336:LEU:HD23	1:A:340:PRO:HA	1.96	0.48
1:A:385:MET:CB	1:A:407:LEU:HD11	2.44	0.48
1:A:529:ARG:HG3	1:A:557:TRP:CE3	2.49	0.48
1:A:488:CYS:HB2	1:A:502:CYS:N	2.29	0.47
1:A:96:ALA:CB	1:A:207:PHE:HB3	2.44	0.47
1:A:486:GLU:HG3	1:A:501:LEU:HD13	1.96	0.47
1:A:271:GLN:NE2	1:A:307:LEU:HB2	2.30	0.47
1:A:229:LEU:HD21	1:A:244:TRP:CH2	2.50	0.47
1:A:411:MET:SD	1:A:605:ARG:CA	2.96	0.47
1:A:605:ARG:HB3	1:A:646:LYS:HG2	1.96	0.47
1:A:542:HIS:HB2	1:A:581:TYR:HB3	1.96	0.47
1:A:25:ASP:HA	1:A:28:GLN:OE1	2.14	0.47
1:A:628:PHE:HD1	1:A:637:PHE:HB3	1.79	0.47
1:A:117:THR:HB	1:A:190:GLY:H	1.79	0.47
1:A:355:LYS:HB2	1:A:373:VAL:CG2	2.44	0.47
1:A:355:LYS:HG2	1:A:359:ASP:OD2	2.14	0.47
1:A:382:ILE:HA	1:A:385:MET:HG2	1.97	0.47
1:A:548:ASN:HD22	1:A:553:ASN:ND2	1.93	0.47
1:A:651:THR:CG2	1:A:652:THR:H	2.23	0.47
1:A:158:ALA:HB1	1:A:173:GLN:HE22	1.79	0.47
1:A:356:SER:O	1:A:360:ARG:HG2	2.14	0.47
1:A:464:TRP:C	1:A:467:PRO:HD2	2.33	0.47
1:A:112:LYS:HE2	1:A:112:LYS:H	1.79	0.47
1:A:314:MET:CE	1:A:683:LEU:HD11	2.45	0.47
1:A:354:GLU:O	1:A:357:LYS:HB3	2.14	0.47
1:A:138:ILE:HG23	1:A:155:PHE:CG	2.49	0.47
1:A:665:ILE:HG23	1:A:669:LYS:HE3	1.97	0.47
1:A:68:GLY:HA3	1:A:316:SER:OG	2.15	0.47
1:A:80:GLU:OE1	1:A:301:LYS:HB3	2.15	0.46
1:A:119:LEU:O	1:A:121:ARG:N	2.48	0.46
1:A:58:SER:HA	1:A:252:VAL:HA	1.97	0.46
1:A:32:ILE:CG2	1:A:266:PHE:HB2	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:ILE:HA	1:A:55:ASP:OD2	2.16	0.46
1:A:19:LYS:CD	1:A:299:LEU:HB2	2.31	0.46
1:A:335:GLN:HG3	1:A:336:LEU:N	2.30	0.46
1:A:505:SER:HB3	1:A:511:GLU:H	1.80	0.46
1:A:234:GLN:CB	1:A:235:PRO:HD2	2.38	0.46
1:A:458:VAL:O	1:A:458:VAL:HG13	2.15	0.46
1:A:509:PRO:O	1:A:511:GLU:N	2.44	0.46
1:A:418:GLU:OE2	1:A:643:CYS:HA	2.16	0.46
1:A:189:SER:N	1:A:193:GLY:HA3	2.31	0.46
1:A:458:VAL:HG12	1:A:491:GLY:HA3	1.97	0.46
1:A:68:GLY:O	1:A:73:LYS:HA	2.16	0.46
1:A:436:VAL:O	1:A:531:LEU:HD11	2.15	0.46
1:A:314:MET:CE	1:A:682:PHE:HE1	2.29	0.46
1:A:305:ILE:N	1:A:305:ILE:CD1	2.79	0.46
1:A:346:GLN:CD	1:A:347:TRP:N	2.69	0.46
1:A:158:ALA:C	1:A:173:GLN:HE22	2.20	0.46
1:A:286:GLY:HA3	1:A:302:ASP:CG	2.37	0.46
1:A:557:TRP:N	1:A:557:TRP:CD1	2.84	0.46
1:A:140:TRP:NE1	1:A:142:GLY:C	2.64	0.45
1:A:238:ASN:O	1:A:242:CYS:HB3	2.15	0.45
1:A:444:ASN:HA	1:A:569:LEU:HD21	1.97	0.45
1:A:645:PHE:O	1:A:645:PHE:HD1	1.99	0.45
1:A:529:ARG:HG3	1:A:557:TRP:CD2	2.51	0.45
1:A:365:SER:O	1:A:368:ASP:N	2.43	0.45
1:A:297:ASP:HB3	1:A:301:LYS:HA	1.98	0.45
1:A:26:LEU:HD12	1:A:26:LEU:N	2.26	0.45
1:A:479:ASN:HB3	1:A:482:GLU:HB2	1.98	0.45
1:A:174:CYS:CB	1:A:181:LYS:HZ2	2.30	0.45
1:A:611:GLN:OE1	1:A:615:PHE:HB2	2.16	0.45
1:A:54:ALA:O	1:A:255:ARG:NH1	2.49	0.45
1:A:502:CYS:SG	1:A:513:CYS:HA	2.56	0.45
1:A:487:GLY:HA2	1:A:501:LEU:HD22	1.97	0.45
1:A:362:SER:OG	1:A:371:CYS:SG	2.75	0.45
1:A:143:ILE:HA	1:A:147:SER:HA	1.96	0.45
1:A:268:SER:HA	1:A:271:GLN:OE1	2.16	0.45
1:A:117:THR:HG21	1:A:190:GLY:O	2.16	0.45
1:A:410:VAL:HG22	1:A:605:ARG:CG	2.46	0.45
1:A:458:VAL:HG11	1:A:491:GLY:C	2.37	0.45
1:A:589:VAL:HA	1:A:590:PRO:HD3	1.67	0.45
1:A:676:ILE:HG23	1:A:677:LEU:N	2.31	0.45
1:A:445:TRP:CG	1:A:571:THR:HA	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:TRP:CE2	1:A:636:LEU:HD21	2.51	0.45
1:A:102:THR:OG1	1:A:233:ARG:NH1	2.50	0.45
1:A:270:ALA:HA	1:A:274:PHE:CD2	2.51	0.45
1:A:51:ASN:C	1:A:53:GLU:H	2.20	0.45
1:A:70:ALA:HB1	1:A:71:PRO:HA	1.98	0.45
1:A:97:VAL:HB	1:A:226:LEU:CD2	2.35	0.45
1:A:446:ASN:ND2	1:A:446:ASN:N	2.65	0.45
1:A:626:MET:HE1	1:A:628:PHE:HD2	1.82	0.45
1:A:140:TRP:CD1	1:A:141:GLU:N	2.85	0.45
1:A:472:HIS:C	1:A:474:ARG:H	2.21	0.45
1:A:268:SER:O	1:A:271:GLN:HB2	2.17	0.45
1:A:174:CYS:CB	1:A:181:LYS:HG3	2.41	0.44
1:A:433:ALA:O	1:A:586:LEU:N	2.30	0.44
1:A:95:VAL:HG21	1:A:226:LEU:HD22	1.99	0.44
1:A:626:MET:HE3	1:A:628:PHE:HB2	1.99	0.44
1:A:168:GLN:C	1:A:170:LEU:H	2.20	0.44
1:A:350:VAL:H	1:A:354:GLU:CD	2.21	0.44
1:A:365:SER:O	1:A:367:GLY:N	2.51	0.44
1:A:552:LYS:HB2	1:A:552:LYS:HZ3	1.82	0.44
1:A:456:THR:HG21	1:A:460:ARG:HD3	1.99	0.44
1:A:439:LYS:HB2	1:A:565:ASP:HA	2.00	0.44
1:A:127:ILE:CB	1:A:128:PRO:HD3	2.41	0.44
1:A:234:GLN:HB3	1:A:235:PRO:CD	2.42	0.44
1:A:258:ASN:OD1	1:A:259:LYS:HG3	2.17	0.44
1:A:82:TYR:OH	1:A:249:ALA:HB1	2.18	0.44
1:A:345:ILE:CG2	1:A:607:LEU:HD22	2.48	0.44
1:A:477:THR:HG22	1:A:478:CYS:N	2.32	0.44
1:A:659:ASP:C	1:A:661:PHE:H	2.20	0.44
1:A:49:ILE:CG2	1:A:54:ALA:HB3	2.47	0.44
1:A:173:GLN:HB2	1:A:202:LYS:HG2	1.99	0.44
1:A:297:ASP:HA	1:A:302:ASP:H	1.83	0.44
1:A:382:ILE:HD12	1:A:382:ILE:N	2.33	0.44
1:A:456:THR:HG23	1:A:523:GLY:C	2.38	0.44
1:A:147:SER:H	1:A:150:GLN:NE2	2.16	0.44
1:A:432:PHE:CD1	1:A:585:ASN:OD1	2.69	0.44
1:A:558:ALA:O	1:A:559:LYS:C	2.55	0.44
1:A:175:LYS:HG2	1:A:202:LYS:HZ2	1.83	0.44
1:A:27:THR:HB	1:A:266:PHE:CZ	2.53	0.43
1:A:298:LEU:C	1:A:300:PHE:H	2.22	0.43
1:A:49:ILE:HG22	1:A:54:ALA:CB	2.46	0.43
1:A:432:PHE:CE2	1:A:582:ARG:HD2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:PHE:CE1	1:A:69:LEU:HD11	2.53	0.43
1:A:127:ILE:HB	1:A:128:PRO:CD	2.41	0.43
1:A:490:PRO:O	1:A:515:ALA:HB2	2.17	0.43
1:A:415:TYR:CD1	1:A:415:TYR:N	2.84	0.43
1:A:193:GLY:O	1:A:196:HIS:HB2	2.19	0.43
1:A:345:ILE:HG23	1:A:369:VAL:HG13	2.00	0.43
1:A:427:ARG:HH11	1:A:427:ARG:HG2	1.82	0.43
1:A:652:THR:HG22	1:A:655:GLU:HG3	2.00	0.43
1:A:98:VAL:CG2	1:A:99:LYS:H	2.31	0.43
1:A:345:ILE:HG12	1:A:346:GLN:H	1.82	0.43
1:A:611:GLN:OE1	1:A:615:PHE:HD1	2.00	0.43
1:A:291:LYS:HG3	1:A:292:ASP:H	1.83	0.43
1:A:34:LEU:CD2	1:A:36:CYS:SG	3.07	0.43
1:A:458:VAL:HA	1:A:464:TRP:CD2	2.53	0.43
1:A:274:PHE:HA	1:A:278:THR:HB	2.00	0.43
1:A:577:ASN:HD22	1:A:578:VAL:N	2.17	0.43
1:A:158:ALA:HB1	1:A:173:GLN:NE2	2.33	0.43
1:A:633:LYS:HD2	1:A:634:ASP:H	1.84	0.43
1:A:91:SER:O	1:A:92:TYR:CD1	2.72	0.43
1:A:133:LEU:HD11	1:A:140:TRP:CE3	2.54	0.42
1:A:652:THR:HG23	1:A:655:GLU:H	1.83	0.42
1:A:92:TYR:HB3	1:A:209:LYS:NZ	2.34	0.42
1:A:434:VAL:HB	1:A:568:LEU:HD22	2.01	0.42
1:A:258:ASN:HD21	1:A:259:LYS:NZ	2.17	0.42
1:A:217:ALA:HA	1:A:218:PRO:HD2	1.87	0.42
1:A:411:MET:HG2	1:A:646:LYS:HA	2.00	0.42
1:A:146:GLY:HA2	1:A:150:GLN:HB3	2.01	0.42
1:A:514:VAL:C	1:A:516:SER:H	2.21	0.42
1:A:659:ASP:O	1:A:661:PHE:N	2.52	0.42
1:A:285:PHE:CE2	1:A:306:MET:HA	2.54	0.42
1:A:39:LYS:HG3	1:A:45:CYS:HA	2.01	0.42
1:A:445:TRP:HA	1:A:448:LEU:HD13	2.00	0.42
1:A:125:TRP:CZ2	1:A:148:VAL:HG22	2.54	0.42
1:A:292:ASP:O	1:A:295:LEU:N	2.48	0.42
1:A:413:GLU:HB3	1:A:641:THR:HG23	2.01	0.42
1:A:424:THR:HG23	1:A:427:ARG:HH21	1.85	0.42
1:A:458:VAL:CG1	1:A:491:GLY:HA3	2.49	0.42
1:A:659:ASP:C	1:A:661:PHE:N	2.73	0.42
1:A:126:ASN:O	1:A:130:GLY:N	2.48	0.42
1:A:345:ILE:CG2	1:A:369:VAL:HG13	2.50	0.42
1:A:267:LEU:HD12	1:A:270:ALA:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:449:LYS:NZ	1:A:483:TYR:HA	2.34	0.42
1:A:443:VAL:HG12	1:A:451:LYS:HG2	2.02	0.42
1:A:453:SER:HB3	1:A:484:PHE:CE1	2.55	0.42
1:A:486:GLU:HG3	1:A:501:LEU:CD1	2.49	0.42
1:A:293:PRO:HA	1:A:296:LYS:HG2	2.00	0.42
1:A:81:VAL:HG22	1:A:306:MET:O	2.20	0.42
1:A:18:LYS:HB3	1:A:18:LYS:HE3	1.84	0.42
1:A:140:TRP:CE2	1:A:146:GLY:O	2.73	0.41
1:A:458:VAL:HG23	1:A:464:TRP:CZ2	2.54	0.41
1:A:77:ILE:HD12	1:A:78:ALA:CB	2.50	0.41
1:A:267:LEU:O	1:A:270:ALA:N	2.53	0.41
1:A:583:GLU:O	1:A:584:CYS:HB2	2.20	0.41
1:A:423:LYS:HD3	1:A:423:LYS:N	2.36	0.41
1:A:131:THR:OG1	1:A:244:TRP:CZ3	2.63	0.41
1:A:149:GLU:O	1:A:152:VAL:HB	2.20	0.41
1:A:45:CYS:O	1:A:49:ILE:HG12	2.21	0.41
1:A:27:THR:HB	1:A:266:PHE:CE1	2.56	0.41
1:A:96:ALA:HB2	1:A:207:PHE:HB3	2.01	0.41
1:A:615:PHE:HB2	1:A:627:MET:SD	2.61	0.41
1:A:356:SER:O	1:A:360:ARG:N	2.43	0.41
1:A:227:LEU:HD13	1:A:233:ARG:CZ	2.50	0.41
1:A:466:ILE:HG21	1:A:587:ALA:CB	2.50	0.41
1:A:147:SER:O	1:A:151:ALA:N	2.48	0.41
1:A:30:GLU:HG3	1:A:269:LYS:HZ3	1.86	0.41
1:A:394:LEU:HD22	1:A:398:LEU:HB3	2.01	0.41
1:A:378:LYS:HE2	1:A:378:LYS:HB2	1.87	0.41
1:A:246:ARG:HB2	1:A:323:GLU:OE1	2.21	0.41
1:A:402:ALA:O	1:A:405:CYS:N	2.51	0.41
1:A:133:LEU:HD13	1:A:330:SER:O	2.20	0.41
1:A:542:HIS:CG	1:A:543:SER:H	2.39	0.41
1:A:316:SER:C	1:A:318:LEU:N	2.74	0.41
1:A:631:GLN:O	1:A:632:ASN:HB3	2.20	0.41
1:A:653:TYR:HA	1:A:656:PHE:HB3	2.02	0.41
1:A:98:VAL:CG2	1:A:99:LYS:N	2.83	0.41
1:A:13:SER:O	1:A:17:GLU:HB2	2.21	0.41
1:A:350:VAL:HA	1:A:374:VAL:HG22	2.02	0.41
1:A:301:LYS:HE3	1:A:303:SER:HG	1.85	0.41
1:A:421:CYS:HB2	1:A:643:CYS:HB2	1.95	0.41
1:A:396:GLY:O	1:A:399:VAL:HB	2.21	0.41
1:A:439:LYS:HZ3	1:A:439:LYS:CB	2.34	0.41
1:A:62:GLY:HA2	1:A:324:TYR:OH	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:603:LYS:O	1:A:606:ASP:HB2	2.21	0.41
1:A:147:SER:C	1:A:149:GLU:N	2.74	0.41
1:A:79:ALA:HA	1:A:251:ALA:HA	2.03	0.41
1:A:638:LYS:HG2	1:A:640:LEU:H	1.86	0.41
1:A:32:ILE:H	1:A:32:ILE:CD1	2.21	0.40
1:A:113:THR:CB	1:A:158:ALA:HB3	2.51	0.40
1:A:357:LYS:O	1:A:360:ARG:HB2	2.21	0.40
1:A:105:THR:HA	1:A:233:ARG:HH21	1.86	0.40
1:A:250:HIS:ND1	1:A:301:LYS:HB2	2.36	0.40
1:A:269:LYS:C	1:A:271:GLN:N	2.74	0.40
1:A:316:SER:O	1:A:318:LEU:N	2.54	0.40
1:A:293:PRO:HA	1:A:296:LYS:HG3	2.02	0.40
1:A:109:LEU:HD12	1:A:112:LYS:HD2	2.03	0.40
1:A:609:GLU:HA	1:A:612:GLU:HB2	2.02	0.40
1:A:46:ILE:HD13	1:A:49:ILE:HD11	2.03	0.40
1:A:158:ALA:CB	1:A:173:GLN:HE22	2.35	0.40
1:A:380:CYS:O	1:A:384:ILE:HG13	2.21	0.40
1:A:186:ALA:O	1:A:188:TYR:N	2.54	0.40
1:A:386:LYS:HB3	1:A:388:GLU:HG3	2.03	0.40
1:A:243:ASN:ND2	1:A:246:ARG:HH21	2.20	0.40
1:A:461:THR:HA	1:A:465:VAL:HG23	2.03	0.40
1:A:585:ASN:HD22	1:A:585:ASN:H	1.69	0.40
1:A:352:LYS:HB3	1:A:352:LYS:HZ2	1.86	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	684/686 (100%)	450 (66%)	159 (23%)	75 (11%)	0 2

All (75) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	122	SER
1	A	126	ASN
1	A	145	SER
1	A	201	GLY
1	A	219	ASP
1	A	248	ALA
1	A	366	ASN
1	A	427	ARG
1	A	430	SER
1	A	441	SER
1	A	482	GLU
1	A	508	ILE
1	A	561	LEU
1	A	584	CYS
1	A	592	HIS
1	A	601	ALA
1	A	645	PHE
1	A	675	ASP
1	A	2	PRO
1	A	4	LYS
1	A	106	VAL
1	A	115	CYS
1	A	120	GLY
1	A	136	GLY
1	A	250	HIS
1	A	254	ALA
1	A	334	ASP
1	A	417	ASP
1	A	419	SER
1	A	443	VAL
1	A	490	PRO
1	A	559	LYS
1	A	602	ASN
1	A	35	THR
1	A	123	ALA
1	A	173	GLN
1	A	222	ASP
1	A	255	ARG
1	A	317	GLN
1	A	493	PRO
1	A	668	LEU
1	A	52	ASN
1	A	85	THR

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Mol	Chain	Res	Type
1	A	86	GLU
1	A	111	GLY
1	A	127	ILE
1	A	146	GLY
1	A	157	SER
1	A	181	LYS
1	A	362	SER
1	A	464	TRP
1	A	473	ASN
1	A	494	PRO
1	A	504	GLY
1	A	571	THR
1	A	578	VAL
1	A	612	GLU
1	A	24	ARG
1	A	169	LYS
1	A	213	VAL
1	A	284	LEU
1	A	288	PRO
1	A	474	ARG
1	A	510	PRO
1	A	187	PRO
1	A	220	GLN
1	A	235	PRO
1	A	458	VAL
1	A	647	VAL
1	A	507	GLY
1	A	286	GLY
1	A	293	PRO
1	A	364	VAL
1	A	95	VAL
1	A	253	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	580/580 (100%)	467 (80%)	113 (20%)	2 9

All (113) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ARG
1	A	10	CYS
1	A	17	GLU
1	A	20	CYS
1	A	24	ARG
1	A	25	ASP
1	A	31	ARG
1	A	32	ILE
1	A	34	LEU
1	A	37	VAL
1	A	45	CYS
1	A	69	LEU
1	A	83	GLU
1	A	86	GLU
1	A	89	THR
1	A	90	THR
1	A	102	THR
1	A	103	GLU
1	A	108	ASP
1	A	112	LYS
1	A	115	CYS
1	A	119	LEU
1	A	121	ARG
1	A	132	LEU
1	A	133	LEU
1	A	138	ILE
1	A	141	GLU
1	A	145	SER
1	A	148	VAL
1	A	154	LYS
1	A	159	SER
1	A	168	GLN
1	A	170	LEU
1	A	177	ASP
1	A	192	SER
1	A	195	PHE
1	A	198	LEU
1	A	207	PHE

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Mol	Chain	Res	Type
1	A	209	LYS
1	A	219	ASP
1	A	220	GLN
1	A	221	LYS
1	A	225	GLU
1	A	227	LEU
1	A	234	GLN
1	A	243	ASN
1	A	246	ARG
1	A	253	VAL
1	A	269	LYS
1	A	273	ASP
1	A	274	PHE
1	A	276	VAL
1	A	278	THR
1	A	293	PRO
1	A	295	LEU
1	A	299	LEU
1	A	302	ASP
1	A	307	LEU
1	A	309	ARG
1	A	311	PRO
1	A	326	SER
1	A	329	GLN
1	A	332	ARG
1	A	333	LYS
1	A	335	GLN
1	A	353	ASP
1	A	361	TRP
1	A	369	VAL
1	A	375	ASP
1	A	378	LYS
1	A	390	ASP
1	A	395	ASP
1	A	414	ARG
1	A	423	LYS
1	A	425	ASP
1	A	431	TYR
1	A	440	ASP
1	A	441	SER
1	A	446	ASN
1	A	448	LEU

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Mol	Chain	Res	Type
1	A	451	LYS
1	A	468	MET
1	A	478	CYS
1	A	490	PRO
1	A	495	ASN
1	A	497	ARG
1	A	500	GLN
1	A	508	ILE
1	A	531	LEU
1	A	533	GLU
1	A	540	ILE
1	A	552	LYS
1	A	557	TRP
1	A	564	ASP
1	A	577	ASN
1	A	578	VAL
1	A	581	TYR
1	A	585	ASN
1	A	592	HIS
1	A	606	ASP
1	A	607	LEU
1	A	608	LEU
1	A	612	GLU
1	A	618	ASN
1	A	620	SER
1	A	627	MET
1	A	640	LEU
1	A	645	PHE
1	A	648	ARG
1	A	660	LYS
1	A	670	THR
1	A	682	PHE
1	A	684	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	22	ASN
1	A	51	ASN
1	A	110	GLN
1	A	116	HIS

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Mol	Chain	Res	Type
1	A	134	HIS
1	A	150	GLN
1	A	196	HIS
1	A	216	ASN
1	A	243	ASN
1	A	346	GLN
1	A	446	ASN
1	A	447	ASN
1	A	455	HIS
1	A	503	GLN
1	A	548	ASN
1	A	562	GLN
1	A	577	ASN
1	A	602	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 ⓘ

2 carbohydrates are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	A	688	1,2	14,14,15	0.70	0	15,19,21	0.99	1 (6%)
2	NDG	A	689	2	14,14,15	0.62	0	15,19,21	0.98	2 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	688	1,2	-	0/6/23/26	0/1/1/1
2	NDG	A	689	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	688	NAG	C2-N2-C7	-3.07	119.09	123.04
2	A	689	NDG	C2-N2-C7	-2.36	120.00	123.04
2	A	689	NDG	C4-C3-C2	-2.23	107.77	111.23

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	688	NAG	4	0
2	A	689	NDG	3	0

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.