WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 09:02 PM GMT

|		
PDB ID	:	1N54
Title	:	Cap Binding Complex m7GpppG free
Authors	:	Calero, G.; Wilson, K.; Ly, T.; Rios-Steiner, J.; Clardy, J.; Cerione, R.
Deposited on	:	2002-11-04
Resolution	:	2.72 Å(reported)

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 2.72 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	Percentile Ranks	Value
Rfree		0.281
Clashscore		30
Ramachandran outliers		2.6%
Sidechain outliers		6.2%
RSRZ outliers		6.7%

Worse   *Better*

▮ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution
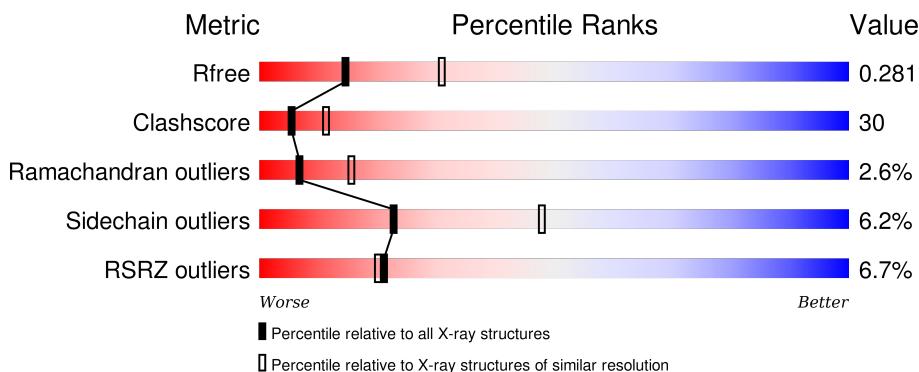
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	91344	2439 (2.74-2.70)
Clashscore	102246	2771 (2.74-2.70)
Ramachandran outliers	100387	2726 (2.74-2.70)
Sidechain outliers	100360	2727 (2.74-2.70)
RSRZ outliers	91569	2443 (2.74-2.70)

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	790	5%	46% 42% • 7%
2	B	156	10%	36% 36% • • 22%
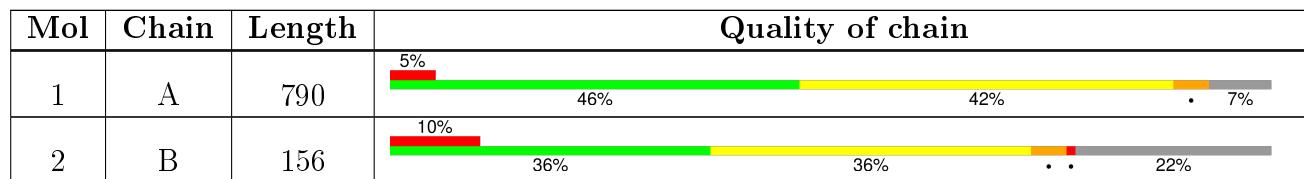
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	A	1556	-	X	-	-
3	GOL	A	1557	-	X	-	-
3	GOL	A	1558	-	X	-	X
3	GOL	A	1560	-	X	-	X
3	GOL	B	1555	-	X	-	-
3	GOL	B	1559	-	X	-	-
3	GOL	B	1561	-	X	-	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 7292 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 80 kDa nuclear cap binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	733	5997	3865	1010	1084	38	0	0	0

- Molecule 2 is a protein called 20 kDa nuclear cap binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	121	998	628	171	193	6	0	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).
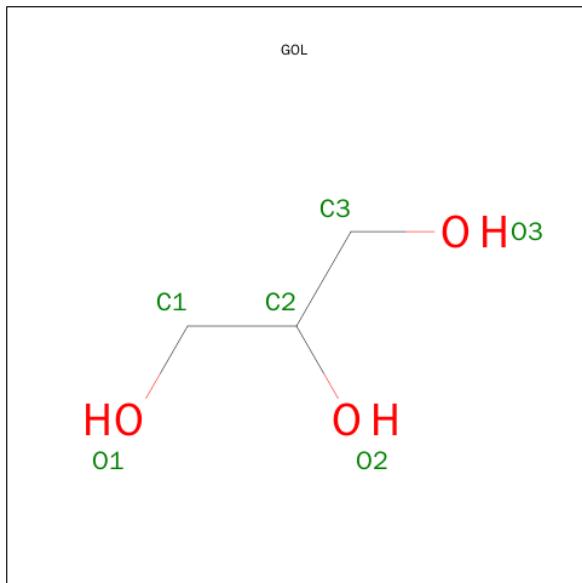
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	B	1	6	3	3	0	0
3	A	1	6	3	3	0	0

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	208	Total 208	O 208	0	0
4	B	47	Total 47	O 47	0	0

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.

- Molecule 1: 80 kDa nuclear cap binding protein

A780 V781   Q784 F785   Q789 A790
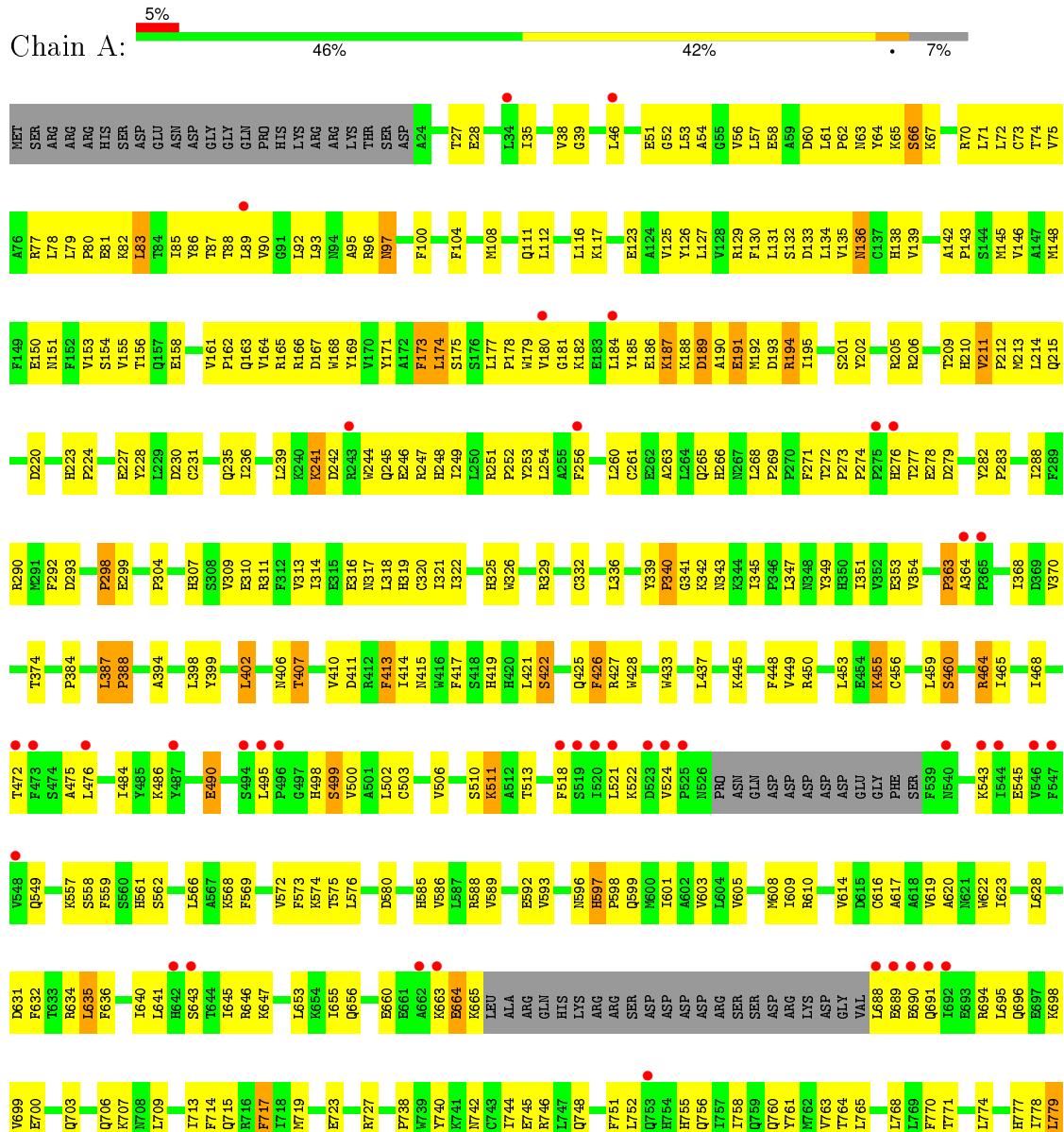
• Molecule 2: 20 kDa nuclear cap binding protein

Chain B:
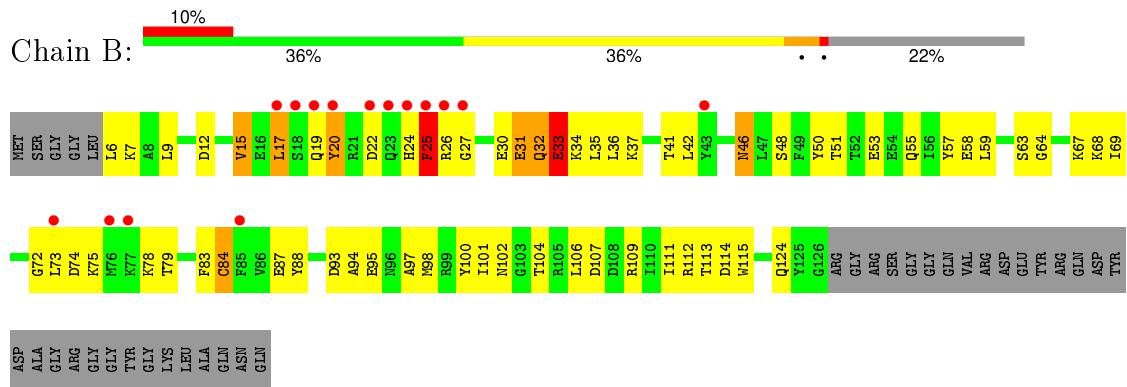
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	111.77Å 111.77Å 175.73Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	24.41 – 2.72 48.40 – 2.59	Depositor EDS
% Data completeness (in resolution range)	72.9 (24.41-2.72) 84.4 (48.40-2.59)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	1.47 (at 2.58Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.263 , 0.282 0.258 , 0.281	Depositor DCC
R_{free} test set	2294 reflections (9.12%)	DCC
Wilson B-factor (Å²)	64.5	Xtriage
Anisotropy	0.264	Xtriage
Bulk solvent k_{sol}(e/Å³), B_{sol}(Å²)	0.30 , 64.3	EDS
Estimated twinning fraction	0.045 for -h,-k,l	Xtriage
L-test for twinning [2]	$< |L| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Outliers	0 of 33886 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	7292	wwPDB-VP
Average B, all atoms (Å²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.61% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: 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	0.53	0/6149	0.70	0/8343
2	B	0.58	0/1015	0.74	1/1356 (0.1%)
All	All	0.54	0/7164	0.71	1/9699 (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})
2	B	25	PHE	N-CA-C	5.10	124.76	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	5997	0	5978	358	1
2	B	998	0	970	64	0
3	A	24	0	19	3	0
3	B	18	0	13	3	0
4	A	208	0	0	50	1
4	B	47	0	0	4	0
All	All	7292	0	6980	418	2

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 30.

All (418) 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)
3:B:1561:GOL:O1	3:B:1561:GOL:C1	1.63	1.44
3:A:1556:GOL:C1	3:A:1556:GOL:O1	1.63	1.42
1:A:187:LYS:HE3	1:A:188:LYS:N	1.45	1.31
1:A:187:LYS:CE	1:A:188:LYS:H	1.53	1.22
1:A:513:THR:HG21	4:A:1743:HOH:O	1.37	1.20
2:B:32:GLN:HG3	2:B:33:GLU:N	1.58	1.08
2:B:17:LEU:HD22	2:B:37:LYS:HG3	1.36	1.07
1:A:187:LYS:HE3	1:A:188:LYS:H	0.91	1.06
1:A:428:TRP:HA	4:A:1701:HOH:O	1.54	1.06
2:B:32:GLN:HG3	2:B:33:GLU:H	0.89	1.05
1:A:129:ARG:HD3	1:A:179:TRP:CZ3	1.94	1.02
1:A:269:PRO:HB2	4:A:1620:HOH:O	1.59	0.98
1:A:572:VAL:O	1:A:575:THR:HG22	1.63	0.98
1:A:252:PRO:HA	4:A:1688:HOH:O	1.62	0.97
2:B:32:GLN:CG	2:B:33:GLU:H	1.82	0.92
2:B:17:LEU:HD21	2:B:36:LEU:HB3	1.52	0.92
1:A:771:THR:H	1:A:774:LEU:HD13	1.33	0.91
1:A:88:THR:HG1	1:A:253:TYR:HD2	1.17	0.88
1:A:187:LYS:CD	1:A:188:LYS:H	1.89	0.86
1:A:368:ILE:HG12	1:A:370:VAL:HG12	1.57	0.86
1:A:150:GLU:HB3	4:A:1722:HOH:O	1.75	0.86
1:A:175:SER:O	1:A:178:PRO:HD2	1.76	0.85
1:A:187:LYS:HE3	1:A:188:LYS:CA	2.07	0.85
1:A:601:ILE:O	1:A:605:VAL:HG23	1.75	0.84
1:A:417:PHE:HB3	4:A:1695:HOH:O	1.77	0.84
1:A:148:MET:HG3	1:A:271:PHE:HB3	1.60	0.83
1:A:27:THR:OG1	4:A:1627:HOH:O	1.93	0.83
1:A:179:TRP:CD1	1:A:249:ILE:HG21	2.14	0.82
1:A:187:LYS:HG3	1:A:188:LYS:N	1.94	0.82
1:A:71:LEU:HG	4:A:1757:HOH:O	1.80	0.80
1:A:619:VAL:O	1:A:623:ILE:HG12	1.81	0.79
1:A:231:CYS:SG	4:A:1622:HOH:O	2.41	0.79
1:A:634:ARG:HG3	4:A:1732:HOH:O	1.82	0.78
1:A:187:LYS:HG3	1:A:188:LYS:HG2	1.65	0.77
1:A:184:LEU:HD11	4:A:1685:HOH:O	1.83	0.77
1:A:187:LYS:CG	1:A:188:LYS:N	2.47	0.77
2:B:31:GLU:OE2	4:B:1578:HOH:O	2.01	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:ARG:NH2	1:A:274:PRO:O	2.18	0.76
1:A:261:CYS:HB2	4:A:1760:HOH:O	1.88	0.74
1:A:608:MET:HB3	1:A:614:VAL:HG22	1.70	0.74
1:A:142:ALA:HB3	1:A:143:PRO:HD3	1.69	0.74
1:A:374:THR:HG21	2:B:100:TYR:O	1.88	0.73
1:A:399:TYR:O	1:A:402:LEU:HB2	1.89	0.73
1:A:518:PHE:HE1	1:A:575:THR:HG21	1.53	0.73
1:A:709:LEU:O	1:A:713:ILE:HG13	1.90	0.72
1:A:247:ARG:HE	1:A:343:ASN:ND2	1.86	0.72
1:A:61:LEU:HD22	1:A:65:LYS:HG3	1.70	0.72
1:A:187:LYS:CG	1:A:188:LYS:H	2.03	0.72
1:A:251:ARG:NH2	4:A:1747:HOH:O	2.16	0.71
1:A:689:GLU:C	1:A:691:GLN:H	1.91	0.71
1:A:112:LEU:HD13	1:A:127:LEU:HD12	1.71	0.70
1:A:116:LEU:HB2	4:A:1610:HOH:O	1.90	0.70
1:A:213:MET:CG	1:A:752:LEU:HD21	2.21	0.70
1:A:641:LEU:O	1:A:645:ILE:HG13	1.92	0.69
1:A:185:TYR:OH	1:A:193:ASP:OD2	2.11	0.69
1:A:27:THR:HG21	4:A:1736:HOH:O	1.93	0.69
1:A:135:VAL:HA	4:A:1696:HOH:O	1.92	0.68
1:A:363:PRO:HG2	1:A:364:ALA:H	1.58	0.68
2:B:30:GLU:HA	2:B:33:GLU:HB3	1.76	0.68
1:A:413:PHE:O	4:A:1695:HOH:O	2.11	0.68
1:A:598:PRO:HA	1:A:601:ILE:HD12	1.75	0.68
1:A:580:ASP:OD2	4:A:1645:HOH:O	2.12	0.67
1:A:227:GLU:HB3	1:A:230:ASP:HB2	1.76	0.67
1:A:745:GLU:O	1:A:748:GLN:HB3	1.95	0.67
1:A:558:SER:HB3	4:A:1691:HOH:O	1.95	0.67
1:A:406:ASN:HD21	1:A:748:GLN:HE22	1.43	0.66
1:A:173:PHE:CE2	1:A:177:LEU:HD11	2.31	0.66
2:B:6:LEU:O	2:B:6:LEU:HD23	1.95	0.66
1:A:277:THR:C	1:A:279:ASP:H	1.99	0.66
1:A:325:HIS:O	1:A:332:CYS:HB2	1.96	0.66
1:A:166:ARG:HB2	1:A:202:TYR:OH	1.96	0.66
1:A:572:VAL:O	1:A:575:THR:CG2	2.40	0.65
1:A:299:GLU:HB3	4:A:1690:HOH:O	1.96	0.65
1:A:146:VAL:HG23	4:A:1685:HOH:O	1.95	0.65
1:A:86:TYR:O	1:A:90:VAL:HG23	1.97	0.65
1:A:339:TYR:CD1	1:A:340:PRO:HD2	2.32	0.65
2:B:32:GLN:O	2:B:34:LYS:N	2.30	0.64
1:A:182:LYS:NZ	1:A:245:GLN:HG2	2.13	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:ILE:O	1:A:38:VAL:HG22	1.97	0.64
1:A:74:THR:HG22	1:A:78:LEU:HD12	1.79	0.64
1:A:406:ASN:ND2	1:A:748:GLN:HE22	1.96	0.63
1:A:153:VAL:HG21	1:A:195:ILE:CG2	2.28	0.63
1:A:168:TRP:O	1:A:171:TYR:N	2.31	0.63
1:A:173:PHE:CE1	1:A:177:LEU:HD21	2.34	0.63
1:A:292:PHE:HB2	1:A:353:GLU:OE2	1.99	0.63
1:A:191:GLU:HG3	1:A:194:ARG:HE	1.64	0.62
2:B:32:GLN:CG	2:B:33:GLU:N	2.44	0.62
2:B:74:ASP:O	2:B:78:LYS:HD3	1.97	0.62
1:A:58:GLU:OE2	1:A:96:ARG:HD3	1.99	0.62
1:A:319:HIS:CE1	1:A:354:VAL:HG13	2.33	0.62
1:A:85:ILE:HA	1:A:252:PRO:HG2	1.80	0.62
1:A:771:THR:N	1:A:774:LEU:HD13	2.11	0.62
1:A:146:VAL:O	1:A:150:GLU:HG3	1.99	0.61
1:A:213:MET:SD	1:A:752:LEU:HD21	2.40	0.61
1:A:518:PHE:CE1	1:A:575:THR:HG21	2.35	0.61
1:A:117:LYS:HE3	4:A:1625:HOH:O	1.99	0.61
1:A:125:VAL:CG1	1:A:129:ARG:HH21	2.14	0.61
1:A:187:LYS:CE	1:A:188:LYS:N	2.29	0.61
1:A:510:SER:O	1:A:511:LYS:HB2	2.01	0.60
1:A:572:VAL:C	1:A:575:THR:HG22	2.21	0.60
1:A:689:GLU:C	1:A:691:GLN:N	2.54	0.60
1:A:223:HIS:HE1	1:A:293:ASP:HB3	1.64	0.60
1:A:93:LEU:HD23	1:A:100:PHE:CE2	2.36	0.60
1:A:597:HIS:O	1:A:601:ILE:HG13	2.02	0.59
1:A:572:VAL:HG12	1:A:576:LEU:HD12	1.85	0.59
2:B:30:GLU:HG2	2:B:33:GLU:HG2	1.84	0.59
1:A:399:TYR:HA	1:A:402:LEU:HD22	1.84	0.59
1:A:145:MET:HB3	4:A:1685:HOH:O	2.01	0.59
1:A:188:LYS:C	1:A:190:ALA:N	2.55	0.59
1:A:165:ARG:NH1	1:A:276:HIS:HA	2.18	0.59
1:A:635:LEU:N	4:A:1603:HOH:O	2.35	0.59
1:A:90:VAL:HG11	1:A:104:PHE:CE2	2.37	0.59
1:A:191:GLU:O	1:A:195:ILE:HG12	2.02	0.59
1:A:173:PHE:O	1:A:175:SER:N	2.35	0.59
1:A:75:VAL:HG11	1:A:86:TYR:CE1	2.39	0.58
3:A:1556:GOL:HO1	3:A:1556:GOL:C1	2.07	0.58
2:B:17:LEU:HD21	2:B:36:LEU:CB	2.31	0.58
1:A:450:ARG:HD3	1:A:476:LEU:HD22	1.84	0.58
2:B:114:ASP:HB2	4:B:1594:HOH:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:VAL:O	1:A:156:THR:HG23	2.03	0.58
1:A:77:ARG:HG3	1:A:78:LEU:HG	1.86	0.58
2:B:83:PHE:O	2:B:84:CYS:HB3	2.03	0.58
1:A:179:TRP:NE1	1:A:249:ILE:HG21	2.18	0.58
1:A:292:PHE:HD2	1:A:353:GLU:HB2	1.67	0.58
1:A:173:PHE:CZ	1:A:177:LEU:HD11	2.39	0.58
1:A:188:LYS:C	1:A:190:ALA:H	2.04	0.58
1:A:206:ARG:HB2	4:A:1632:HOH:O	2.04	0.58
2:B:88:TYR:OH	2:B:97:ALA:HB2	2.03	0.58
1:A:71:LEU:O	1:A:75:VAL:HG23	2.04	0.57
1:A:165:ARG:NH1	1:A:276:HIS:CA	2.67	0.57
1:A:256:PHE:O	1:A:260:LEU:HB2	2.03	0.57
1:A:211:VAL:O	1:A:215:GLN:HG3	2.04	0.57
1:A:495:LEU:O	1:A:498:HIS:HB2	2.03	0.57
1:A:292:PHE:CD2	1:A:353:GLU:HB2	2.39	0.57
1:A:213:MET:HG2	1:A:752:LEU:HD21	1.87	0.57
1:A:398:LEU:O	1:A:402:LEU:HD13	2.04	0.57
1:A:415:ASN:HD21	1:A:455:LYS:NZ	2.03	0.57
1:A:572:VAL:HG12	1:A:576:LEU:CD1	2.34	0.57
1:A:643:SER:OG	1:A:647:LYS:NZ	2.38	0.57
1:A:96:ARG:NE	4:A:1683:HOH:O	2.33	0.56
3:B:1561:GOL:HO1	3:B:1561:GOL:C1	2.07	0.56
1:A:660:GLU:O	1:A:664:GLU:HG2	2.05	0.56
1:A:588:ARG:O	1:A:592:GLU:HG2	2.05	0.56
1:A:242:ASP:O	1:A:245:GLN:NE2	2.39	0.56
2:B:67:LYS:HD3	2:B:87:GLU:OE1	2.05	0.56
1:A:609:ILE:HG12	1:A:614:VAL:O	2.06	0.56
1:A:169:TYR:CZ	1:A:273:PRO:HB3	2.41	0.56
1:A:61:LEU:HB2	1:A:62:PRO:HD3	1.88	0.56
1:A:566:LEU:HD23	1:A:573:PHE:CE1	2.41	0.56
1:A:95:ALA:HB2	1:A:263:ALA:HB2	1.89	0.55
1:A:290:ARG:HH11	1:A:311:ARG:NH2	2.04	0.55
1:A:426:PHE:CE1	1:A:456:CYS:HB3	2.41	0.55
1:A:406:ASN:HD21	1:A:748:GLN:NE2	2.04	0.55
1:A:174:LEU:O	1:A:236:ILE:HD11	2.05	0.55
1:A:319:HIS:ND1	1:A:354:VAL:HG13	2.21	0.55
1:A:180:VAL:O	1:A:184:LEU:HB2	2.06	0.55
1:A:235:GLN:O	1:A:309:VAL:HG13	2.06	0.55
1:A:696:GLN:O	1:A:700:GLU:HG2	2.07	0.55
1:A:132:SER:HB3	1:A:180:VAL:HB	1.89	0.55
1:A:329:ARG:HH21	2:B:100:TYR:HA	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:557:LYS:HB3	1:A:561:HIS:HD2	1.72	0.55
1:A:129:ARG:HD3	1:A:179:TRP:HZ3	1.68	0.54
1:A:38:VAL:HG23	1:A:39:GLY:N	2.22	0.54
1:A:88:THR:OG1	1:A:253:TYR:HD2	1.83	0.54
2:B:57:TYR:CD2	2:B:69:ILE:HD12	2.43	0.54
1:A:425:GLN:O	1:A:427:ARG:HG2	2.07	0.54
1:A:709:LEU:CD1	1:A:713:ILE:HD11	2.37	0.54
1:A:179:TRP:HA	1:A:251:ARG:HH22	1.72	0.54
1:A:236:ILE:O	1:A:239:LEU:HB3	2.08	0.54
1:A:87:THR:HG21	1:A:133:ASP:HB3	1.90	0.54
1:A:453:LEU:HB2	4:A:1735:HOH:O	2.08	0.53
1:A:623:ILE:HA	1:A:628:LEU:HD12	1.90	0.53
1:A:709:LEU:HD11	1:A:713:ILE:HD11	1.91	0.53
2:B:72:GLY:HA3	2:B:83:PHE:CE1	2.43	0.53
1:A:186:GLU:HB3	4:A:1729:HOH:O	2.09	0.53
1:A:407:THR:OG1	1:A:745:GLU:OE1	2.27	0.53
1:A:131:LEU:O	1:A:134:LEU:HB2	2.08	0.53
1:A:188:LYS:O	1:A:192:MET:N	2.31	0.53
1:A:179:TRP:CD1	1:A:249:ILE:HD13	2.44	0.53
1:A:79:LEU:N	1:A:80:PRO:HD3	2.24	0.53
1:A:181:GLY:HA2	1:A:184:LEU:HB3	1.90	0.53
1:A:213:MET:HB2	1:A:784:GLN:OE1	2.09	0.53
1:A:655:ILE:HG22	1:A:699:VAL:HG22	1.91	0.53
1:A:513:THR:CG2	4:A:1743:HOH:O	2.18	0.52
1:A:271:PHE:HE1	1:A:273:PRO:HG3	1.73	0.52
2:B:83:PHE:HD1	2:B:84:CYS:N	2.07	0.52
2:B:42:LEU:HD22	2:B:98:MET:SD	2.49	0.52
1:A:646:ARG:HG3	1:A:646:ARG:HH11	1.75	0.52
1:A:698:LYS:HE2	4:A:1767:HOH:O	2.09	0.52
1:A:88:THR:OG1	1:A:252:PRO:HB2	2.10	0.52
2:B:32:GLN:O	2:B:33:GLU:C	2.48	0.52
1:A:188:LYS:O	1:A:191:GLU:N	2.41	0.52
1:A:608:MET:HB3	1:A:614:VAL:CG2	2.38	0.51
1:A:182:LYS:HZ2	1:A:245:GLN:HG2	1.73	0.51
1:A:319:HIS:CD2	4:A:1699:HOH:O	2.63	0.51
2:B:17:LEU:HD12	2:B:115:TRP:CD1	2.46	0.51
1:A:66:SER:HB3	1:A:70:ARG:HH11	1.74	0.51
1:A:241:LYS:O	1:A:241:LYS:HG2	2.11	0.50
1:A:231:CYS:O	1:A:235:GLN:HG3	2.12	0.50
1:A:277:THR:C	1:A:279:ASP:N	2.64	0.50
1:A:90:VAL:HG11	1:A:104:PHE:CD2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:VAL:HB	1:A:212:PRO:HD3	1.94	0.50
2:B:41:THR:O	2:B:41:THR:HG23	2.10	0.50
1:A:63:ASN:ND2	4:A:1637:HOH:O	2.45	0.50
1:A:460:SER:HA	2:B:55:GLN:NE2	2.26	0.50
1:A:764:THR:HG23	1:A:768:LEU:HD12	1.93	0.50
1:A:575:THR:HG23	1:A:576:LEU:N	2.26	0.50
1:A:417:PHE:CB	4:A:1695:HOH:O	2.47	0.50
1:A:622:TRP:NE1	1:A:628:LEU:HD21	2.27	0.50
1:A:52:GLY:O	1:A:56:VAL:HG23	2.12	0.50
1:A:164:VAL:HG13	1:A:790:ALA:O	2.11	0.49
2:B:46:ASN:ND2	2:B:109:ARG:HH12	2.10	0.49
2:B:46:ASN:ND2	2:B:109:ARG:NH1	2.59	0.49
1:A:445:LYS:O	1:A:448:PHE:HB3	2.12	0.49
1:A:75:VAL:HG11	1:A:86:TYR:CD1	2.47	0.49
1:A:689:GLU:O	1:A:691:GLN:N	2.46	0.49
2:B:111:ILE:O	2:B:111:ILE:HG13	2.12	0.49
1:A:179:TRP:HE1	1:A:249:ILE:CG2	2.25	0.49
1:A:269:PRO:CG	4:A:1686:HOH:O	2.59	0.49
1:A:631:ASP:HA	1:A:634:ARG:HD3	1.94	0.49
1:A:425:GLN:NE2	1:A:425:GLN:N	2.60	0.49
1:A:486:LYS:HB2	1:A:549:GLN:NE2	2.27	0.49
1:A:688:LEU:HD12	1:A:688:LEU:C	2.31	0.49
1:A:415:ASN:HD21	1:A:455:LYS:HZ3	1.61	0.49
1:A:609:ILE:HD11	1:A:619:VAL:HG21	1.93	0.49
1:A:486:LYS:NZ	4:A:1644:HOH:O	2.44	0.49
2:B:48:SER:HB3	2:B:51:THR:OG1	2.12	0.49
1:A:125:VAL:CG2	1:A:168:TRP:HE1	2.25	0.49
1:A:53:LEU:O	1:A:57:LEU:HG	2.13	0.49
1:A:384:PRO:HD2	4:A:1606:HOH:O	2.12	0.49
1:A:123:GLU:HA	1:A:126:TYR:CD2	2.47	0.49
1:A:213:MET:HE1	1:A:785:PHE:N	2.26	0.49
1:A:740:TYR:O	1:A:744:ILE:HG22	2.13	0.49
2:B:97:ALA:CB	2:B:101:ILE:HD12	2.42	0.48
1:A:585:HIS:O	1:A:588:ARG:HB3	2.13	0.48
2:B:102:ASN:HB2	2:B:113:THR:OG1	2.12	0.48
1:A:202:TYR:CE2	1:A:206:ARG:HD2	2.49	0.48
1:A:269:PRO:HG3	4:A:1686:HOH:O	2.13	0.48
1:A:61:LEU:CD2	1:A:65:LYS:HG3	2.42	0.48
1:A:460:SER:HA	2:B:55:GLN:HE21	1.79	0.48
1:A:179:TRP:NE1	1:A:249:ILE:CG2	2.76	0.48
1:A:598:PRO:O	1:A:601:ILE:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:GLN:HA	1:A:307:HIS:O	2.12	0.48
1:A:210:HIS:HB2	1:A:214:LEU:CD1	2.43	0.48
1:A:426:PHE:HE1	1:A:456:CYS:HB3	1.78	0.48
1:A:727:ARG:NH1	4:A:1631:HOH:O	2.45	0.48
1:A:175:SER:O	1:A:178:PRO:CD	2.57	0.48
1:A:290:ARG:NH1	1:A:311:ARG:NH2	2.62	0.48
1:A:213:MET:HG2	1:A:213:MET:O	2.13	0.48
1:A:394:ALA:O	1:A:398:LEU:HG	2.14	0.47
1:A:688:LEU:O	1:A:688:LEU:HD12	2.13	0.47
2:B:64:GLY:HA3	2:B:93:ASP:HB3	1.96	0.47
1:A:744:ILE:HG23	1:A:745:GLU:N	2.29	0.47
2:B:17:LEU:O	2:B:17:LEU:HD23	2.14	0.47
2:B:59:LEU:HD22	2:B:106:LEU:HD13	1.96	0.47
1:A:129:ARG:HH12	1:A:316:GLU:HG2	1.78	0.47
1:A:399:TYR:CG	1:A:433:TRP:NE1	2.83	0.47
1:A:163:GLN:HB3	1:A:790:ALA:OXT	2.15	0.47
1:A:321:ILE:CG2	1:A:336:LEU:HD13	2.44	0.47
1:A:499:SER:HA	1:A:502:LEU:HD12	1.97	0.47
1:A:518:PHE:O	1:A:522:LYS:HG3	2.14	0.47
1:A:417:PHE:CE2	1:A:421:LEU:HD11	2.49	0.47
1:A:714:PHE:O	1:A:717:PHE:N	2.47	0.47
1:A:210:HIS:HB2	1:A:214:LEU:HD12	1.96	0.47
1:A:38:VAL:HG11	1:A:53:LEU:HD22	1.97	0.47
3:A:1556:GOL:O1	2:B:68:LYS:HD2	2.14	0.47
1:A:189:ASP:O	1:A:193:ASP:OD1	2.32	0.47
1:A:148:MET:HG3	1:A:271:PHE:CB	2.39	0.47
1:A:691:GLN:HE22	1:A:694:ARG:NH1	2.11	0.47
1:A:51:GLU:O	1:A:54:ALA:HB3	2.15	0.47
1:A:260:LEU:O	1:A:263:ALA:HB3	2.15	0.47
1:A:329:ARG:NH2	2:B:100:TYR:HA	2.29	0.47
1:A:643:SER:N	4:A:1684:HOH:O	2.47	0.47
1:A:425:GLN:CD	1:A:425:GLN:N	2.68	0.47
1:A:419:HIS:O	1:A:422:SER:OG	2.31	0.46
1:A:182:LYS:HA	1:A:244:TRP:CB	2.45	0.46
1:A:502:LEU:O	1:A:506:VAL:HG23	2.15	0.46
1:A:321:ILE:HG21	1:A:336:LEU:HD13	1.98	0.46
1:A:146:VAL:CG2	4:A:1685:HOH:O	2.60	0.46
1:A:789:GLN:HA	1:A:789:GLN:OE1	2.15	0.46
2:B:12:ASP:HB3	2:B:15:VAL:HG12	1.97	0.46
1:A:696:GLN:OE1	1:A:700:GLU:OE1	2.34	0.46
1:A:125:VAL:HG23	1:A:168:TRP:HE1	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:ASP:OD1	1:A:206:ARG:NE	2.49	0.46
2:B:83:PHE:C	2:B:83:PHE:CD1	2.89	0.46
1:A:179:TRP:HA	1:A:251:ARG:NH2	2.31	0.46
2:B:15:VAL:HG13	2:B:15:VAL:O	2.15	0.46
2:B:7:LYS:HE2	2:B:7:LYS:HB3	1.65	0.46
1:A:220:ASP:O	1:A:224:PRO:HG3	2.16	0.46
1:A:585:HIS:O	1:A:586:VAL:C	2.53	0.46
1:A:559:PHE:HB2	2:B:53:GLU:OE1	2.15	0.46
1:A:248:HIS:HA	1:A:342:LYS:HB3	1.99	0.45
1:A:518:PHE:HB3	1:A:522:LYS:NZ	2.31	0.45
1:A:290:ARG:HA	4:A:1614:HOH:O	2.16	0.45
1:A:437:LEU:HD13	1:A:472:THR:HB	1.98	0.45
1:A:179:TRP:HE1	1:A:249:ILE:HG23	1.82	0.45
1:A:165:ARG:NH1	1:A:276:HIS:N	2.64	0.45
2:B:63:SER:OG	2:B:97:ALA:HB2	2.16	0.45
1:A:239:LEU:HG	1:A:244:TRP:HA	1.97	0.45
1:A:521:LEU:HB3	1:A:543:LYS:HE3	1.97	0.45
1:A:46:LEU:HD21	1:A:85:ILE:HG12	1.99	0.45
1:A:271:PHE:CE1	1:A:273:PRO:HG3	2.51	0.45
1:A:185:TYR:HB3	4:A:1730:HOH:O	2.16	0.45
1:A:742:ASN:O	1:A:746:ARG:HG2	2.16	0.45
1:A:459:LEU:CD2	2:B:58:GLU:HG2	2.47	0.45
2:B:75:LYS:HB3	4:B:1593:HOH:O	2.15	0.45
1:A:317:ASN:O	1:A:320:CYS:HB2	2.17	0.45
1:A:318:LEU:HD22	1:A:336:LEU:HD12	1.99	0.45
1:A:738:PRO:O	1:A:742:ASN:ND2	2.50	0.45
2:B:32:GLN:O	2:B:35:LEU:N	2.41	0.44
1:A:304:PRO:HB3	1:A:310:GLU:HB2	1.99	0.44
1:A:248:HIS:CE1	1:A:345:ILE:HD13	2.51	0.44
1:A:640:ILE:O	1:A:641:LEU:C	2.54	0.44
1:A:72:LEU:HD21	1:A:89:LEU:HD23	1.98	0.44
1:A:148:MET:O	1:A:151:ASN:N	2.51	0.44
1:A:60:ASP:O	1:A:63:ASN:O	2.34	0.44
1:A:589:VAL:O	1:A:593:VAL:HG23	2.17	0.44
1:A:298:PRO:HG2	1:A:299:GLU:H	1.82	0.44
1:A:201:SER:O	1:A:205:ARG:HD3	2.17	0.44
1:A:185:TYR:HE1	1:A:192:MET:CB	2.31	0.44
1:A:387:LEU:O	1:A:388:PRO:C	2.55	0.44
1:A:780:ALA:O	1:A:784:GLN:HG3	2.16	0.44
1:A:459:LEU:HD23	2:B:58:GLU:HG2	2.00	0.44
1:A:653:LEU:HD23	1:A:656:GLN:OE1	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:755:HIS:ND1	1:A:756:GLN:N	2.66	0.44
1:A:777:HIS:CE1	4:A:1734:HOH:O	2.71	0.44
1:A:309:VAL:HG23	1:A:310:GLU:OE2	2.17	0.44
2:B:88:TYR:OH	2:B:97:ALA:CB	2.65	0.44
1:A:131:LEU:HA	1:A:134:LEU:HD12	1.98	0.44
1:A:521:LEU:HD22	1:A:543:LYS:HG2	1.99	0.44
1:A:475:ALA:HB1	4:A:1656:HOH:O	2.17	0.43
1:A:758:ILE:C	1:A:760:GLN:N	2.71	0.43
1:A:277:THR:O	1:A:279:ASP:N	2.51	0.43
2:B:97:ALA:HA	2:B:101:ILE:HG13	1.99	0.43
1:A:778:ILE:O	1:A:779:LEU:C	2.56	0.43
1:A:703:GLN:O	1:A:706:GLN:N	2.51	0.43
1:A:410:VAL:HG12	1:A:414:ILE:HD11	2.00	0.43
1:A:609:ILE:HA	1:A:614:VAL:O	2.18	0.43
1:A:310:GLU:CD	1:A:310:GLU:H	2.21	0.43
2:B:64:GLY:HA3	2:B:93:ASP:OD2	2.19	0.43
1:A:136:ASN:N	1:A:136:ASN:ND2	2.66	0.43
1:A:347:LEU:HG	1:A:351:ILE:HD11	1.99	0.43
1:A:97:ASN:HD22	1:A:100:PHE:H	1.65	0.43
1:A:559:PHE:CZ	1:A:599:GLN:HG2	2.54	0.43
1:A:484:ILE:HD11	1:A:596:ASN:ND2	2.33	0.43
2:B:73:LEU:HA	2:B:79:THR:O	2.18	0.43
1:A:695:LEU:O	1:A:699:VAL:HG23	2.19	0.43
2:B:58:GLU:OE1	3:B:1555:GOL:O2	2.36	0.43
2:B:83:PHE:CD1	2:B:84:CYS:N	2.86	0.42
1:A:568:LYS:HD3	1:A:569:PHE:CE1	2.54	0.42
1:A:738:PRO:CD	4:A:1707:HOH:O	2.68	0.42
2:B:72:GLY:CA	2:B:83:PHE:CE1	3.02	0.42
1:A:322:ILE:O	1:A:326:TRP:HB3	2.20	0.42
1:A:770:PHE:HA	1:A:774:LEU:HD22	2.01	0.42
1:A:127:LEU:O	1:A:130:PHE:N	2.52	0.42
1:A:313:VAL:HG12	1:A:314:ILE:N	2.35	0.42
2:B:30:GLU:O	2:B:34:LYS:HB3	2.19	0.42
1:A:598:PRO:HA	1:A:601:ILE:CD1	2.47	0.42
2:B:50:TYR:HB2	4:B:1596:HOH:O	2.19	0.42
1:A:707:LYS:HG3	1:A:761:TYR:CD2	2.55	0.42
1:A:245:GLN:NE2	4:A:1611:HOH:O	2.52	0.42
2:B:112:ARG:O	2:B:112:ARG:HG3	2.20	0.42
1:A:173:PHE:O	1:A:174:LEU:C	2.57	0.42
1:A:173:PHE:CD2	1:A:174:LEU:N	2.88	0.42
1:A:260:LEU:HD23	4:A:1655:HOH:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:585:HIS:O	1:A:588:ARG:N	2.52	0.42
2:B:15:VAL:HG21	2:B:95:GLU:HB3	2.02	0.42
1:A:719:MET:O	1:A:723:GLU:HB2	2.19	0.42
1:A:153:VAL:HG21	1:A:195:ILE:HG22	2.01	0.42
1:A:185:TYR:CE1	1:A:192:MET:HB2	2.54	0.42
2:B:101:ILE:O	2:B:104:THR:HG23	2.19	0.42
1:A:559:PHE:HZ	1:A:599:GLN:HG2	1.85	0.42
1:A:465:ILE:HA	1:A:468:ILE:HG12	2.00	0.42
1:A:758:ILE:HG23	1:A:765:LEU:HD11	2.02	0.42
1:A:209:THR:O	1:A:212:PRO:HD2	2.20	0.42
1:A:92:LEU:HD22	1:A:92:LEU:N	2.35	0.42
1:A:714:PHE:O	1:A:715:GLN:C	2.59	0.41
2:B:88:TYR:CD2	2:B:94:ALA:HA	2.55	0.41
1:A:464:ARG:O	1:A:468:ILE:HG23	2.19	0.41
1:A:500:VAL:HG21	1:A:524:VAL:HG22	2.02	0.41
1:A:318:LEU:HD22	1:A:336:LEU:CD1	2.51	0.41
1:A:228:TYR:HA	1:A:288:ILE:HD11	2.02	0.41
1:A:155:VAL:HG13	4:A:1759:HOH:O	2.19	0.41
1:A:293:ASP:OD1	1:A:293:ASP:C	2.55	0.41
1:A:410:VAL:O	1:A:413:PHE:HB3	2.21	0.41
1:A:635:LEU:O	1:A:636:PHE:C	2.58	0.41
2:B:19:GLN:NE2	2:B:114:ASP:OD1	2.53	0.41
1:A:28:GLU:HB3	1:A:67:LYS:HE2	2.03	0.41
1:A:138:HIS:HE1	4:A:1754:HOH:O	2.03	0.41
1:A:617:ALA:O	1:A:620:ALA:HB3	2.21	0.41
1:A:182:LYS:HA	1:A:244:TRP:HB2	2.01	0.41
1:A:619:VAL:O	1:A:619:VAL:HG12	2.20	0.41
1:A:410:VAL:O	1:A:411:ASP:C	2.58	0.41
1:A:545:GLU:O	1:A:549:GLN:HB2	2.21	0.41
1:A:187:LYS:HE3	1:A:188:LYS:HA	1.98	0.41
1:A:73:CYS:HG	1:A:104:PHE:HE1	1.67	0.41
1:A:713:ILE:O	1:A:717:PHE:HB2	2.20	0.41
1:A:247:ARG:HH21	1:A:343:ASN:ND2	2.18	0.41
1:A:83:LEU:HD12	1:A:130:PHE:HD2	1.85	0.41
1:A:646:ARG:HG3	1:A:646:ARG:NH1	2.36	0.41
1:A:486:LYS:O	1:A:490:GLU:OE1	2.39	0.41
1:A:139:VAL:O	1:A:266:HIS:N	2.54	0.41
1:A:610:ARG:HD3	4:A:1616:HOH:O	2.20	0.41
1:A:173:PHE:CG	1:A:174:LEU:N	2.88	0.41
1:A:309:VAL:O	1:A:310:GLU:C	2.60	0.41
2:B:25:PHE:N	2:B:25:PHE:CD2	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:GLU:CD	1:A:161:VAL:HG11	2.41	0.41
1:A:145:MET:SD	1:A:268:LEU:HD11	2.61	0.40
1:A:80:PRO:HD2	1:A:81:GLU:OE1	2.21	0.40
1:A:599:GLN:O	1:A:603:VAL:HG13	2.21	0.40
1:A:751:PHE:CD2	1:A:781:VAL:HG12	2.56	0.40
1:A:663:LYS:C	1:A:665:LYS:H	2.24	0.40
1:A:185:TYR:HE1	1:A:192:MET:HB2	1.85	0.40
1:A:108:MET:O	1:A:111:GLN:HB3	2.21	0.40
1:A:191:GLU:C	1:A:193:ASP:H	2.24	0.40
1:A:349:TYR:O	1:A:353:GLU:HB2	2.22	0.40
1:A:321:ILE:HD12	1:A:336:LEU:HD12	2.02	0.40
1:A:161:VAL:HA	1:A:162:PRO:HD3	1.96	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:LYS:CD	1:A:187:LYS:CD[5_675]	1.70	0.50
4:A:1599:HOH:O	4:A:1599:HOH:O[6_555]	1.77	0.43

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	727/790 (92%)	622 (86%)	87 (12%)	18 (2%)	7	17
2	B	119/156 (76%)	98 (82%)	17 (14%)	4 (3%)	5	10
All	All	846/946 (89%)	720 (85%)	104 (12%)	22 (3%)	7	15

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	66	SER
1	A	83	LEU
1	A	174	LEU
1	A	341	GLY
1	A	363	PRO
2	B	20	TYR
2	B	33	GLU
1	A	64	TYR
1	A	173	PHE
1	A	278	GLU
1	A	632	PHE
2	B	24	HIS
1	A	664	GLU
1	A	298	PRO
1	A	426	PHE
1	A	460	SER
1	A	511	LYS
2	B	27	GLY
1	A	265	GLN
1	A	388	PRO
1	A	690	GLU
1	A	211	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	672/724 (93%)	638 (95%)	34 (5%)	29	57
2	B	106/130 (82%)	92 (87%)	14 (13%)	5	11
All	All	778/854 (91%)	730 (94%)	48 (6%)	23	48

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	82	LYS
1	A	97	ASN

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Mol	Chain	Res	Type
1	A	136	ASN
1	A	154	SER
1	A	187	LYS
1	A	189	ASP
1	A	191	GLU
1	A	194	ARG
1	A	241	LYS
1	A	246	GLU
1	A	254	LEU
1	A	272	THR
1	A	282	TYR
1	A	283	PRO
1	A	340	PRO
1	A	387	LEU
1	A	402	LEU
1	A	407	THR
1	A	413	PHE
1	A	422	SER
1	A	449	VAL
1	A	455	LYS
1	A	464	ARG
1	A	490	GLU
1	A	499	SER
1	A	503	CYS
1	A	562	SER
1	A	574	LYS
1	A	597	HIS
1	A	616	CYS
1	A	635	LEU
1	A	717	PHE
1	A	763	VAL
1	A	779	LEU
2	B	9	LEU
2	B	15	VAL
2	B	17	LEU
2	B	20	TYR
2	B	22	ASP
2	B	25	PHE
2	B	26	ARG
2	B	31	GLU
2	B	32	GLN
2	B	33	GLU

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Mol	Chain	Res	Type
2	B	46	ASN
2	B	84	CYS
2	B	107	ASP
2	B	124	GLN

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	63	ASN
1	A	97	ASN
1	A	120	ASN
1	A	223	HIS
1	A	245	GLN
1	A	343	ASN
1	A	415	ASN
1	A	420	HIS
1	A	425	GLN
1	A	439	GLN
1	A	463	GLN
1	A	493	ASN
1	A	561	HIS
1	A	596	ASN
1	A	612	GLN
1	A	642	HIS
1	A	649	ASN
1	A	691	GLN
1	A	696	GLN
1	A	703	GLN
1	A	742	ASN
1	A	748	GLN
1	A	759	GLN
2	B	46	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

7 ligands 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	$\#|Z| > 2$
3	GOL	A	1556	-	5,5,5	4.69	5 (100%)	5,5,5	5.40	3 (60%)
3	GOL	A	1557	-	5,5,5	4.75	5 (100%)	5,5,5	5.74	3 (60%)
3	GOL	A	1558	-	5,5,5	4.81	5 (100%)	5,5,5	6.02	3 (60%)
3	GOL	A	1560	-	5,5,5	4.78	5 (100%)	5,5,5	5.84	3 (60%)
3	GOL	B	1555	-	5,5,5	4.82	5 (100%)	5,5,5	5.78	3 (60%)
3	GOL	B	1559	-	5,5,5	4.71	4 (80%)	5,5,5	5.34	3 (60%)
3	GOL	B	1561	-	5,5,5	4.51	4 (80%)	5,5,5	5.78	3 (60%)

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	1556	-	-	0/4/4/4	0/0/0/0
3	GOL	A	1557	-	-	0/4/4/4	0/0/0/0
3	GOL	A	1558	-	-	0/4/4/4	0/0/0/0
3	GOL	A	1560	-	-	0/4/4/4	0/0/0/0
3	GOL	B	1555	-	-	0/4/4/4	0/0/0/0
3	GOL	B	1559	-	-	0/4/4/4	0/0/0/0
3	GOL	B	1561	-	-	0/4/4/4	0/0/0/0

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1560	GOL	C3-C2	-8.35	1.20	1.52
3	B	1555	GOL	C3-C2	-8.35	1.20	1.52
3	A	1557	GOL	C3-C2	-8.02	1.21	1.52
3	A	1558	GOL	C3-C2	-7.84	1.22	1.52
3	A	1556	GOL	C3-C2	-7.76	1.22	1.52
3	B	1559	GOL	C3-C2	-7.59	1.23	1.52
3	B	1561	GOL	C3-C2	-7.10	1.25	1.52
3	B	1559	GOL	C1-C2	-4.80	1.34	1.52
3	A	1558	GOL	C1-C2	-4.71	1.34	1.52
3	A	1557	GOL	C1-C2	-3.84	1.37	1.52
3	A	1560	GOL	C1-C2	-3.30	1.39	1.52
3	B	1555	GOL	O2-C2	-3.13	1.34	1.43
3	A	1556	GOL	C1-C2	-2.80	1.41	1.52
3	B	1561	GOL	O2-C2	-2.76	1.35	1.43
3	A	1556	GOL	O2-C2	-2.40	1.36	1.43
3	A	1557	GOL	O2-C2	-2.17	1.37	1.43
3	A	1560	GOL	O2-C2	-2.08	1.37	1.43
3	A	1558	GOL	O2-C2	-2.05	1.37	1.43
3	B	1555	GOL	C1-C2	-2.04	1.44	1.52
3	B	1555	GOL	O3-C3	3.15	1.55	1.42
3	A	1557	GOL	O3-C3	3.30	1.56	1.42
3	A	1560	GOL	O3-C3	3.31	1.56	1.42
3	B	1559	GOL	O3-C3	3.36	1.56	1.42
3	A	1556	GOL	O3-C3	3.48	1.57	1.42
3	A	1558	GOL	O1-C1	3.68	1.58	1.42
3	A	1558	GOL	O3-C3	3.79	1.58	1.42
3	B	1559	GOL	O1-C1	4.09	1.60	1.42
3	B	1561	GOL	O3-C3	4.11	1.60	1.42
3	A	1557	GOL	O1-C1	4.24	1.60	1.42
3	A	1560	GOL	O1-C1	4.28	1.60	1.42
3	B	1555	GOL	O1-C1	4.76	1.62	1.42
3	B	1561	GOL	O1-C1	4.90	1.63	1.42
3	A	1556	GOL	O1-C1	4.91	1.63	1.42

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1558	GOL	O1-C1-C2	3.15	125.47	110.18
3	B	1555	GOL	O1-C1-C2	3.37	126.53	110.18
3	A	1557	GOL	O1-C1-C2	3.51	127.20	110.18
3	A	1556	GOL	O1-C1-C2	3.54	127.37	110.18
3	A	1560	GOL	O1-C1-C2	3.57	127.48	110.18
3	B	1561	GOL	O1-C1-C2	3.73	128.30	110.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1559	GOL	O1-C1-C2	3.88	129.02	110.18
3	A	1556	GOL	O2-C2-C3	6.32	137.62	108.65
3	B	1559	GOL	O2-C2-C3	6.36	137.83	108.65
3	A	1557	GOL	O2-C2-C3	6.52	138.53	108.65
3	A	1558	GOL	O2-C2-C3	6.63	139.05	108.65
3	A	1560	GOL	O2-C2-C3	6.66	139.19	108.65
3	B	1561	GOL	O2-C2-C3	6.87	140.17	108.65
3	B	1555	GOL	O2-C2-C3	7.22	141.78	108.65
3	B	1559	GOL	O3-C3-C2	9.24	154.99	110.18
3	A	1556	GOL	O3-C3-C2	9.62	156.82	110.18
3	B	1555	GOL	O3-C3-C2	10.13	159.31	110.18
3	B	1561	GOL	O3-C3-C2	10.27	159.99	110.18
3	A	1557	GOL	O3-C3-C2	10.44	160.81	110.18
3	A	1560	GOL	O3-C3-C2	10.56	161.42	110.18
3	A	1558	GOL	O3-C3-C2	11.24	164.70	110.18

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1556	GOL	3	0
3	B	1555	GOL	1	0
3	B	1561	GOL	2	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	733/790 (92%)	0.39	42 (5%)	27	26	20, 73, 102, 129	0
2	B	121/156 (77%)	0.74	15 (12%)	5	4	31, 74, 101, 114	0
All	All	854/946 (90%)	0.44	57 (6%)	21	20	20, 73, 102, 129	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	25	PHE	7.0
2	B	22	ASP	6.4
2	B	17	LEU	6.3
2	B	23	GLN	5.7
2	B	24	HIS	5.3
2	B	20	TYR	4.9
1	A	790	ALA	4.4
1	A	473	PHE	4.4
1	A	89	LEU	4.4
1	A	487	TYR	4.1
1	A	275	PRO	4.1
1	A	662	ALA	3.9
1	A	256	PHE	3.8
1	A	540	ASN	3.8
1	A	691	GLN	3.8
1	A	520	ILE	3.7
1	A	663	LYS	3.7
1	A	543	LYS	3.6
2	B	26	ARG	3.4
1	A	524	VAL	3.4
1	A	688	LEU	3.4
1	A	495	LEU	3.3
1	A	243	ARG	3.2
1	A	753	GLN	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	521	LEU	3.1
1	A	692	ILE	3.1
2	B	27	GLY	2.8
1	A	525	PRO	2.7
2	B	19	GLN	2.7
1	A	180	VAL	2.7
2	B	18	SER	2.7
1	A	547	PHE	2.7
1	A	476	LEU	2.6
1	A	276	HIS	2.6
2	B	43	TYR	2.6
1	A	690	GLU	2.5
2	B	76	MET	2.5
1	A	365	PRO	2.4
1	A	548	VAL	2.4
1	A	546	VAL	2.4
1	A	523	ASP	2.4
1	A	494	SER	2.4
1	A	642	HIS	2.3
1	A	518	PHE	2.3
2	B	77	LYS	2.3
1	A	544	ILE	2.2
2	B	85	PHE	2.2
1	A	519	SER	2.2
1	A	689	GLU	2.2
1	A	643	SER	2.1
2	B	73	LEU	2.1
1	A	364	ALA	2.1
1	A	46	LEU	2.1
1	A	184	LEU	2.0
1	A	34	LEU	2.0
1	A	472	THR	2.0
1	A	496	PRO	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å²)	Q<0.9
3	GOL	A	1558	6/6	0.76	0.45	3.62	52,56,56,57	0
3	GOL	A	1560	6/6	0.95	0.24	2.21	66,68,70,72	0
3	GOL	B	1555	6/6	0.90	0.27	0.63	56,57,58,61	0
3	GOL	B	1559	6/6	0.85	0.22	-	74,76,76,77	0
3	GOL	A	1556	6/6	0.80	0.23	-	75,78,79,81	0
3	GOL	A	1557	6/6	0.71	0.24	-	78,80,81,83	0
3	GOL	B	1561	6/6	0.81	0.35	-	58,59,59,61	0

6.5 Other polymers (i)

There are no such residues in this entry.