Full wwPDB X-ray Structure Validation Report (i)

Oct 15, 2023 – 04:11 PM EDT

PDB ID	:	1WN7
Title	:	Crystal structure of archaeal family B DNA polymerase mutant
Authors	:	Kuroita, T.; Matsumura, H.; Yokota, N.; Hashimoto, H.; Imanaka, T.; Inoue, T.; Kai, Y.
Deposited on	:	2004-07-28
Resolution	:	2.75 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 (i) 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 (i)) were used in the production of this report:

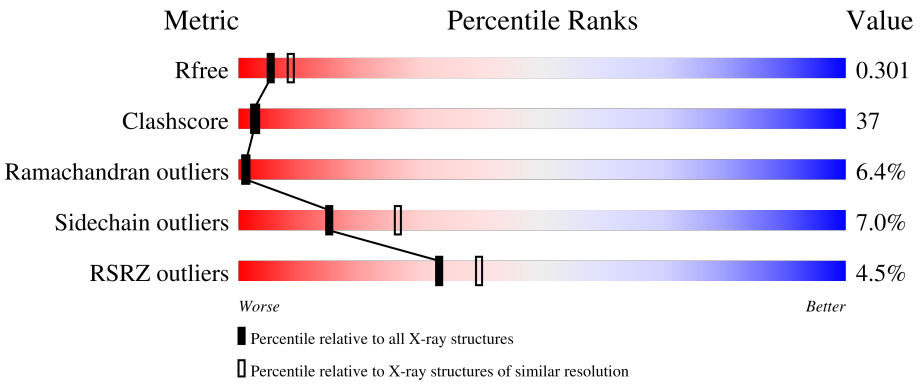
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.75 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}	130704	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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 <=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	774	4% 39% 47% 7% • 6%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6157 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.

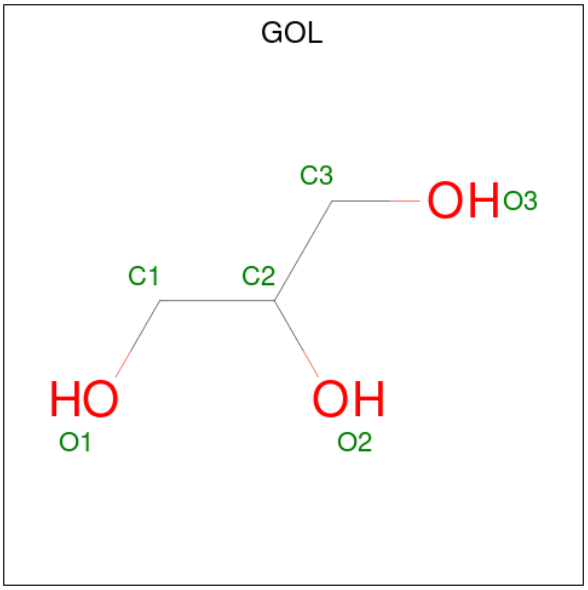
- Molecule 1 is a protein called Family B DNA Polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	729	5873	3778	985	1094	16	0	0	0

- Molecule 2 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ni		
2	A	1	1	1	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 4 is water.

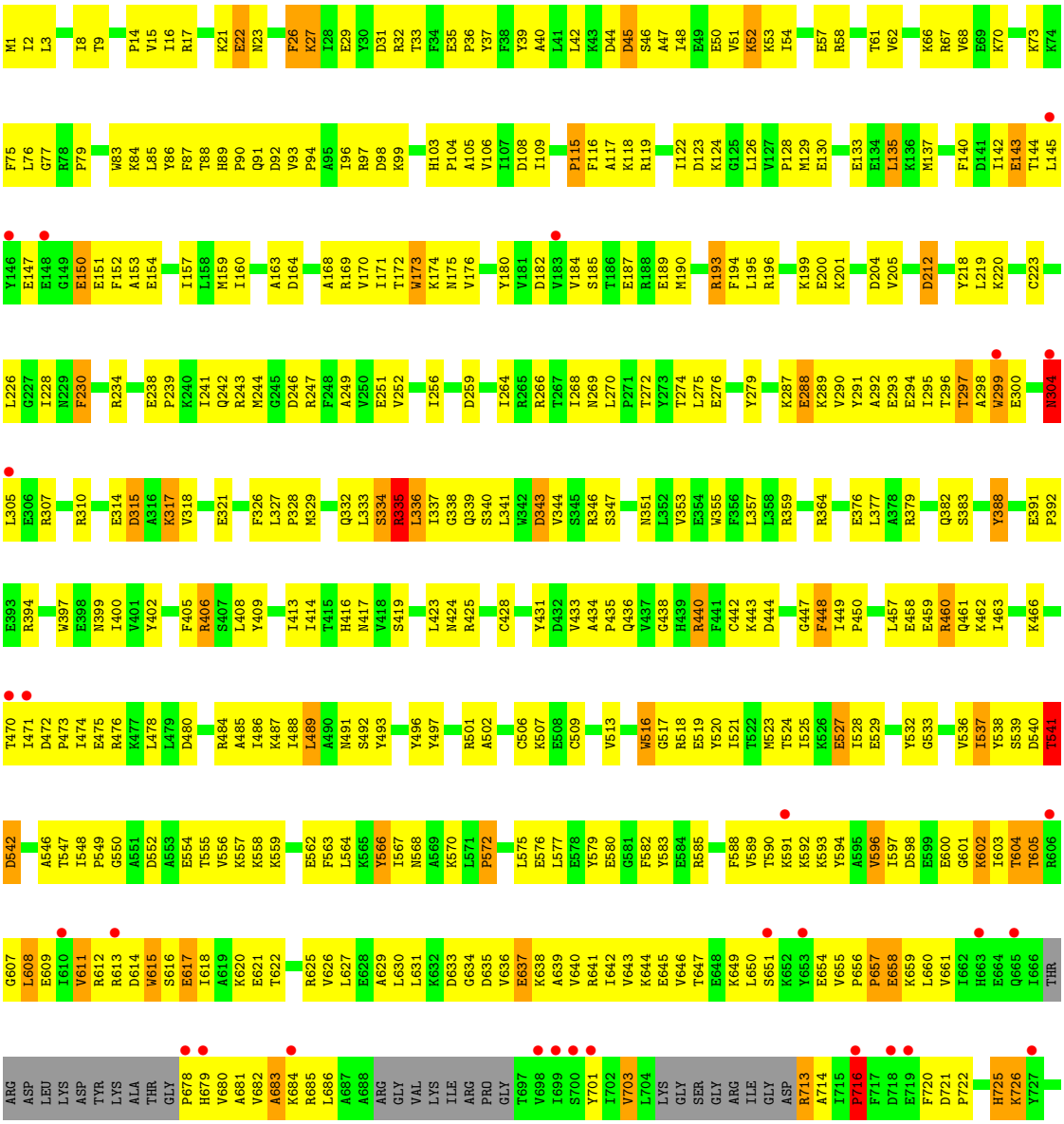
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	277	277	277	0	0

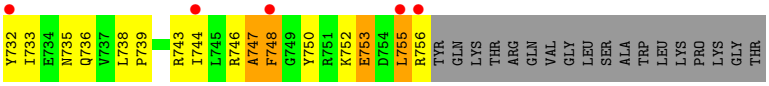
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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: Family B DNA Polymerase

Chain A:




Y732
I733
E734
N735
Q736
V737
L738
P739
R743
I744
L745
R746
A747
F748
G749
Y750
R751
K752
E753
D754
L755
R756
TYR
GLN
LYS
THR
ARG
GLN
VAL
GLY
LEU
SER
ALA
TRP
LEU
LYS
PRO
LYS
GLY
THR

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	74.34Å 111.13Å 111.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.26 – 2.75 33.26 – 2.72	Depositor EDS
% Data completeness (in resolution range)	(Not available) (33.26-2.75) 89.3 (33.26-2.72)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.94 (at 2.72Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.226 , 0.306 0.221 , 0.301	Depositor DCC
R_{free} test set	1103 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å^2)	41.1	Xtriage
Anisotropy	0.588	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 62.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.031 for -h,l,k	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	6157	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.74% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NI, 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	0.40	0/6002	0.61	1/8110 (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	304	ASN	N-CA-C	-5.32	96.64	111.00

There are no chirality outliers.

There are no planarity outliers.

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	5873	0	5752	429	0
2	A	1	0	0	0	0
3	A	6	0	8	1	0
4	A	277	0	0	35	0
All	All	6157	0	5760	429	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 37.

All (429) 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:590:THR:HG22	1:A:591:LYS:H	1.19	1.05
1:A:594:TYR:H	1:A:607:GLY:HA3	1.18	1.04
1:A:392:PRO:HA	4:A:2144:HOH:O	1.60	1.02
1:A:525:ILE:HG23	1:A:536:VAL:HG21	1.39	1.01
1:A:299:TRP:HA	1:A:305:LEU:HD11	1.40	1.00
1:A:76:LEU:HB3	4:A:2070:HOH:O	1.59	1.00
1:A:61:THR:HG22	1:A:62:VAL:H	1.29	0.96
1:A:428:CYS:HB2	1:A:431:TYR:CZ	2.02	0.94
1:A:611:VAL:HG12	1:A:612:ARG:H	1.33	0.94
1:A:276:GLU:HG3	1:A:287:LYS:HD2	1.46	0.93
1:A:720:PHE:O	1:A:722:PRO:HD3	1.71	0.91
1:A:622:THR:HA	1:A:625:ARG:HG3	1.54	0.90
1:A:640:VAL:HG21	1:A:748:PHE:HE1	1.37	0.89
1:A:417:ASN:HD21	1:A:447:GLY:H	1.14	0.89
1:A:51:VAL:O	1:A:54:ILE:HG22	1.73	0.87
1:A:171:ILE:HG22	1:A:190:MET:HG3	1.55	0.86
1:A:738:LEU:HB3	1:A:739:PRO:HD3	1.55	0.86
1:A:680:VAL:HA	1:A:683:ALA:HB3	1.57	0.85
1:A:15:VAL:HG22	1:A:32:ARG:HB3	1.59	0.84
1:A:593:LYS:HA	1:A:607:GLY:CA	2.08	0.83
1:A:541:THR:O	1:A:542:ASP:HB3	1.79	0.83
1:A:590:THR:HG22	1:A:591:LYS:N	1.93	0.83
1:A:103:HIS:CD2	1:A:105:ALA:H	1.97	0.82
1:A:339:GLN:N	4:A:2104:HOH:O	2.11	0.81
1:A:143:GLU:HB2	4:A:2225:HOH:O	1.80	0.81
1:A:48:ILE:HD11	1:A:68:VAL:HG11	1.62	0.80
1:A:594:TYR:N	1:A:607:GLY:HA3	1.96	0.79
1:A:93:VAL:HB	1:A:94:PRO:HD3	1.65	0.78
1:A:635:ASP:HB3	1:A:638:LYS:HB2	1.64	0.78
1:A:244:MET:HG3	1:A:249:ALA:HB2	1.66	0.78
1:A:196:ARG:O	1:A:200:GLU:HB2	1.85	0.77
1:A:590:THR:CG2	1:A:591:LYS:H	1.97	0.77
1:A:627:LEU:HD21	1:A:744:ILE:HD13	1.66	0.77
1:A:650:LEU:HD12	1:A:651:SER:N	1.99	0.76
1:A:608:LEU:HD22	1:A:608:LEU:O	1.86	0.76
1:A:332:GLN:HB3	4:A:2105:HOH:O	1.85	0.76
1:A:701:TYR:HA	1:A:716:PRO:HD3	1.68	0.75
1:A:720:PHE:O	1:A:726:LYS:HG3	1.87	0.75
1:A:296:THR:HG23	1:A:297:THR:H	1.52	0.74
1:A:540:ASP:HB3	4:A:2256:HOH:O	1.86	0.74
1:A:185:SER:HB2	1:A:189:GLU:HG3	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:611:VAL:HG13	1:A:620:LYS:HD2	1.69	0.74
1:A:537:ILE:HD11	1:A:547:THR:HG22	1.71	0.73
1:A:638:LYS:HZ2	1:A:641:ARG:HH21	1.38	0.72
1:A:402:TYR:HD2	1:A:580:GLU:HG2	1.55	0.72
1:A:466:LYS:HD3	1:A:466:LYS:O	1.90	0.72
1:A:159:MET:HG2	1:A:172:THR:HB	1.71	0.71
1:A:594:TYR:O	1:A:605:THR:HG23	1.90	0.71
1:A:117:ALA:HB3	4:A:2024:HOH:O	1.90	0.71
1:A:266:ARG:HD2	4:A:2028:HOH:O	1.91	0.70
1:A:472:ASP:OD2	1:A:475:GLU:HB2	1.90	0.70
1:A:97:ARG:HG3	1:A:98:ASP:H	1.56	0.70
1:A:417:ASN:ND2	1:A:447:GLY:H	1.90	0.69
1:A:622:THR:HA	1:A:625:ARG:CG	2.21	0.69
1:A:440:ARG:HH11	1:A:440:ARG:HB3	1.55	0.69
1:A:626:VAL:HG13	1:A:639:ALA:HB1	1.74	0.69
1:A:596:VAL:HG23	1:A:604:THR:OG1	1.93	0.69
1:A:115:PRO:HB2	1:A:118:LYS:HD3	1.73	0.69
1:A:187:GLU:HB3	4:A:2091:HOH:O	1.92	0.69
1:A:123:ASP:OD2	4:A:2062:HOH:O	2.09	0.69
1:A:379:ARG:HA	1:A:382:GLN:HE21	1.56	0.69
1:A:620:LYS:HE3	4:A:2263:HOH:O	1.93	0.69
1:A:76:LEU:HD12	1:A:76:LEU:O	1.92	0.69
1:A:713:ARG:HD3	1:A:713:ARG:N	2.08	0.68
1:A:173:TRP:CD1	1:A:173:TRP:N	2.61	0.68
1:A:317:LYS:O	1:A:321:GLU:HG3	1.94	0.68
1:A:75:PHE:O	1:A:76:LEU:HG	1.94	0.68
1:A:460:ARG:HH12	1:A:487:LYS:HE2	1.58	0.67
1:A:591:LYS:HG2	4:A:2122:HOH:O	1.93	0.67
1:A:484:ARG:O	1:A:488:ILE:HG13	1.95	0.67
1:A:61:THR:HG22	1:A:62:VAL:N	2.07	0.66
1:A:472:ASP:OD1	1:A:474:ILE:HG22	1.95	0.66
1:A:287:LYS:HE2	1:A:318:VAL:HG21	1.78	0.66
1:A:97:ARG:HG3	1:A:98:ASP:N	2.11	0.65
1:A:449:ILE:HB	1:A:450:PRO:HD3	1.78	0.65
1:A:338:GLY:N	4:A:2104:HOH:O	2.29	0.65
1:A:746:ARG:HA	1:A:746:ARG:NE	2.12	0.65
1:A:212:ASP:HB2	1:A:259:ASP:OD1	1.96	0.65
1:A:638:LYS:O	1:A:642:ILE:HG13	1.97	0.65
1:A:537:ILE:HG12	1:A:546:ALA:HA	1.79	0.65
1:A:199:LYS:HE2	4:A:2133:HOH:O	1.97	0.64
1:A:147:GLU:HG3	1:A:150:GLU:HB2	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:638:LYS:NZ	1:A:641:ARG:HH21	1.94	0.64
1:A:135:LEU:HD12	4:A:2015:HOH:O	1.98	0.63
1:A:517:GLY:O	1:A:521:ILE:HG13	1.98	0.63
1:A:703:VAL:HA	1:A:714:ALA:HB3	1.80	0.63
1:A:205:VAL:HG22	1:A:256:ILE:HB	1.79	0.63
1:A:701:TYR:HA	1:A:716:PRO:CD	2.28	0.63
1:A:26:PHE:CZ	1:A:234:ARG:HG2	2.33	0.63
1:A:556:VAL:HG13	1:A:557:LYS:N	2.13	0.62
1:A:376:GLU:OE2	1:A:379:ARG:NH2	2.32	0.62
1:A:419:SER:HB2	1:A:450:PRO:HD3	1.81	0.62
1:A:118:LYS:HG3	1:A:339:GLN:NE2	2.13	0.62
1:A:615:TRP:O	1:A:620:LYS:HB2	2.00	0.62
1:A:150:GLU:HG3	1:A:154:GLU:HB2	1.80	0.62
1:A:174:LYS:HD2	1:A:299:TRP:CE3	2.35	0.62
1:A:296:THR:HG23	1:A:297:THR:N	2.14	0.62
1:A:752:LYS:NZ	1:A:755:LEU:HD12	2.14	0.62
1:A:291:TYR:O	1:A:295:ILE:HG13	1.99	0.62
1:A:402:TYR:O	1:A:580:GLU:HB3	2.00	0.62
1:A:44:ASP:C	1:A:46:SER:H	2.02	0.61
1:A:593:LYS:HA	1:A:607:GLY:HA2	1.80	0.61
1:A:738:LEU:HD21	1:A:750:TYR:CD2	2.34	0.61
1:A:460:ARG:NH1	1:A:487:LYS:HE2	2.15	0.61
1:A:157:ILE:HG22	1:A:190:MET:HE1	1.83	0.61
1:A:243:ARG:HD2	1:A:243:ARG:O	2.00	0.61
1:A:611:VAL:HG12	1:A:612:ARG:N	2.10	0.61
1:A:118:LYS:HG2	1:A:355:TRP:CH2	2.36	0.60
1:A:636:VAL:HG23	1:A:637:GLU:H	1.66	0.60
1:A:417:ASN:HD21	1:A:447:GLY:N	1.92	0.60
1:A:615:TRP:O	1:A:617:GLU:N	2.30	0.60
1:A:629:ALA:HA	1:A:633:ASP:OD2	2.02	0.60
1:A:130:GLU:HG2	1:A:335:ARG:HG3	1.84	0.60
1:A:402:TYR:CD2	1:A:580:GLU:HG2	2.35	0.60
1:A:173:TRP:H	1:A:173:TRP:HD1	1.48	0.59
1:A:42:LEU:HD12	1:A:83:TRP:CD1	2.38	0.59
1:A:122:ILE:HG23	1:A:359:ARG:HA	1.83	0.59
1:A:733:ILE:O	1:A:738:LEU:HB2	2.03	0.59
1:A:58:ARG:HH11	1:A:91:GLN:HB2	1.67	0.59
1:A:428:CYS:HB2	1:A:431:TYR:OH	2.03	0.59
1:A:579:TYR:OH	1:A:582:PHE:HB2	2.03	0.59
1:A:645:GLU:O	1:A:649:LYS:HG2	2.02	0.59
1:A:16:ILE:HG22	1:A:31:ASP:HB3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:474:ILE:O	1:A:478:LEU:HB2	2.03	0.58
1:A:164:ASP:OD1	1:A:201:LYS:HD3	2.03	0.58
1:A:615:TRP:C	1:A:620:LYS:HG3	2.24	0.58
1:A:340:SER:OG	1:A:343:ASP:HB2	2.04	0.58
1:A:44:ASP:O	1:A:46:SER:N	2.37	0.58
1:A:459:GLU:O	1:A:463:ILE:HG12	2.04	0.58
1:A:750:TYR:HA	1:A:753:GLU:CD	2.24	0.58
1:A:541:THR:O	1:A:542:ASP:CB	2.51	0.57
1:A:1:MET:CE	1:A:135:LEU:HD21	2.34	0.57
1:A:29:GLU:HB3	4:A:2003:HOH:O	2.03	0.57
1:A:31:ASP:OD1	1:A:33:THR:HB	2.05	0.57
1:A:54:ILE:HA	4:A:2183:HOH:O	2.05	0.57
1:A:647:THR:HG21	1:A:753:GLU:O	2.04	0.57
1:A:640:VAL:HG21	1:A:748:PHE:CE1	2.29	0.57
1:A:470:THR:O	1:A:471:ILE:HB	2.05	0.57
1:A:525:ILE:O	1:A:529:GLU:HG3	2.04	0.57
1:A:538:TYR:HA	4:A:2144:HOH:O	2.04	0.57
1:A:506:CYS:HA	4:A:2251:HOH:O	2.05	0.56
1:A:567:ILE:HD12	1:A:568:ASN:N	2.20	0.56
1:A:679:HIS:ND1	1:A:680:VAL:N	2.52	0.56
1:A:637:GLU:O	1:A:641:ARG:HG3	2.05	0.56
1:A:638:LYS:NZ	1:A:641:ARG:NH2	2.54	0.56
1:A:735:ASN:O	1:A:736:GLN:HG2	2.05	0.56
1:A:397:TRP:HB2	1:A:400:ILE:HD11	1.88	0.56
1:A:89:HIS:O	1:A:92:ASP:HB2	2.04	0.56
1:A:145:LEU:HD22	4:A:2228:HOH:O	2.06	0.56
1:A:603:ILE:O	1:A:603:ILE:HG13	2.06	0.56
1:A:1:MET:HE2	1:A:135:LEU:HD21	1.88	0.56
1:A:151:GLU:HG2	1:A:154:GLU:CG	2.36	0.56
1:A:752:LYS:HZ1	1:A:755:LEU:HD12	1.70	0.56
1:A:145:LEU:HD13	4:A:2228:HOH:O	2.06	0.55
1:A:36:PRO:HD2	1:A:87:PHE:O	2.07	0.55
1:A:159:MET:CE	1:A:170:VAL:HG11	2.35	0.55
1:A:163:ALA:HA	1:A:168:ALA:HA	1.88	0.55
1:A:746:ARG:HA	1:A:746:ARG:CZ	2.36	0.55
1:A:54:ILE:HD11	1:A:99:LYS:HB3	1.87	0.55
1:A:333:LEU:O	1:A:337:ILE:HG12	2.06	0.55
1:A:558:LYS:O	1:A:562:GLU:HG3	2.07	0.55
1:A:650:LEU:HD12	1:A:651:SER:H	1.71	0.55
1:A:58:ARG:NH1	1:A:91:GLN:HB2	2.22	0.54
1:A:279:TYR:CD1	1:A:318:VAL:HG13	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:ALA:HA	1:A:218:TYR:CZ	2.42	0.54
1:A:409:TYR:O	1:A:413:ILE:HG12	2.05	0.54
1:A:701:TYR:HA	1:A:716:PRO:HG3	1.87	0.54
1:A:118:LYS:HG3	1:A:339:GLN:HE22	1.73	0.54
1:A:142:ILE:HG13	1:A:142:ILE:O	2.07	0.54
1:A:21:LYS:HE2	1:A:204:ASP:OD2	2.08	0.54
1:A:635:ASP:OD1	1:A:638:LYS:HD3	2.08	0.54
1:A:142:ILE:HG22	1:A:160:ILE:HG12	1.89	0.54
1:A:597:ILE:HB	1:A:631:LEU:HD13	1.90	0.54
1:A:608:LEU:HD21	1:A:744:ILE:CG1	2.38	0.54
1:A:22:GLU:O	1:A:133:GLU:OE1	2.26	0.54
1:A:296:THR:O	1:A:300:GLU:HG3	2.07	0.54
1:A:122:ILE:CG2	1:A:359:ARG:HA	2.38	0.54
1:A:346:ARG:HG3	1:A:346:ARG:HH11	1.72	0.54
1:A:388:TYR:HD1	1:A:518:ARG:HD3	1.73	0.53
1:A:272:THR:HG22	1:A:274:THR:HG23	1.88	0.53
1:A:288:GLU:CB	1:A:310:ARG:HH22	2.22	0.53
1:A:657:PRO:HG2	1:A:658:GLU:H	1.73	0.53
1:A:564:LEU:HD22	1:A:577:LEU:O	2.09	0.53
1:A:288:GLU:HB3	1:A:310:ARG:HH22	1.73	0.53
1:A:470:THR:H	1:A:476:ARG:HH11	1.55	0.53
1:A:630:LEU:O	1:A:634:GLY:HA2	2.09	0.53
1:A:563:PHE:O	1:A:566:TYR:HB3	2.09	0.53
1:A:585:ARG:HD2	1:A:631:LEU:O	2.09	0.53
1:A:460:ARG:HB3	1:A:486:ILE:HG21	1.91	0.52
1:A:684:LYS:C	1:A:686:LEU:H	2.13	0.52
1:A:3:LEU:HD22	1:A:256:ILE:HD11	1.91	0.52
1:A:461:GLN:HA	1:A:461:GLN:OE1	2.10	0.52
1:A:567:ILE:O	1:A:570:LYS:HB3	2.09	0.52
1:A:77:GLY:HA3	1:A:425:ARG:HH22	1.73	0.52
1:A:144:THR:HG21	1:A:218:TYR:CE2	2.45	0.52
1:A:276:GLU:HG3	1:A:287:LYS:HB3	1.92	0.52
1:A:568:ASN:ND2	1:A:576:GLU:HG3	2.25	0.52
1:A:334:SER:HA	1:A:344:VAL:HG21	1.92	0.52
1:A:33:THR:HG22	4:A:2061:HOH:O	2.09	0.52
1:A:292:ALA:O	1:A:295:ILE:N	2.43	0.52
1:A:434:ALA:O	1:A:438:GLY:HA2	2.11	0.51
1:A:643:VAL:O	1:A:647:THR:HG23	2.09	0.51
1:A:33:THR:HG21	4:A:2055:HOH:O	2.09	0.51
1:A:103:HIS:HD2	1:A:105:ALA:H	1.54	0.51
1:A:135:LEU:HD12	1:A:135:LEU:H	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:590:THR:HG22	1:A:591:LYS:HG3	1.91	0.51
1:A:636:VAL:HG23	1:A:637:GLU:N	2.25	0.51
1:A:738:LEU:HB3	1:A:739:PRO:CD	2.34	0.51
1:A:618:ILE:HG13	1:A:659:LYS:O	2.10	0.51
1:A:51:VAL:C	1:A:53:LYS:H	2.14	0.51
1:A:79:PRO:HA	4:A:2073:HOH:O	2.10	0.51
1:A:341:LEU:HD12	1:A:341:LEU:O	2.10	0.51
1:A:399:ASN:HA	1:A:582:PHE:CZ	2.46	0.51
1:A:593:LYS:HA	1:A:607:GLY:HA3	1.90	0.51
1:A:678:PRO:HB2	4:A:2138:HOH:O	2.11	0.51
1:A:26:PHE:CE1	1:A:234:ARG:HG2	2.46	0.51
1:A:37:TYR:CD1	1:A:37:TYR:C	2.84	0.51
1:A:171:ILE:HD13	1:A:193:ARG:HB3	1.93	0.51
1:A:471:ILE:O	1:A:473:PRO:HD3	2.11	0.51
1:A:103:HIS:CG	1:A:104:PRO:HD2	2.46	0.50
1:A:151:GLU:OE2	1:A:154:GLU:HG3	2.10	0.50
1:A:659:LYS:O	1:A:660:LEU:HD23	2.11	0.50
1:A:147:GLU:HG3	1:A:150:GLU:CB	2.40	0.50
1:A:559:LYS:HA	1:A:562:GLU:OE1	2.12	0.50
1:A:33:THR:HG21	4:A:2215:HOH:O	2.11	0.50
1:A:169:ARG:HD2	1:A:180:TYR:C	2.32	0.50
1:A:722:PRO:HD2	1:A:726:LYS:H	1.77	0.50
1:A:137:MET:HG2	1:A:205:VAL:HB	1.93	0.50
1:A:701:TYR:HA	1:A:716:PRO:CG	2.42	0.50
1:A:332:GLN:NE2	1:A:332:GLN:HA	2.27	0.50
1:A:388:TYR:CD1	1:A:518:ARG:HD3	2.46	0.49
1:A:122:ILE:HB	4:A:2195:HOH:O	2.11	0.49
1:A:428:CYS:HB2	1:A:431:TYR:CE1	2.47	0.49
1:A:639:ALA:HA	1:A:642:ILE:HD12	1.93	0.49
1:A:103:HIS:CD2	1:A:105:ALA:N	2.74	0.49
1:A:646:VAL:O	1:A:650:LEU:HG	2.11	0.49
1:A:650:LEU:CD1	1:A:733:ILE:HB	2.43	0.49
1:A:591:LYS:O	1:A:593:LYS:N	2.46	0.49
1:A:743:ARG:O	1:A:746:ARG:NH1	2.45	0.49
1:A:567:ILE:HA	1:A:570:LYS:HB3	1.94	0.49
1:A:405:PHE:HB2	1:A:408:LEU:HB2	1.94	0.49
1:A:641:ARG:O	1:A:645:GLU:HG3	2.13	0.49
1:A:16:ILE:CG2	1:A:31:ASP:HB3	2.42	0.49
1:A:601:GLY:O	1:A:602:LYS:O	2.31	0.49
1:A:722:PRO:HG3	1:A:725:HIS:CB	2.43	0.49
1:A:44:ASP:C	1:A:46:SER:N	2.65	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:608:LEU:CD1	1:A:608:LEU:H	2.25	0.48
1:A:642:ILE:O	1:A:646:VAL:HG23	2.13	0.48
1:A:84:LYS:HD3	1:A:86:TYR:OH	2.12	0.48
1:A:193:ARG:HA	1:A:193:ARG:HD2	1.60	0.48
1:A:399:ASN:N	1:A:399:ASN:HD22	2.10	0.48
1:A:423:LEU:CD1	1:A:424:ASN:ND2	2.76	0.48
1:A:470:THR:N	1:A:476:ARG:HH11	2.12	0.48
1:A:556:VAL:CG1	1:A:557:LYS:N	2.77	0.48
1:A:394:ARG:CZ	1:A:746:ARG:HD3	2.44	0.48
1:A:713:ARG:N	1:A:713:ARG:CD	2.72	0.47
1:A:406:ARG:NH2	1:A:460:ARG:HH12	2.12	0.47
1:A:327:LEU:N	1:A:328:PRO:CD	2.77	0.47
1:A:585:ARG:HH11	1:A:634:GLY:HA3	1.79	0.47
1:A:644:LYS:HE2	1:A:755:LEU:HD22	1.97	0.47
1:A:14:PRO:HG3	1:A:90:PRO:HD3	1.95	0.47
1:A:171:ILE:HG23	1:A:184:VAL:HG11	1.96	0.47
1:A:346:ARG:HG3	1:A:346:ARG:NH1	2.29	0.47
1:A:419:SER:HB2	1:A:450:PRO:CD	2.43	0.47
1:A:147:GLU:O	1:A:150:GLU:HB3	2.15	0.47
1:A:304:ASN:O	1:A:307:ARG:HB2	2.14	0.47
1:A:47:ALA:HB3	1:A:105:ALA:HB1	1.97	0.47
1:A:84:LYS:HD3	1:A:86:TYR:CZ	2.49	0.47
1:A:150:GLU:CG	1:A:154:GLU:HB2	2.45	0.47
1:A:187:GLU:HG2	1:A:226:LEU:HD11	1.95	0.47
1:A:272:THR:CG2	1:A:274:THR:HG23	2.45	0.47
1:A:353:VAL:O	1:A:357:LEU:HG	2.15	0.47
1:A:555:THR:HA	4:A:2148:HOH:O	2.13	0.47
1:A:218:TYR:O	1:A:220:LYS:N	2.47	0.47
1:A:244:MET:O	1:A:247:ARG:HG2	2.14	0.47
1:A:289:LYS:HD2	1:A:290:VAL:N	2.29	0.47
1:A:475:GLU:HA	1:A:475:GLU:OE1	2.14	0.47
1:A:26:PHE:O	1:A:27:LYS:HB2	2.15	0.47
1:A:172:THR:O	1:A:184:VAL:HG22	2.14	0.47
1:A:471:ILE:N	1:A:471:ILE:HD12	2.30	0.47
1:A:489:LEU:HD22	1:A:493:TYR:HE1	1.80	0.47
1:A:682:VAL:HG21	1:A:714:ALA:C	2.35	0.47
1:A:720:PHE:O	1:A:722:PRO:CD	2.54	0.47
1:A:119:ARG:HD2	1:A:119:ARG:HA	1.73	0.46
1:A:402:TYR:HD2	1:A:580:GLU:CG	2.25	0.46
1:A:618:ILE:HD11	1:A:660:LEU:CD2	2.45	0.46
1:A:684:LYS:O	1:A:686:LEU:N	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:471:ILE:H	1:A:476:ARG:NH1	2.13	0.46
1:A:22:GLU:O	1:A:133:GLU:CD	2.53	0.46
1:A:42:LEU:CD2	1:A:106:VAL:HG22	2.45	0.46
1:A:527:GLU:HG3	1:A:566:TYR:HE2	1.79	0.46
1:A:509:CYS:O	1:A:513:VAL:HG23	2.15	0.46
1:A:556:VAL:HG13	1:A:557:LYS:H	1.78	0.46
1:A:616:SER:O	1:A:617:GLU:CB	2.64	0.46
1:A:296:THR:CG2	1:A:297:THR:H	2.26	0.46
1:A:618:ILE:HD11	1:A:660:LEU:HD21	1.98	0.46
1:A:738:LEU:CB	1:A:739:PRO:HD3	2.37	0.46
1:A:489:LEU:O	1:A:492:SER:HB2	2.15	0.46
1:A:533:GLY:O	1:A:548:ILE:HG23	2.16	0.46
1:A:334:SER:O	4:A:2104:HOH:O	2.20	0.46
1:A:61:THR:CG2	1:A:62:VAL:H	2.10	0.45
1:A:608:LEU:CD1	1:A:608:LEU:N	2.79	0.45
1:A:159:MET:HE1	1:A:170:VAL:HG11	1.98	0.45
1:A:338:GLY:CA	4:A:2104:HOH:O	2.63	0.45
1:A:151:GLU:HG2	1:A:154:GLU:HG2	1.98	0.45
1:A:223:CYS:HA	1:A:228:ILE:HG22	1.98	0.45
1:A:593:LYS:HA	1:A:607:GLY:C	2.37	0.45
1:A:621:GLU:O	1:A:625:ARG:HG2	2.17	0.45
1:A:629:ALA:O	1:A:633:ASP:HB2	2.16	0.45
1:A:242:GLN:NE2	1:A:251:GLU:OE1	2.48	0.45
1:A:442:CYS:SG	1:A:444:ASP:HB2	2.56	0.45
1:A:594:TYR:H	1:A:607:GLY:CA	2.09	0.45
1:A:598:ASP:OD1	1:A:600:GLU:HG3	2.16	0.45
1:A:269:ASN:O	1:A:270:LEU:HD23	2.17	0.45
1:A:458:GLU:O	1:A:461:GLN:HB2	2.17	0.45
1:A:87:PHE:CE2	1:A:96:ILE:HG21	2.51	0.45
1:A:440:ARG:NE	4:A:2245:HOH:O	2.36	0.45
1:A:160:ILE:HG21	1:A:194:PHE:CG	2.52	0.44
1:A:8:ILE:HG22	1:A:9:THR:N	2.32	0.44
1:A:26:PHE:CE2	1:A:234:ARG:HG2	2.53	0.44
1:A:124:LYS:CB	1:A:126:LEU:HD13	2.47	0.44
1:A:171:ILE:HG12	1:A:182:ASP:HB2	1.99	0.44
1:A:480:ASP:O	1:A:484:ARG:HG3	2.17	0.44
1:A:336:LEU:HD12	1:A:485:ALA:HB1	1.99	0.44
1:A:585:ARG:NH1	1:A:634:GLY:HA3	2.33	0.44
1:A:47:ALA:CB	1:A:105:ALA:CB	2.95	0.44
1:A:103:HIS:HD2	1:A:105:ALA:N	2.13	0.44
1:A:220:LYS:NZ	1:A:241:ILE:CD1	2.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:ALA:O	1:A:293:GLU:C	2.56	0.44
1:A:314:GLU:O	1:A:315:ASP:C	2.55	0.44
1:A:616:SER:OG	1:A:736:GLN:NE2	2.50	0.44
1:A:142:ILE:HG22	1:A:160:ILE:HA	1.99	0.44
1:A:423:LEU:HD13	1:A:424:ASN:ND2	2.33	0.44
1:A:90:PRO:O	1:A:94:PRO:HD3	2.18	0.43
1:A:246:ASP:N	1:A:246:ASP:OD2	2.51	0.43
1:A:292:ALA:HA	1:A:295:ILE:HD12	1.98	0.43
1:A:298:ALA:HB1	1:A:304:ASN:HB3	1.99	0.43
1:A:564:LEU:O	1:A:567:ILE:HD12	2.18	0.43
1:A:746:ARG:O	1:A:747:ALA:HB2	2.18	0.43
1:A:491:ASN:HB3	3:A:2001:GOL:O3	2.18	0.43
1:A:501:ARG:NH2	4:A:2045:HOH:O	2.51	0.43
1:A:540:ASP:O	1:A:541:THR:C	2.55	0.43
1:A:57:GLU:HG3	1:A:61:THR:O	2.18	0.43
1:A:243:ARG:O	1:A:244:MET:HG2	2.19	0.43
1:A:264:ILE:HD11	1:A:326:PHE:CE1	2.53	0.43
1:A:379:ARG:HG2	1:A:379:ARG:HH11	1.83	0.43
1:A:45:ASP:OD2	1:A:70:LYS:HD2	2.19	0.43
1:A:193:ARG:NH1	1:A:193:ARG:HG3	2.33	0.43
1:A:364:ARG:HD3	1:A:448:PHE:HE1	1.82	0.43
1:A:726:LYS:HA	1:A:726:LYS:HZ3	1.83	0.43
1:A:204:ASP:HA	1:A:234:ARG:NH1	2.34	0.43
1:A:528:ILE:HG23	1:A:529:GLU:N	2.34	0.43
1:A:703:VAL:CB	1:A:714:ALA:H	2.32	0.43
1:A:52:LYS:O	1:A:52:LYS:HG3	2.18	0.43
1:A:416:HIS:O	1:A:417:ASN:C	2.57	0.43
1:A:527:GLU:OE1	1:A:527:GLU:HA	2.19	0.43
1:A:567:ILE:HD12	1:A:568:ASN:H	1.83	0.43
1:A:660:LEU:HB3	1:A:732:TYR:CZ	2.54	0.43
1:A:150:GLU:HG3	1:A:154:GLU:CB	2.46	0.43
1:A:414:ILE:HD12	1:A:457:LEU:HD12	2.00	0.43
1:A:516:TRP:CD1	1:A:520:TYR:HE1	2.36	0.43
1:A:622:THR:O	1:A:626:VAL:HG23	2.19	0.43
1:A:434:ALA:HA	1:A:435:PRO:HD3	1.94	0.42
1:A:39:TYR:CZ	1:A:73:LYS:HE3	2.53	0.42
1:A:36:PRO:O	1:A:37:TYR:HB3	2.18	0.42
1:A:423:LEU:HD11	1:A:424:ASN:ND2	2.35	0.42
1:A:428:CYS:HA	1:A:444:ASP:OD2	2.18	0.42
1:A:35:GLU:HA	1:A:36:PRO:HD3	1.84	0.42
1:A:175:ASN:HA	4:A:2086:HOH:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:PHE:HD2	1:A:230:PHE:HA	1.72	0.42
1:A:521:ILE:HG13	1:A:521:ILE:H	1.64	0.42
1:A:471:ILE:H	1:A:476:ARG:HH11	1.66	0.42
1:A:487:LYS:HG3	1:A:491:ASN:HD21	1.85	0.42
1:A:589:VAL:O	1:A:590:THR:HB	2.19	0.42
1:A:223:CYS:HA	1:A:228:ILE:CG2	2.50	0.42
1:A:329:MET:CE	1:A:484:ARG:CZ	2.98	0.42
1:A:556:VAL:CG1	1:A:557:LYS:H	2.33	0.42
1:A:614:ASP:C	1:A:616:SER:H	2.23	0.42
1:A:294:GLU:O	1:A:298:ALA:HB2	2.19	0.42
1:A:391:GLU:HA	1:A:392:PRO:HD3	1.88	0.42
1:A:151:GLU:H	1:A:151:GLU:CD	2.21	0.42
1:A:276:GLU:HG2	1:A:289:LYS:HB2	2.02	0.42
1:A:552:ASP:C	1:A:554:GLU:H	2.23	0.42
1:A:611:VAL:CG1	1:A:612:ARG:H	2.15	0.42
1:A:654:GLU:HA	4:A:2162:HOH:O	2.20	0.42
1:A:115:PRO:O	1:A:116:PHE:C	2.58	0.42
1:A:604:THR:O	1:A:605:THR:HB	2.20	0.42
1:A:443:LYS:HB3	1:A:443:LYS:HE2	1.89	0.41
1:A:618:ILE:HD13	1:A:655:VAL:HG21	2.01	0.41
1:A:220:LYS:NZ	1:A:241:ILE:HD11	2.35	0.41
1:A:27:LYS:HE2	4:A:2214:HOH:O	2.20	0.41
1:A:40:ALA:HA	1:A:109:ILE:HA	2.02	0.41
1:A:218:TYR:C	1:A:220:LYS:N	2.74	0.41
1:A:89:HIS:HA	1:A:90:PRO:HD3	1.96	0.41
1:A:238:GLU:O	1:A:239:PRO:C	2.56	0.41
1:A:497:TYR:CD1	1:A:506:CYS:HB3	2.55	0.41
1:A:2:ILE:HB	1:A:128:PRO:HA	2.02	0.41
1:A:142:ILE:CG2	1:A:160:ILE:HG12	2.49	0.41
1:A:496:TYR:CZ	1:A:502:ALA:HB1	2.56	0.41
1:A:518:ARG:O	1:A:519:GLU:C	2.58	0.41
1:A:650:LEU:HD11	1:A:733:ILE:HB	2.03	0.41
1:A:755:LEU:O	1:A:756:ARG:HB2	2.20	0.41
1:A:1:MET:HE3	1:A:129:MET:SD	2.60	0.41
1:A:347:SER:OG	1:A:351:ASN:HB2	2.20	0.41
1:A:423:LEU:HD13	1:A:423:LEU:C	2.41	0.41
1:A:583:TYR:CD2	1:A:596:VAL:HB	2.56	0.41
1:A:268:ILE:HG22	1:A:269:ASN:N	2.35	0.41
1:A:528:ILE:O	1:A:532:TYR:HB2	2.21	0.41
1:A:636:VAL:C	1:A:638:LYS:H	2.23	0.41
1:A:291:TYR:CD1	1:A:291:TYR:N	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:GLU:O	1:A:317:LYS:N	2.53	0.41
1:A:726:LYS:HA	1:A:726:LYS:NZ	2.35	0.41
1:A:523:MET:O	1:A:527:GLU:HB2	2.21	0.41
1:A:537:ILE:HG21	1:A:588:PHE:CE1	2.56	0.41
1:A:413:ILE:HD11	1:A:513:VAL:HG21	2.03	0.40
1:A:470:THR:H	1:A:476:ARG:NH1	2.18	0.40
1:A:538:TYR:CD1	1:A:539:SER:N	2.89	0.40
1:A:608:LEU:HD21	1:A:744:ILE:HG12	2.01	0.40
1:A:14:PRO:CD	1:A:88:THR:O	2.69	0.40
1:A:193:ARG:HG3	1:A:193:ARG:HH11	1.85	0.40
1:A:460:ARG:HH12	1:A:487:LYS:CE	2.31	0.40
1:A:22:GLU:HB3	1:A:23:ASN:H	1.69	0.40
1:A:153:ALA:HA	1:A:218:TYR:CE1	2.56	0.40
1:A:433:VAL:O	1:A:434:ALA:C	2.58	0.40
1:A:521:ILE:O	1:A:524:THR:N	2.51	0.40
1:A:8:ILE:HD11	1:A:17:ARG:NH2	2.37	0.40
1:A:37:TYR:HB2	1:A:85:LEU:O	2.22	0.40
1:A:180:TYR:HD1	1:A:180:TYR:O	2.05	0.40
1:A:537:ILE:HB	1:A:538:TYR:H	1.74	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	721/774 (93%)	572 (79%)	103 (14%)	46 (6%)	1 1

All (46) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	66	LYS
1	A	304	ASN

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Mol	Chain	Res	Type
1	A	572	PRO
1	A	592	LYS
1	A	602	LYS
1	A	617	GLU
1	A	721	ASP
1	A	45	ASP
1	A	150	GLU
1	A	219	LEU
1	A	335	ARG
1	A	542	ASP
1	A	566	TYR
1	A	611	VAL
1	A	656	PRO
1	A	685	ARG
1	A	725	HIS
1	A	747	ALA
1	A	52	LYS
1	A	334	SER
1	A	383	SER
1	A	436	GLN
1	A	537	ILE
1	A	550	GLY
1	A	605	THR
1	A	683	ALA
1	A	152	PHE
1	A	448	PHE
1	A	541	THR
1	A	604	THR
1	A	609	GLU
1	A	613	ARG
1	A	615	TRP
1	A	637	GLU
1	A	657	PRO
1	A	681	ALA
1	A	26	PHE
1	A	27	LYS
1	A	716	PRO
1	A	755	LEU
1	A	252	VAL
1	A	661	VAL
1	A	115	PRO
1	A	549	PRO

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Mol	Chain	Res	Type
1	A	176	VAL
1	A	703	VAL

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	602/674 (89%)	560 (93%)	42 (7%)	15 26

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	GLU
1	A	50	GLU
1	A	67	ARG
1	A	108	ASP
1	A	135	LEU
1	A	140	PHE
1	A	143	GLU
1	A	173	TRP
1	A	193	ARG
1	A	195	LEU
1	A	212	ASP
1	A	230	PHE
1	A	275	LEU
1	A	288	GLU
1	A	297	THR
1	A	299	TRP
1	A	315	ASP
1	A	317	LYS
1	A	335	ARG
1	A	336	LEU
1	A	343	ASP
1	A	377	LEU
1	A	388	TYR
1	A	406	ARG

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Mol	Chain	Res	Type
1	A	440	ARG
1	A	460	ARG
1	A	462	LYS
1	A	489	LEU
1	A	507	LYS
1	A	516	TRP
1	A	527	GLU
1	A	541	THR
1	A	572	PRO
1	A	575	LEU
1	A	596	VAL
1	A	608	LEU
1	A	658	GLU
1	A	713	ARG
1	A	716	PRO
1	A	726	LYS
1	A	748	PHE
1	A	753	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	HIS
1	A	229	ASN
1	A	339	GLN
1	A	382	GLN
1	A	399	ASN
1	A	416	HIS
1	A	417	ASN
1	A	424	ASN
1	A	491	ASN
1	A	736	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 1 is 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	$\#\|Z\| > 2$
3	GOL	A	2001	-	5,5,5	0.91	0	5,5,5	0.39	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
3	GOL	A	2001	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2001	GOL	O2-C2-C3-O3
3	A	2001	GOL	C1-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2001	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 (i)

6.1 Protein, DNA and RNA chains (i)

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	729/774 (94%)	-0.05	33 (4%) 33 39	11, 50, 105, 116	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	699	ILE	5.2
1	A	305	LEU	3.9
1	A	701	TYR	3.8
1	A	727	TYR	3.5
1	A	653	TYR	3.5
1	A	719	GLU	3.4
1	A	651	SER	3.0
1	A	610	ILE	2.9
1	A	591	LYS	2.9
1	A	700	SER	2.8
1	A	304	ASN	2.7
1	A	718	ASP	2.7
1	A	732	TYR	2.5
1	A	146	TYR	2.5
1	A	471	ILE	2.4
1	A	755	LEU	2.3
1	A	698	VAL	2.3
1	A	148	GLU	2.3
1	A	470	THR	2.3
1	A	678	PRO	2.2
1	A	145	LEU	2.2
1	A	183	VAL	2.2
1	A	756	ARG	2.2
1	A	748	PHE	2.2
1	A	663	HIS	2.1
1	A	679	HIS	2.1
1	A	744	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	716	PRO	2.1
1	A	665	GLN	2.1
1	A	606	ARG	2.0
1	A	613	ARG	2.0
1	A	299	TRP	2.0
1	A	684	LYS	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides 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	GOL	A	2001	6/6	0.85	0.22	70,72,73,74	0
2	NI	A	1001	1/1	0.99	0.22	41,41,41,41	0

6.5 Other polymers (i)

There are no such residues in this entry.