



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 11:25 PM UTC

PDB ID : 6KXW / pdb_00006kxw
Title : Crystal structure of human aquaporin AQP7 in bound to glycerol
Authors : Zhang, L.; Yao, D.; Zhou, F.; Zhang, Q.; Zhou, L.; Cao, Y.
Deposited on : 2019-09-13
Resolution : 3.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

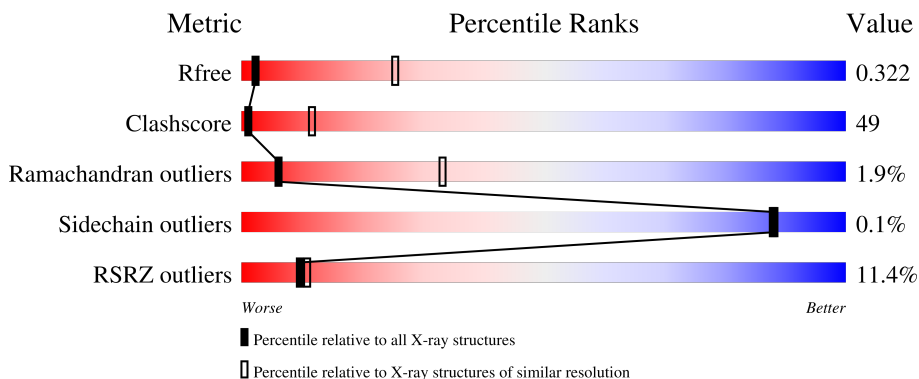
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1131 (3.80-3.60)
Clashscore	190562	1171 (3.80-3.60)
Ramachandran outliers	187476	1129 (3.80-3.60)
Sidechain outliers	187428	1126 (3.80-3.60)
RSRZ outliers	180081	1130 (3.80-3.60)

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

Mol	Chain	Length	Quality of chain
1	A	342	4% 26% 45% 26%
1	B	342	12% 32% 40% 27%
1	C	342	2% 21% 49% 27%
1	D	342	15% 28% 44% 27%

2 Entry composition [i](#)

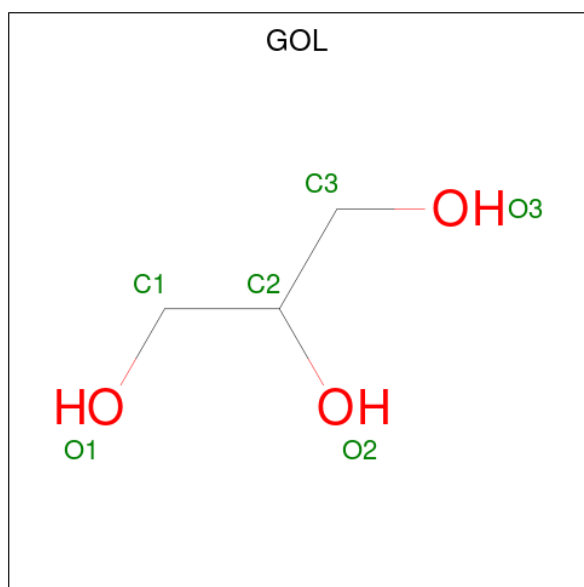
There are 2 unique types of molecules in this entry. The entry contains 7586 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

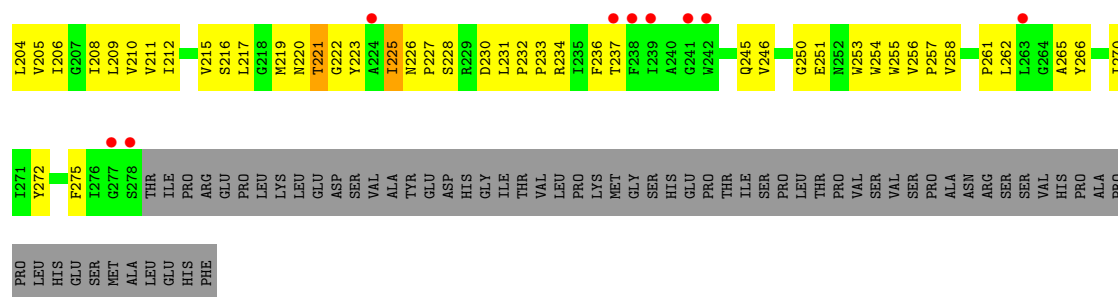
- Molecule 1 is a protein called Aquaporin-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	252	Total	C	N	O	S	0	0	0
			1925	1278	312	322	13			
1	B	249	Total	C	N	O	S	0	0	0
			1890	1253	308	316	13			
1	C	249	Total	C	N	O	S	0	0	0
			1894	1258	306	317	13			
1	D	249	Total	C	N	O	S	0	0	0
			1865	1234	302	316	13			

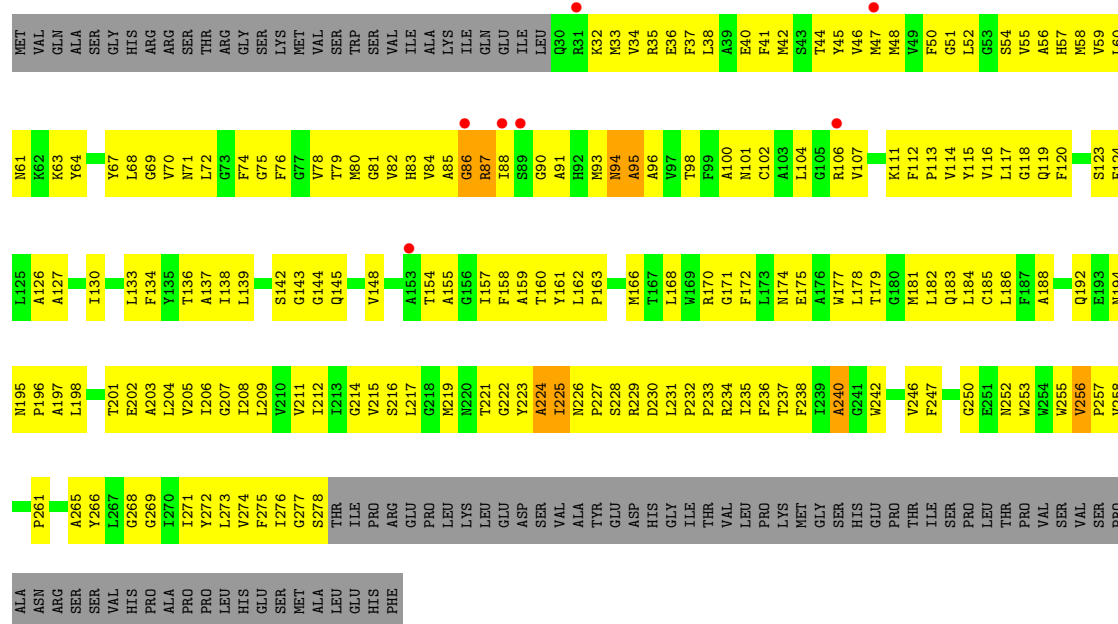
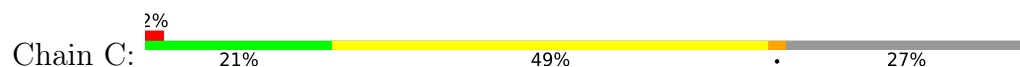
- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$) (labeled as "Ligand of Interest" by depositor).



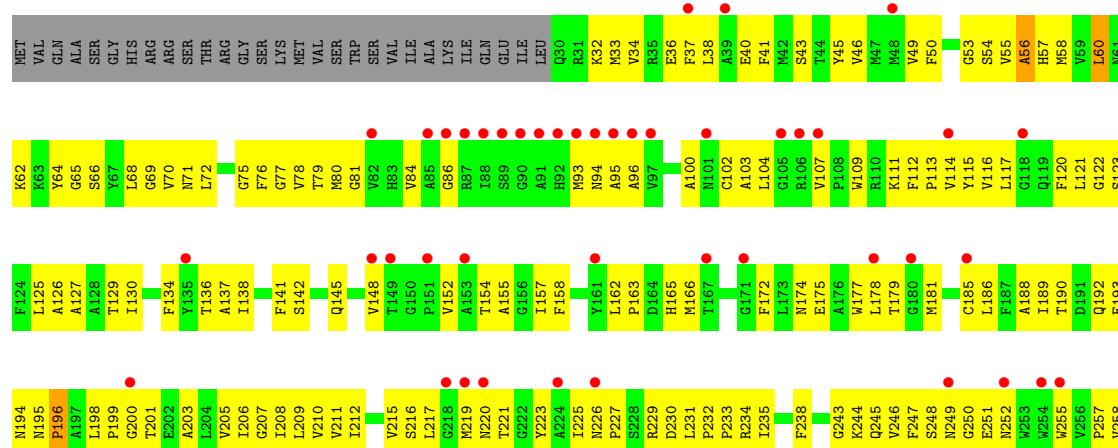
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		



• Molecule 1: Aquaporin-7



• Molecule 1: Aquaporin-7



[illegible]

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	93.51Å 106.29Å 214.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.61 – 3.70 47.61 – 3.70	Depositor EDS
% Data completeness (in resolution range)	71.9 (47.61-3.70) 72.0 (47.61-3.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.62 (at 3.67Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.268 , 0.322 0.270 , 0.322	Depositor DCC
R_{free} test set	883 reflections (3.50%)	wwPDB-VP
Wilson B-factor (Å ²)	55.0	Xtriage
Anisotropy	0.443	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 174.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.79	EDS
Total number of atoms	7586	wwPDB-VP
Average B, all atoms (Å ²)	109.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.73	0/1982	1.10	8/2702 (0.3%)
1	B	0.52	0/1946	0.87	0/2652
1	C	0.78	2/1951 (0.1%)	1.18	6/2661 (0.2%)
1	D	0.51	0/1918	0.88	0/2617
All	All	0.65	2/7797 (0.0%)	1.02	14/10632 (0.1%)

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	2
1	B	0	1
1	C	0	1
1	D	0	2
All	All	0	6

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	195	ASN	C-N	6.99	1.42	1.33
1	C	256	VAL	C-N	5.52	1.46	1.33

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	135	TYR	CA-C-N	6.54	129.34	120.44
1	A	135	TYR	C-N-CA	6.54	129.34	120.44
1	A	86	GLY	CA-C-N	5.98	132.96	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	86	GLY	C-N-CA	5.98	132.96	121.54
1	C	87	ARG	N-CA-C	5.85	123.25	110.80
1	C	86	GLY	CA-C-N	5.72	132.47	121.54
1	C	86	GLY	C-N-CA	5.72	132.47	121.54
1	A	60	LEU	CA-C-N	-5.54	111.04	121.63
1	A	60	LEU	C-N-CA	-5.54	111.04	121.63
1	A	135	TYR	CA-CB-CG	5.43	123.68	113.90
1	C	94	ASN	CA-C-N	5.29	131.65	121.54
1	C	94	ASN	C-N-CA	5.29	131.65	121.54
1	A	47	MET	CB-CG-SD	-5.07	97.51	112.70
1	C	87	ARG	CB-CG-CD	5.03	122.87	111.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	120	PHE	Peptide
1	A	251	GLU	Peptide
1	B	119	GLN	Peptide
1	C	224	ALA	Peptide
1	D	221	THR	Peptide
1	D	86	GLY	Peptide

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	1925	0	1930	200	0
1	B	1890	0	1888	186	0
1	C	1894	0	1891	243	0
1	D	1865	0	1856	211	0
2	A	6	0	8	1	0
2	C	6	0	8	1	0
All	All	7586	0	7581	744	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 49.

All (744) 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:C:48:MET:HE1	1:C:229:ARG:HA	1.31	1.13
1:A:177:TRP:CZ3	1:D:129:THR:HB	1.89	1.07
1:B:38:LEU:HD23	1:D:275:PHE:HA	1.34	1.07
1:A:31:ARG:O	1:A:32:LYS:HG2	1.62	1.00
1:D:41:PHE:HZ	1:D:125:LEU:HD12	1.27	0.99
1:D:33:MET:HA	1:D:36:GLU:HG3	1.42	0.98
1:C:163:PRO:HD2	1:C:166:MET:HG3	1.46	0.93
1:D:75:GLY:HA2	1:D:210:VAL:HB	1.51	0.91
1:A:192:GLN:HA	1:A:196:PRO:HG3	1.50	0.91
1:C:227:PRO:HB3	1:C:258:VAL:HA	1.52	0.91
1:C:68:LEU:HA	1:C:71:ASN:HD21	1.36	0.90
1:C:157:ILE:HG13	1:C:158:PHE:CD1	2.06	0.90
1:C:96:ALA:HB2	1:C:227:PRO:HD2	1.54	0.89
1:A:147:MET:HG2	1:A:152:VAL:HG23	1.52	0.89
1:B:38:LEU:HB3	1:D:275:PHE:HD1	1.39	0.88
1:B:219:MET:HB2	1:C:57:HIS:CE1	2.09	0.86
1:D:68:LEU:O	1:D:70:VAL:N	2.08	0.86
1:A:177:TRP:HH2	1:D:129:THR:HG21	1.39	0.86
1:B:94:ASN:HB2	1:B:97:VAL:HG22	1.58	0.86
1:C:192:GLN:HA	1:C:196:PRO:HG3	1.57	0.85
1:A:177:TRP:CZ3	1:D:129:THR:CB	2.60	0.85
1:D:100:ALA:HB2	1:D:265:ALA:HB1	1.58	0.85
1:A:204:LEU:HD13	1:C:205:VAL:HG12	1.59	0.84
1:C:157:ILE:HG13	1:C:158:PHE:HD1	1.41	0.84
1:D:186:LEU:O	1:D:190:THR:OG1	1.97	0.83
1:A:178:LEU:HG	1:A:217:LEU:HD23	1.60	0.82
1:D:96:ALA:HB2	1:D:227:PRO:HD2	1.61	0.82
1:C:37:PHE:O	1:C:41:PHE:N	2.13	0.81
1:C:233:PRO:HA	1:C:236:PHE:HB3	1.62	0.81
1:A:177:TRP:CH2	1:D:129:THR:HB	2.17	0.80
1:C:33:MET:HE3	1:C:111:LYS:HD2	1.61	0.80
1:C:95:ALA:HB1	1:C:116:VAL:HG22	1.64	0.80
1:A:231:LEU:HD22	1:A:235:ILE:HD11	1.64	0.79
1:A:177:TRP:CH2	1:D:129:THR:CB	2.65	0.79
1:A:80:MET:HE2	1:C:209:LEU:HG	1.65	0.79
1:D:102:CYS:SG	1:D:112:PHE:HB2	2.22	0.79
1:A:57:HIS:O	1:A:65:GLY:HA3	1.82	0.78
1:C:80:MET:SD	1:C:80:MET:N	2.57	0.78
1:C:163:PRO:HD2	1:C:166:MET:CG	2.12	0.78
1:D:95:ALA:HA	1:D:116:VAL:HG22	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:TRP:CH2	1:D:129:THR:HG21	2.18	0.78
1:A:51:GLY:HA3	1:A:74:PHE:CD1	2.19	0.77
1:A:175:GLU:O	1:A:179:THR:OG1	2.01	0.77
1:D:79:THR:HG22	1:D:203:ALA:O	1.85	0.77
1:B:37:PHE:HE2	1:B:118:GLY:HA3	1.49	0.76
1:A:100:ALA:HB2	1:A:265:ALA:HB1	1.67	0.76
1:C:61:ASN:OD1	1:C:64:TYR:N	2.18	0.76
1:D:148:VAL:HG23	1:D:155:ALA:HB3	1.67	0.76
1:D:37:PHE:O	1:D:41:PHE:N	2.17	0.75
1:B:197:ALA:HB1	1:B:201:THR:O	1.87	0.75
1:A:219:MET:HB2	1:D:57:HIS:HD1	1.52	0.74
1:B:160:THR:HG23	1:B:253:TRP:HE1	1.53	0.74
1:D:227:PRO:HG3	1:D:258:VAL:HA	1.69	0.74
1:D:216:SER:HB2	1:D:217:LEU:HD12	1.68	0.74
1:B:72:LEU:HA	1:B:211:VAL:HG22	1.70	0.74
1:B:83:HIS:CD2	1:D:189:ILE:HG12	2.22	0.74
1:A:116:VAL:O	1:A:120:PHE:HB3	1.87	0.74
1:B:73:GLY:HA2	1:D:212:ILE:HD11	1.70	0.74
1:A:224:ALA:HB1	1:A:230:ASP:OD2	1.88	0.73
1:B:202:GLU:O	1:B:206:ILE:HG12	1.88	0.73
1:D:72:LEU:HA	1:D:211:VAL:HG22	1.70	0.73
1:A:57:HIS:HA	1:C:219:MET:HE2	1.71	0.73
1:A:37:PHE:HD1	1:A:38:LEU:HD12	1.53	0.73
1:A:129:THR:HB	1:C:177:TRP:CZ3	2.23	0.73
1:C:197:ALA:HB1	1:C:201:THR:HB	1.68	0.73
1:B:41:PHE:HZ	1:B:125:LEU:HD11	1.53	0.73
1:A:42:MET:HB2	1:A:84:VAL:HG11	1.71	0.72
1:C:40:GLU:OE1	1:C:93:MET:N	2.23	0.72
1:B:178:LEU:HD21	1:B:217:LEU:HB2	1.71	0.71
1:C:44:THR:HG21	1:C:119:GLN:O	1.89	0.71
1:D:41:PHE:CZ	1:D:125:LEU:HD12	2.18	0.71
1:D:55:VAL:HG22	1:D:70:VAL:HG21	1.71	0.71
1:B:219:MET:HB2	1:C:57:HIS:ND1	2.05	0.71
1:A:177:TRP:CH2	1:D:129:THR:CG2	2.74	0.71
1:A:219:MET:HB2	1:D:57:HIS:ND1	2.05	0.71
1:B:38:LEU:HD23	1:D:275:PHE:CA	2.15	0.71
1:A:121:LEU:HD13	1:A:125:LEU:HD23	1.71	0.70
1:D:94:ASN:HB3	1:D:226:ASN:HD22	1.54	0.70
1:A:98:THR:HG22	1:A:112:PHE:CD1	2.26	0.70
1:B:275:PHE:HB2	1:C:38:LEU:HB3	1.72	0.69
1:C:223:TYR:HB2	1:C:225:ILE:HG23	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:189:ILE:HD13	1:D:205:VAL:HG12	1.75	0.69
1:B:38:LEU:CD2	1:D:275:PHE:HA	2.17	0.69
1:D:102:CYS:O	1:D:109:TRP:NE1	2.25	0.69
1:B:212:ILE:HD13	1:C:76:PHE:HB3	1.73	0.68
1:C:272:TYR:CD1	1:C:273:LEU:HD23	2.28	0.68
1:C:120:PHE:O	1:C:123:SER:OG	2.09	0.68
1:D:79:THR:HG23	1:D:207:GLY:HA3	1.73	0.68
1:C:98:THR:O	1:C:102:CYS:HB2	1.93	0.68
1:B:75:GLY:O	1:B:78:VAL:HG12	1.94	0.68
1:C:214:GLY:HA2	1:C:223:TYR:CE1	2.29	0.68
1:D:198:LEU:H	1:D:201:THR:HB	1.59	0.68
1:C:127:ALA:HB2	1:C:233:PRO:HB3	1.74	0.68
1:B:37:PHE:CZ	1:B:114:VAL:HG22	2.29	0.67
1:C:54:SER:OG	1:C:69:GLY:O	2.11	0.67
1:A:200:GLY:HA3	1:C:198:LEU:HG	1.77	0.67
1:C:154:THR:OG1	1:C:242:TRP:NE1	2.27	0.67
1:C:246:VAL:HG23	1:C:247:PHE:CD1	2.29	0.67
1:B:158:PHE:HB3	1:B:233:PRO:HB2	1.77	0.67
1:B:163:PRO:HD2	1:B:166:MET:HE1	1.77	0.67
1:B:163:PRO:O	1:B:166:MET:SD	2.53	0.66
1:A:166:MET:HE1	1:A:220:ASN:HB3	1.75	0.66
1:B:37:PHE:CE2	1:B:118:GLY:HA3	2.31	0.66
1:C:68:LEU:HA	1:C:71:ASN:ND2	2.08	0.66
1:C:56:ALA:HA	1:C:59:VAL:HG12	1.76	0.66
1:D:53:GLY:O	1:D:57:HIS:HB3	1.97	0.65
1:C:205:VAL:HA	1:C:208:ILE:HG22	1.77	0.65
1:A:205:VAL:HG12	1:A:206:ILE:HD12	1.76	0.65
1:C:175:GLU:OE1	1:C:221:THR:HG21	1.96	0.65
1:D:75:GLY:HA2	1:D:210:VAL:CB	2.24	0.65
1:D:75:GLY:O	1:D:78:VAL:HB	1.97	0.65
1:A:98:THR:HG21	1:A:115:TYR:HB3	1.79	0.65
1:C:48:MET:HE2	1:C:123:SER:CB	2.26	0.65
1:C:78:VAL:O	1:C:81:GLY:N	2.29	0.65
1:D:53:GLY:HA2	1:D:56:ALA:HB3	1.77	0.64
1:D:104:LEU:HD23	1:D:273:LEU:HD12	1.79	0.64
1:B:195:ASN:CG	1:C:87:ARG:HG2	2.22	0.64
1:C:51:GLY:O	1:C:54:SER:N	2.29	0.64
1:C:116:VAL:O	1:C:120:PHE:N	2.31	0.64
1:A:37:PHE:CD1	1:A:38:LEU:HD12	2.32	0.64
1:A:46:VAL:HG13	1:C:181:MET:HE1	1.80	0.64
1:B:209:LEU:HA	1:C:80:MET:HE2	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:94:ASN:HB2	1:C:226:ASN:CB	2.27	0.64
1:B:85:ALA:HB1	1:B:90:GLY:O	1.98	0.64
1:C:139:LEU:HD12	1:C:144:GLY:HA2	1.78	0.64
1:C:71:ASN:HB2	1:C:214:GLY:HA3	1.79	0.64
1:C:216:SER:HB3	1:C:217:LEU:HD13	1.79	0.64
1:D:55:VAL:C	1:D:57:HIS:H	2.06	0.63
1:C:178:LEU:CD2	1:C:217:LEU:HD23	2.28	0.63
1:B:38:LEU:HB3	1:D:275:PHE:CD1	2.30	0.63
1:D:162:LEU:HB2	1:D:166:MET:HE2	1.80	0.63
1:A:95:ALA:HB1	1:A:116:VAL:HG22	1.80	0.63
1:A:181:MET:HE3	1:D:49:VAL:HB	1.80	0.63
1:B:212:ILE:HA	1:B:215:VAL:HG22	1.80	0.63
1:D:37:PHE:O	1:D:40:GLU:N	2.32	0.63
1:B:231:LEU:HD12	1:B:258:VAL:HG21	1.79	0.62
1:D:60:LEU:HD11	1:D:137:ALA:O	2.00	0.62
1:D:37:PHE:CE1	1:D:114:VAL:HB	2.33	0.62
1:A:129:THR:HB	1:C:177:TRP:HZ3	1.64	0.62
1:D:178:LEU:HD22	1:D:225:ILE:HD11	1.80	0.62
1:D:37:PHE:HE1	1:D:114:VAL:HB	1.65	0.62
1:A:165:HIS:O	1:D:136:THR:OG1	2.17	0.62
1:C:56:ALA:HB2	1:C:157:ILE:HD12	1.81	0.62
1:C:272:TYR:O	1:C:274:VAL:N	2.33	0.62
1:D:95:ALA:HB2	1:D:116:VAL:HG13	1.80	0.62
1:A:98:THR:HG22	1:A:112:PHE:HD1	1.64	0.62
1:A:60:LEU:HD11	1:A:138:ILE:HG22	1.82	0.62
1:D:94:ASN:CB	1:D:226:ASN:HD22	2.13	0.62
1:B:114:VAL:HG13	1:B:115:TYR:CD1	2.35	0.61
1:C:201:THR:O	1:C:205:VAL:HG22	1.99	0.61
1:B:212:ILE:HG13	1:C:50:PHE:HE2	1.65	0.61
1:B:227:PRO:HG2	1:B:262:LEU:HD21	1.82	0.61
1:C:274:VAL:HG23	1:C:275:PHE:N	2.15	0.61
1:D:78:VAL:HG21	1:D:210:VAL:HG21	1.81	0.61
1:B:220:ASN:O	1:B:222:GLY:N	2.34	0.61
1:C:272:TYR:HD1	1:C:273:LEU:HD23	1.65	0.61
1:B:219:MET:HE2	1:C:134:PHE:HE1	1.65	0.61
1:D:81:GLY:O	1:D:84:VAL:N	2.27	0.61
1:B:189:ILE:HG21	1:B:206:ILE:HD11	1.80	0.61
1:A:235:ILE:O	1:A:239:ILE:HG13	2.00	0.61
1:A:109:TRP:O	1:A:111:LYS:N	2.34	0.61
1:A:116:VAL:HG12	1:A:117:LEU:HD23	1.83	0.61
1:A:215:VAL:HG11	1:D:72:LEU:HD21	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:48:MET:HE2	1:C:123:SER:HB3	1.82	0.60
1:D:79:THR:CG2	1:D:207:GLY:HA3	2.30	0.60
1:D:255:TRP:CE3	1:D:259:VAL:HG21	2.36	0.60
1:C:71:ASN:ND2	1:C:71:ASN:H	1.97	0.60
1:D:198:LEU:HB3	1:D:199:PRO:HD2	1.83	0.60
1:B:75:GLY:HA2	1:B:210:VAL:HB	1.83	0.60
1:B:80:MET:HE2	1:D:209:LEU:HD13	1.83	0.60
1:B:156:GLY:HA2	1:B:161:TYR:CE2	2.35	0.60
1:B:212:ILE:HD13	1:C:76:PHE:CB	2.30	0.60
1:B:253:TRP:O	1:B:255:TRP:N	2.34	0.60
1:D:60:LEU:HD21	1:D:138:ILE:HG12	1.82	0.60
1:A:54:SER:HB2	1:A:70:VAL:HG22	1.83	0.60
1:B:43:SER:OG	1:B:93:MET:SD	2.59	0.60
1:A:51:GLY:HA3	1:A:74:PHE:CE1	2.36	0.60
1:A:181:MET:HE1	1:D:46:VAL:HA	1.82	0.60
1:B:45:TYR:HE1	1:B:129:THR:HG21	1.67	0.60
1:C:157:ILE:HG13	1:C:158:PHE:CE1	2.36	0.60
1:C:224:ALA:O	1:C:226:ASN:N	2.35	0.60
1:A:36:GLU:O	1:A:40:GLU:N	2.34	0.59
1:A:148:VAL:HG12	1:A:149:THR:HG23	1.83	0.59
1:C:70:VAL:O	1:C:74:PHE:HB2	2.01	0.59
1:C:94:ASN:O	1:C:96:ALA:N	2.35	0.59
1:B:58:MET:HG3	1:B:59:VAL:N	2.17	0.59
1:B:124:PHE:HD1	1:B:236:PHE:HB2	1.66	0.59
1:B:219:MET:HE2	1:C:134:PHE:CE1	2.38	0.59
1:B:228:SER:HA	1:B:232:PRO:HG2	1.84	0.59
1:C:226:ASN:HD22	1:C:228:SER:HB2	1.66	0.59
1:A:83:HIS:O	1:C:188:ALA:HB1	2.02	0.59
1:B:80:MET:HG2	1:D:185:CYS:SG	2.43	0.59
1:B:100:ALA:O	1:B:102:CYS:N	2.30	0.59
1:A:172:PHE:CZ	1:A:259:VAL:HG12	2.37	0.59
1:B:138:ILE:O	1:B:142:SER:N	2.20	0.59
1:A:138:ILE:HG13	1:A:139:LEU:HD23	1.84	0.59
1:B:217:LEU:HD23	1:C:133:LEU:HD22	1.85	0.59
1:B:100:ALA:C	1:B:102:CYS:H	2.09	0.59
1:D:178:LEU:HB3	1:D:225:ILE:HG12	1.85	0.59
1:A:34:VAL:O	1:A:38:LEU:HD13	2.02	0.58
1:A:138:ILE:O	1:A:141:PHE:N	2.35	0.58
1:C:85:ALA:O	1:C:91:ALA:HB2	2.02	0.58
1:C:114:VAL:HG23	1:C:115:TYR:HD1	1.67	0.58
1:B:163:PRO:HD2	1:B:166:MET:CE	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:138:ILE:HA	1:D:141:PHE:HB3	1.85	0.58
1:C:75:GLY:HA3	1:C:211:VAL:CG1	2.32	0.58
1:B:129:THR:HB	1:D:177:TRP:CZ3	2.39	0.58
1:D:179:THR:HB	1:D:261:PRO:HA	1.84	0.58
1:D:189:ILE:HD12	1:D:206:ILE:CD1	2.34	0.58
1:A:175:GLU:HB3	1:A:260:ALA:HB1	1.86	0.58
1:D:76:PHE:O	1:D:79:THR:OG1	2.12	0.58
1:C:76:PHE:O	1:C:79:THR:HB	2.04	0.57
1:D:205:VAL:HA	1:D:208:ILE:HG22	1.85	0.57
1:C:94:ASN:HB2	1:C:226:ASN:CG	2.29	0.57
1:D:268:GLY:O	1:D:271:ILE:N	2.36	0.57
1:B:35:ARG:HH11	1:D:276:ILE:HD11	1.69	0.57
1:C:256:VAL:C	1:C:258:VAL:H	2.13	0.57
1:B:35:ARG:HE	1:D:276:ILE:CD1	2.17	0.57
1:C:41:PHE:O	1:C:45:TYR:N	2.33	0.57
1:D:185:CYS:O	1:D:189:ILE:HG13	2.05	0.57
1:D:189:ILE:HD12	1:D:206:ILE:HD13	1.85	0.57
1:A:202:GLU:O	1:A:206:ILE:HD13	2.05	0.57
1:C:159:ALA:HB1	1:C:234:ARG:CZ	2.35	0.57
1:D:194:ASN:ND2	1:D:272:TYR:OH	2.23	0.57
1:B:205:VAL:O	1:B:209:LEU:N	2.37	0.56
1:A:94:ASN:O	1:A:96:ALA:N	2.39	0.56
1:B:57:HIS:NE2	1:B:65:GLY:HA2	2.21	0.56
1:D:234:ARG:HD2	1:D:247:PHE:HD1	1.71	0.56
1:A:181:MET:HE1	1:D:46:VAL:HG13	1.86	0.56
1:B:40:GLU:OE2	1:B:115:TYR:CD2	2.58	0.56
1:C:68:LEU:O	1:C:72:LEU:HD23	2.06	0.56
1:C:162:LEU:HD11	1:C:250:GLY:HA2	1.85	0.56
1:C:185:CYS:HB2	1:C:209:LEU:HD11	1.87	0.56
1:D:68:LEU:HB3	1:D:72:LEU:HD22	1.87	0.56
1:A:184:LEU:HD13	1:A:268:GLY:O	2.06	0.56
1:B:87:ARG:HB2	1:D:195:ASN:CG	2.30	0.56
1:A:160:THR:HG23	1:A:253:TRP:HE1	1.71	0.56
1:C:85:ALA:HB1	1:C:90:GLY:O	2.05	0.56
1:A:138:ILE:HG13	1:A:139:LEU:CD2	2.36	0.56
1:A:238:PHE:HB2	1:A:246:VAL:HG21	1.87	0.56
1:B:41:PHE:CZ	1:B:125:LEU:HD11	2.39	0.56
1:C:160:THR:HG21	1:C:222:GLY:O	2.06	0.56
1:A:120:PHE:HE2	1:A:227:PRO:O	1.88	0.56
1:B:111:LYS:O	1:B:114:VAL:HG12	2.05	0.56
1:C:231:LEU:HD22	1:C:235:ILE:CD1	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:68:LEU:HD22	1:D:71:ASN:HB2	1.86	0.56
1:B:54:SER:O	1:B:57:HIS:HB3	2.06	0.56
1:A:136:THR:HG22	1:C:170:ARG:HG3	1.87	0.56
1:B:57:HIS:O	1:B:65:GLY:HA3	2.06	0.56
1:C:41:PHE:O	1:C:45:TYR:HB2	2.05	0.56
1:C:154:THR:HG1	1:C:242:TRP:NE1	2.04	0.56
1:C:237:THR:HA	1:C:240:ALA:HB3	1.87	0.56
1:B:104:LEU:HG	1:B:106:ARG:H	1.71	0.56
1:D:209:LEU:O	1:D:212:ILE:N	2.39	0.55
1:B:230:ASP:CB	1:B:257:PRO:HB2	2.37	0.55
1:C:256:VAL:HB	1:C:257:PRO:CD	2.36	0.55
1:C:80:MET:O	1:C:84:VAL:HG23	2.06	0.55
1:C:106:ARG:O	1:C:107:VAL:HG23	2.05	0.55
1:C:166:MET:HE1	1:C:170:ARG:HB2	1.87	0.55
1:D:205:VAL:HG12	1:D:205:VAL:O	2.06	0.55
1:A:109:TRP:O	1:A:112:PHE:N	2.34	0.55
1:C:209:LEU:O	1:C:212:ILE:N	2.27	0.55
1:C:142:SER:OG	1:C:145:GLN:O	2.23	0.55
1:D:175:GLU:HG2	1:D:257:PRO:HB3	1.88	0.55
1:A:82:VAL:C	1:A:84:VAL:H	2.15	0.55
1:A:225:ILE:O	1:A:227:PRO:HD3	2.07	0.55
1:A:226:ASN:HB3	1:A:229:ARG:HG2	1.89	0.55
1:C:179:THR:HG22	1:C:265:ALA:HB2	1.89	0.55
1:D:257:PRO:HA	1:D:261:PRO:HD3	1.89	0.55
1:B:234:ARG:NH1	1:B:246:VAL:O	2.36	0.55
1:C:162:LEU:HB2	1:C:166:MET:HB2	1.88	0.55
1:A:30:GLN:HA	1:A:30:GLN:OE1	2.07	0.55
1:A:58:MET:SD	1:A:67:TYR:HA	2.46	0.55
1:A:129:THR:HB	1:C:177:TRP:CH2	2.41	0.55
1:B:126:ALA:O	1:B:129:THR:N	2.40	0.55
1:D:120:PHE:CZ	1:D:232:PRO:HD3	2.42	0.55
1:D:275:PHE:CD2	1:D:276:ILE:HG22	2.42	0.55
1:A:189:ILE:HB	1:A:206:ILE:HD11	1.89	0.54
1:B:75:GLY:CA	1:B:210:VAL:HB	2.37	0.54
1:B:109:TRP:O	1:B:112:PHE:HB3	2.07	0.54
1:B:124:PHE:CD1	1:B:236:PHE:HB2	2.42	0.54
1:C:256:VAL:HB	1:C:257:PRO:HD3	1.87	0.54
1:D:230:ASP:OD1	1:D:234:ARG:NH2	2.35	0.54
1:A:76:PHE:CE2	1:C:208:ILE:HD11	2.41	0.54
1:A:240:ALA:HB3	1:A:242:TRP:HZ3	1.72	0.54
1:B:76:PHE:C	1:D:212:ILE:HG12	2.32	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:LEU:HD11	1:D:174:ASN:HA	1.88	0.54
1:B:231:LEU:HD12	1:B:258:VAL:HG11	1.90	0.54
1:D:49:VAL:HG23	1:D:126:ALA:HB1	1.88	0.54
1:D:223:TYR:HB2	1:D:225:ILE:HG13	1.89	0.54
1:A:121:LEU:HD22	1:A:124:PHE:HD2	1.72	0.54
1:B:103:ALA:CB	1:B:266:TYR:HD1	2.21	0.54
1:A:200:GLY:HA3	1:C:198:LEU:CG	2.37	0.54
1:B:67:TYR:O	1:B:71:ASN:ND2	2.40	0.54
1:A:58:MET:HB3	1:A:66:SER:O	2.07	0.54
1:A:219:MET:SD	1:D:57:HIS:HA	2.48	0.54
1:C:202:GLU:O	1:C:206:ILE:HG13	2.08	0.54
1:A:189:ILE:HD11	1:D:80:MET:HE3	1.89	0.54
1:B:80:MET:HE3	1:D:189:ILE:HD11	1.88	0.54
1:D:71:ASN:HB3	1:D:211:VAL:HG13	1.90	0.54
1:A:96:ALA:O	1:A:99:PHE:N	2.41	0.54
2:A:401:GOL:H11	1:D:64:TYR:CE2	2.43	0.54
1:B:71:ASN:HA	1:B:223:TYR:OH	2.08	0.54
1:D:130:ILE:HD11	1:D:134:PHE:HE2	1.71	0.54
1:C:94:ASN:HB2	1:C:226:ASN:HB3	1.88	0.53
1:C:231:LEU:CD2	1:C:235:ILE:HD11	2.37	0.53
1:A:75:GLY:O	1:A:207:GLY:HA3	2.08	0.53
1:C:112:PHE:HB3	1:C:113:PRO:HD3	1.89	0.53
1:C:194:ASN:CG	1:C:276:ILE:HD11	2.32	0.53
1:D:123:SER:HB2	1:D:232:PRO:CG	2.38	0.53
1:B:35:ARG:HE	1:D:276:ILE:HD11	1.73	0.53
1:B:102:CYS:HB3	1:B:109:TRP:CD1	2.43	0.53
1:D:123:SER:HB2	1:D:232:PRO:HG2	1.91	0.53
1:B:114:VAL:HG13	1:B:115:TYR:HD1	1.72	0.53
1:A:219:MET:HE2	1:D:134:PHE:HE1	1.74	0.53
1:B:227:PRO:HB3	1:B:258:VAL:HA	1.91	0.53
1:C:139:LEU:O	1:C:143:GLY:N	2.42	0.53
1:C:204:LEU:O	1:C:208:ILE:HB	2.09	0.53
1:D:178:LEU:HD21	1:D:217:LEU:HB2	1.90	0.53
1:D:250:GLY:C	1:D:252:ASN:H	2.16	0.53
1:B:216:SER:OG	1:C:54:SER:HB2	2.08	0.52
1:A:40:GLU:OE1	1:A:92:HIS:N	2.42	0.52
1:A:214:GLY:HA2	1:A:223:TYR:HE2	1.74	0.52
1:A:237:THR:O	1:A:242:TRP:HE3	1.92	0.52
1:B:128:ALA:O	1:B:131:TYR:N	2.42	0.52
1:B:275:PHE:HA	1:C:38:LEU:HD22	1.92	0.52
1:C:75:GLY:HA3	1:C:211:VAL:HG12	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:138:ILE:CG2	1:D:154:THR:HG21	2.39	0.52
1:A:136:THR:CG2	1:C:170:ARG:HG3	2.40	0.52
1:A:275:PHE:HA	1:D:38:LEU:HD23	1.92	0.52
1:C:37:PHE:N	1:C:37:PHE:CD1	2.77	0.52
1:C:130:ILE:HD11	1:C:134:PHE:CE2	2.44	0.52
1:B:45:TYR:HA	1:B:122:GLY:O	2.10	0.52
1:B:73:GLY:HA2	1:D:212:ILE:CD1	2.38	0.52
1:B:231:LEU:CD1	1:B:258:VAL:HG21	2.39	0.52
1:C:55:VAL:HG22	1:C:157:ILE:HG22	1.92	0.52
1:C:271:ILE:O	1:C:274:VAL:HG22	2.09	0.52
1:D:62:LYS:HA	1:D:65:GLY:O	2.10	0.52
1:A:177:TRP:HH2	1:D:129:THR:CG2	2.11	0.52
1:A:33:MET:SD	1:A:111:LYS:HB3	2.49	0.51
1:A:47:MET:HE1	1:A:226:ASN:ND2	2.25	0.51
1:B:148:VAL:HB	1:B:245:GLN:OE1	2.10	0.51
1:B:275:PHE:HB2	1:C:38:LEU:CB	2.39	0.51
1:D:117:LEU:C	1:D:121:LEU:HG	2.36	0.51
1:B:160:THR:CG2	1:B:253:TRP:HE1	2.22	0.51
1:C:114:VAL:HG23	1:C:115:TYR:CD1	2.44	0.51
1:A:104:LEU:HD21	1:A:270:ILE:HG13	1.93	0.51
1:C:82:VAL:CG1	1:C:203:ALA:HB2	2.40	0.51
1:B:223:TYR:C	1:B:225:ILE:H	2.17	0.51
1:D:117:LEU:O	1:D:121:LEU:HG	2.10	0.51
1:B:162:LEU:HD23	1:B:162:LEU:H	1.75	0.51
1:B:148:VAL:HG21	1:B:245:GLN:HB2	1.91	0.51
1:B:272:TYR:CE1	1:B:275:PHE:HE1	2.29	0.51
1:C:226:ASN:O	1:C:228:SER:N	2.42	0.51
1:C:33:MET:O	1:C:36:GLU:HB2	2.10	0.51
1:D:138:ILE:HG21	1:D:154:THR:HG21	1.93	0.51
1:A:189:ILE:HD13	1:A:205:VAL:CG1	2.40	0.51
1:B:172:PHE:HD1	1:B:256:VAL:HG23	1.76	0.51
1:B:182:LEU:O	1:B:186:LEU:HB2	2.11	0.51
1:B:217:LEU:HD12	1:B:217:LEU:N	2.26	0.51
1:D:198:LEU:HB2	1:D:201:THR:OG1	2.11	0.51
1:B:272:TYR:CZ	1:B:275:PHE:HE1	2.29	0.51
1:C:178:LEU:HD21	1:C:217:LEU:HD23	1.91	0.51
1:C:183:GLN:HA	1:C:183:GLN:OE1	2.10	0.50
1:D:172:PHE:CD2	1:D:260:ALA:HB2	2.45	0.50
1:A:50:PHE:HD2	1:A:77:GLY:HA2	1.75	0.50
1:A:159:ALA:HB2	1:A:234:ARG:HB2	1.94	0.50
1:D:75:GLY:HA2	1:D:210:VAL:CG1	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:116:VAL:O	1:D:120:PHE:HB2	2.11	0.50
1:A:56:ALA:O	1:A:60:LEU:HB3	2.10	0.50
1:A:98:THR:HG21	1:A:115:TYR:CB	2.42	0.50
1:A:135:TYR:HB3	1:C:170:ARG:NH2	2.26	0.50
1:D:103:ALA:HB2	1:D:109:TRP:HZ2	1.75	0.50
1:B:225:ILE:HD12	1:B:226:ASN:N	2.26	0.50
1:C:48:MET:HG3	1:C:123:SER:HA	1.94	0.50
1:D:32:LYS:HD3	1:D:33:MET:H	1.76	0.50
1:A:71:ASN:HA	1:A:223:TYR:OH	2.11	0.50
1:B:115:TYR:O	1:B:119:GLN:HB2	2.12	0.50
1:B:227:PRO:HG2	1:B:262:LEU:CD2	2.41	0.50
1:C:55:VAL:HB	1:C:70:VAL:HG13	1.94	0.50
1:A:60:LEU:HD21	1:A:137:ALA:O	2.11	0.50
1:B:51:GLY:HA2	1:B:74:PHE:HA	1.94	0.50
1:B:124:PHE:HE1	1:B:236:PHE:HD1	1.59	0.50
1:D:33:MET:CA	1:D:36:GLU:HG3	2.28	0.50
1:D:234:ARG:HD3	1:D:246:VAL:O	2.11	0.50
1:A:205:VAL:HA	1:A:208:ILE:HG22	1.93	0.49
1:A:157:ILE:HB	1:A:158:PHE:CD1	2.47	0.49
1:A:189:ILE:HG21	1:A:205:VAL:HG11	1.94	0.49
1:C:48:MET:HE2	1:C:123:SER:HB2	1.92	0.49
1:A:202:GLU:OE1	1:A:202:GLU:N	2.42	0.49
1:C:208:ILE:O	1:C:212:ILE:HG12	2.11	0.49
1:A:120:PHE:CE2	1:A:227:PRO:O	2.65	0.49
1:A:189:ILE:HD13	1:A:205:VAL:HG11	1.94	0.49
1:B:226:ASN:O	1:B:228:SER:N	2.42	0.49
1:C:124:PHE:HE1	1:C:236:PHE:HD1	1.60	0.49
1:D:212:ILE:HD12	1:D:215:VAL:HG21	1.94	0.49
1:B:55:VAL:HA	1:B:70:VAL:HG22	1.94	0.49
1:D:245:GLN:HA	1:D:248:SER:OG	2.11	0.49
1:A:33:MET:O	1:A:36:GLU:N	2.39	0.49
1:A:75:GLY:O	1:A:79:THR:HG23	2.13	0.49
1:B:45:TYR:CE1	1:B:129:THR:HG21	2.47	0.49
1:C:67:TYR:O	1:C:70:VAL:N	2.43	0.49
1:C:85:ALA:HB3	1:C:91:ALA:HA	1.94	0.49
1:D:117:LEU:O	1:D:121:LEU:N	2.27	0.49
1:A:90:GLY:HA2	1:A:115:TYR:OH	2.13	0.49
1:B:100:ALA:HB2	1:B:265:ALA:HB1	1.95	0.49
1:A:31:ARG:O	1:A:32:LYS:CG	2.49	0.49
1:B:37:PHE:HZ	1:B:114:VAL:O	1.96	0.49
1:D:45:TYR:HA	1:D:126:ALA:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:LEU:O	1:A:235:ILE:HG13	2.13	0.49
1:B:181:MET:O	1:B:185:CYS:HB2	2.12	0.49
1:C:118:GLY:H	1:C:120:PHE:H	1.60	0.49
1:C:211:VAL:HG23	1:C:212:ILE:HD13	1.95	0.49
1:C:219:MET:HE3	1:C:219:MET:HB3	1.76	0.49
1:A:75:GLY:HA2	1:A:210:VAL:HB	1.94	0.48
1:B:128:ALA:HA	1:B:131:TYR:HB3	1.94	0.48
1:D:34:VAL:C	1:D:36:GLU:H	2.19	0.48
1:D:267:LEU:O	1:D:271:ILE:HG12	2.13	0.48
1:A:121:LEU:HD22	1:A:124:PHE:CD2	2.47	0.48
1:B:131:TYR:CD2	1:B:236:PHE:HZ	2.30	0.48
1:D:252:ASN:OD1	1:D:252:ASN:N	2.47	0.48
1:C:72:LEU:HA	1:C:211:VAL:HG12	1.94	0.48
1:C:162:LEU:O	1:C:162:LEU:HD12	2.13	0.48
1:C:226:ASN:ND2	1:C:228:SER:HB2	2.29	0.48
1:D:163:PRO:HD2	1:D:166:MET:SD	2.54	0.48
1:A:79:THR:HG22	1:A:207:GLY:H	1.79	0.48
1:A:163:PRO:C	1:A:165:HIS:H	2.21	0.48
1:C:172:PHE:CD2	1:C:256:VAL:HG13	2.49	0.48
1:C:182:LEU:O	1:C:186:LEU:HB2	2.14	0.48
1:A:128:ALA:HB2	1:A:236:PHE:CE1	2.49	0.48
1:A:275:PHE:CE2	1:A:276:ILE:HB	2.49	0.48
1:B:50:PHE:O	1:B:54:SER:OG	2.17	0.48
1:B:76:PHE:O	1:D:212:ILE:HG12	2.13	0.48
1:C:68:LEU:CA	1:C:71:ASN:HD21	2.18	0.48
1:C:124:PHE:C	1:C:126:ALA:H	2.22	0.48
1:D:226:ASN:OD1	1:D:226:ASN:N	2.45	0.48
1:A:228:SER:O	1:A:232:PRO:HG2	2.14	0.48
1:C:37:PHE:O	1:C:41:PHE:HB2	2.14	0.48
1:C:255:TRP:CD1	1:C:256:VAL:N	2.82	0.48
1:D:104:LEU:HD21	1:D:269:GLY:C	2.39	0.48
1:C:78:VAL:O	1:C:79:THR:C	2.56	0.47
1:D:122:GLY:O	1:D:125:LEU:N	2.47	0.47
1:D:192:GLN:HA	1:D:196:PRO:HG3	1.95	0.47
1:A:60:LEU:CD1	1:A:138:ILE:HG22	2.43	0.47
1:C:231:LEU:O	1:C:235:ILE:HG13	2.14	0.47
1:C:250:GLY:C	1:C:252:ASN:H	2.22	0.47
1:A:256:VAL:O	1:A:260:ALA:N	2.33	0.47
1:C:71:ASN:OD1	1:C:215:VAL:CG1	2.62	0.47
1:A:95:ALA:CB	1:A:116:VAL:HG22	2.44	0.47
1:A:172:PHE:HZ	1:A:259:VAL:HG12	1.75	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:231:LEU:HD23	1:C:235:ILE:HG13	1.96	0.47
1:A:107:VAL:HG12	1:A:108:PRO:O	2.15	0.47
1:A:177:TRP:HZ3	1:D:129:THR:CB	2.24	0.47
1:C:161:TYR:OH	1:C:246:VAL:HG12	2.15	0.47
1:C:171:GLY:O	1:C:256:VAL:HG11	2.14	0.47
1:C:78:VAL:HB	1:C:207:GLY:HA2	1.96	0.47
1:D:123:SER:CB	1:D:232:PRO:HG2	2.44	0.47
1:C:162:LEU:HB2	1:C:166:MET:CB	2.44	0.47
1:C:269:GLY:O	1:C:272:TYR:HB3	2.15	0.47
1:D:179:THR:OG1	1:D:225:ILE:HG23	2.15	0.47
1:A:204:LEU:HD21	1:C:204:LEU:HD12	1.96	0.47
1:B:45:TYR:O	1:B:45:TYR:CG	2.68	0.47
1:D:78:VAL:HG22	1:D:93:MET:HE1	1.96	0.47
1:A:85:ALA:O	1:A:91:ALA:HB2	2.16	0.47
1:D:234:ARG:HD2	1:D:247:PHE:CD1	2.48	0.47
1:A:76:PHE:HD2	1:C:212:ILE:HD11	1.80	0.46
1:A:254:TRP:CD1	1:A:255:TRP:N	2.83	0.46
1:A:142:SER:OG	1:A:145:GLN:O	2.32	0.46
1:B:172:PHE:HD1	1:B:256:VAL:CG2	2.28	0.46
1:B:208:ILE:HD12	1:C:204:LEU:HD21	1.97	0.46
1:C:42:MET:O	1:C:46:VAL:HG23	2.16	0.46
1:A:162:LEU:HD23	1:A:253:TRP:CE3	2.51	0.46
1:B:40:GLU:OE1	1:B:119:GLN:HG3	2.16	0.46
1:C:47:MET:HE1	1:C:226:ASN:OD1	2.16	0.46
1:C:186:LEU:HA	1:C:186:LEU:HD22	1.75	0.46
1:D:227:PRO:HB3	1:D:258:VAL:HG13	1.96	0.46
1:A:48:MET:HE1	1:A:229:ARG:CB	2.46	0.46
1:B:46:VAL:HG22	1:D:181:MET:CE	2.46	0.46
1:D:142:SER:OG	1:D:145:GLN:O	2.20	0.46
1:A:46:VAL:HG13	1:C:181:MET:CE	2.46	0.46
1:B:83:HIS:CE1	1:D:205:VAL:HG11	2.50	0.46
1:C:56:ALA:HB2	1:C:157:ILE:CD1	2.45	0.46
1:C:166:MET:HE1	1:C:170:ARG:CB	2.46	0.46
1:A:84:VAL:O	1:A:84:VAL:HG12	2.15	0.46
1:A:85:ALA:O	1:A:87:ARG:N	2.49	0.46
1:A:183:GLN:OE1	1:A:183:GLN:HA	2.16	0.46
1:C:154:THR:OG1	1:C:155:ALA:N	2.49	0.46
1:D:157:ILE:HG13	1:D:158:PHE:H	1.81	0.46
1:B:253:TRP:C	1:B:255:TRP:H	2.24	0.46
1:D:219:MET:HE2	1:D:219:MET:HB3	1.77	0.46
1:B:160:THR:HG23	1:B:253:TRP:NE1	2.26	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:198:LEU:N	1:D:201:THR:HB	2.28	0.46
1:A:74:PHE:O	1:A:78:VAL:HG23	2.16	0.46
1:A:209:LEU:HG	1:D:80:MET:HE2	1.97	0.46
1:D:76:PHE:HA	1:D:79:THR:HG23	1.98	0.46
1:D:275:PHE:CE2	1:D:276:ILE:HG22	2.51	0.46
1:A:200:GLY:HA3	1:C:198:LEU:CD2	2.45	0.45
1:C:134:PHE:O	1:C:138:ILE:HG12	2.16	0.45
1:B:85:ALA:HB1	1:B:91:ALA:HA	1.97	0.45
1:C:41:PHE:O	1:C:45:TYR:CB	2.64	0.45
1:C:184:LEU:HD12	1:C:268:GLY:O	2.15	0.45
1:D:95:ALA:CB	1:D:116:VAL:HG13	2.45	0.45
1:D:107:VAL:HG12	1:D:111:LYS:HB2	1.97	0.45
1:A:92:HIS:CE1	1:A:115:TYR:HE2	2.34	0.45
1:A:126:ALA:HA	1:A:129:THR:OG1	2.17	0.45
1:A:159:ALA:HB1	1:A:234:ARG:NH2	2.32	0.45
1:C:52:LEU:HA	1:C:55:VAL:HG12	1.98	0.45
1:C:71:ASN:HA	1:C:223:TYR:OH	2.17	0.45
1:C:148:VAL:HG22	1:C:242:TRP:HD1	1.81	0.45
1:C:183:GLN:O	1:C:184:LEU:C	2.58	0.45
1:A:162:LEU:O	1:A:162:LEU:HD12	2.17	0.45
1:A:216:SER:HA	1:D:54:SER:HA	1.98	0.45
1:C:95:ALA:CB	1:C:116:VAL:HG22	2.42	0.45
1:C:104:LEU:CD2	1:C:266:TYR:HE1	2.30	0.45
1:C:227:PRO:HD3	1:C:261:PRO:CB	2.47	0.45
1:A:79:THR:CG2	1:A:207:GLY:HA3	2.47	0.45
1:A:205:VAL:O	1:A:208:ILE:HG22	2.17	0.45
1:B:191:ASP:C	1:B:193:GLU:H	2.25	0.45
1:C:117:LEU:HA	1:C:120:PHE:HB2	1.99	0.45
1:D:193:GLU:HG3	1:D:194:ASN:H	1.80	0.45
1:A:184:LEU:HD21	1:A:271:ILE:HG22	1.98	0.45
1:B:225:ILE:CD1	1:B:226:ASN:HD22	2.30	0.45
1:C:75:GLY:HA3	1:C:211:VAL:HG13	1.97	0.45
1:C:205:VAL:HA	1:C:208:ILE:CG2	2.44	0.45
1:B:41:PHE:HZ	1:B:125:LEU:CD1	2.25	0.45
1:C:272:TYR:CD1	1:C:276:ILE:HG23	2.52	0.45
1:A:170:ARG:HG3	1:D:136:THR:CG2	2.47	0.45
1:B:116:VAL:HG12	1:B:120:PHE:CZ	2.51	0.45
1:B:45:TYR:CD1	1:B:126:ALA:HB2	2.52	0.45
1:B:208:ILE:HD13	1:C:76:PHE:CZ	2.52	0.45
1:C:222:GLY:HA2	2:C:400:GOL:H2	1.98	0.45
1:D:71:ASN:HD21	1:D:215:VAL:HA	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:112:PHE:CZ	1:D:116:VAL:HG21	2.52	0.45
1:D:231:LEU:O	1:D:235:ILE:N	2.42	0.45
1:A:48:MET:HE1	1:A:229:ARG:HB3	1.98	0.44
1:A:171:GLY:O	1:A:256:VAL:HG11	2.16	0.44
1:B:148:VAL:HG11	1:B:245:GLN:HB3	2.00	0.44
1:B:170:ARG:HG2	1:C:136:THR:HG23	1.99	0.44
1:C:94:ASN:CB	1:C:226:ASN:CG	2.91	0.44
1:D:271:ILE:O	1:D:275:PHE:HB3	2.17	0.44
1:B:100:ALA:HB2	1:B:265:ALA:CB	2.46	0.44
1:B:230:ASP:CB	1:B:257:PRO:HG2	2.48	0.44
1:C:58:MET:HG3	1:C:59:VAL:N	2.32	0.44
1:C:232:PRO:HB2	1:C:233:PRO:HD3	2.00	0.44
1:D:127:ALA:HA	1:D:130:ILE:HG22	2.00	0.44
1:A:213:ILE:HA	1:A:213:ILE:HD13	1.85	0.44
1:C:100:ALA:C	1:C:102:CYS:H	2.26	0.44
1:C:231:LEU:HD22	1:C:235:ILE:HD11	1.96	0.44
1:B:189:ILE:HG21	1:B:206:ILE:CD1	2.45	0.44
1:B:266:TYR:CE1	1:B:270:ILE:HD11	2.52	0.44
1:C:168:LEU:HD21	1:C:253:TRP:HE3	1.83	0.44
1:D:54:SER:C	1:D:70:VAL:HG22	2.41	0.44
1:B:195:ASN:CB	1:C:87:ARG:HG2	2.48	0.44
1:D:60:LEU:HD13	1:D:60:LEU:O	2.17	0.44
1:A:109:TRP:C	1:A:111:LYS:H	2.25	0.44
1:B:127:ALA:HB2	1:B:233:PRO:HB3	2.00	0.44
1:B:206:ILE:O	1:B:210:VAL:HG23	2.17	0.44
1:B:221:THR:HB	1:B:253:TRP:CH2	2.53	0.44
1:C:231:LEU:CD2	1:C:235:ILE:HG13	2.47	0.44
1:A:68:LEU:O	1:A:71:ASN:N	2.51	0.44
1:A:88:ILE:HD11	1:A:190:THR:CG2	2.48	0.44
1:B:226:ASN:C	1:B:228:SER:H	2.24	0.44
1:B:256:VAL:HG12	1:B:257:PRO:HD3	2.00	0.44
1:C:148:VAL:HG22	1:C:242:TRP:CD1	2.53	0.44
1:A:42:MET:HB2	1:A:84:VAL:CG1	2.45	0.44
1:B:83:HIS:HB3	1:D:188:ALA:HB1	1.98	0.44
1:B:100:ALA:C	1:B:102:CYS:N	2.76	0.44
1:B:206:ILE:O	1:B:209:LEU:HB3	2.18	0.44
1:C:168:LEU:HA	1:C:171:GLY:HA3	2.00	0.44
1:D:55:VAL:C	1:D:57:HIS:N	2.75	0.44
1:B:45:TYR:HD1	1:B:126:ALA:HB2	1.81	0.44
1:B:68:LEU:HA	1:B:71:ASN:OD1	2.18	0.44
1:C:37:PHE:CE1	1:C:114:VAL:HB	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:37:PHE:HE1	1:C:114:VAL:HB	1.81	0.44
1:C:68:LEU:C	1:C:72:LEU:HD23	2.43	0.44
1:C:71:ASN:CB	1:C:214:GLY:HA3	2.47	0.44
1:C:157:ILE:CD1	1:C:158:PHE:HE1	2.31	0.44
1:D:127:ALA:O	1:D:130:ILE:HG22	2.18	0.44
1:A:207:GLY:O	1:A:210:VAL:N	2.51	0.43
1:A:208:ILE:O	1:A:212:ILE:HG13	2.17	0.43
1:C:252:ASN:OD1	1:C:252:ASN:N	2.50	0.43
1:C:274:VAL:CG2	1:C:275:PHE:N	2.80	0.43
1:D:212:ILE:HA	1:D:215:VAL:HG22	1.99	0.43
1:B:48:MET:HE3	1:B:228:SER:O	2.18	0.43
1:C:226:ASN:O	1:C:226:ASN:ND2	2.51	0.43
1:D:208:ILE:HG13	1:D:208:ILE:O	2.18	0.43
1:A:76:PHE:CB	1:C:212:ILE:HG13	2.47	0.43
1:D:212:ILE:HD12	1:D:212:ILE:HA	1.83	0.43
1:A:67:TYR:CD2	1:A:67:TYR:C	2.95	0.43
1:B:79:THR:HG22	1:B:203:ALA:O	2.18	0.43
1:D:113:PRO:HA	1:D:116:VAL:HB	1.99	0.43
1:D:195:ASN:H	1:D:195:ASN:ND2	2.15	0.43
1:D:230:ASP:O	1:D:234:ARG:HB2	2.18	0.43
1:A:205:VAL:O	1:A:209:LEU:N	2.51	0.43
1:A:236:PHE:O	1:A:239:ILE:N	2.46	0.43
1:B:253:TRP:C	1:B:255:TRP:N	2.76	0.43
1:C:85:ALA:HB3	1:C:91:ALA:CB	2.49	0.43
1:D:142:SER:CB	1:D:152:VAL:HG11	2.48	0.43
1:D:175:GLU:HG3	1:D:261:PRO:HG3	2.00	0.43
1:D:209:LEU:O	1:D:212:ILE:HG22	2.19	0.43
1:D:238:PHE:CD1	1:D:244:LYS:HA	2.54	0.43
1:A:58:MET:C	1:A:60:LEU:H	2.25	0.43
1:B:68:LEU:HD12	1:B:71:ASN:OD1	2.18	0.43
1:C:35:ARG:HA	1:C:38:LEU:HD13	2.00	0.43
1:D:43:SER:OG	1:D:93:MET:HG2	2.19	0.43
1:D:94:ASN:HD22	1:D:226:ASN:ND2	2.17	0.43
1:A:123:SER:OG	1:A:228:SER:O	2.31	0.43
1:B:228:SER:HA	1:B:232:PRO:CG	2.49	0.43
1:C:114:VAL:HG23	1:C:115:TYR:H	1.82	0.43
1:C:154:THR:O	1:C:157:ILE:HG12	2.18	0.43
1:A:32:LYS:HD3	1:A:32:LYS:HA	1.55	0.43
1:A:209:LEU:CG	1:D:80:MET:HE2	2.49	0.43
1:B:162:LEU:HD22	1:B:253:TRP:CE3	2.53	0.43
1:C:36:GLU:OE1	1:C:115:TYR:OH	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:231:LEU:CD2	1:C:235:ILE:CD1	2.96	0.43
1:D:81:GLY:H	1:D:84:VAL:HG23	1.84	0.43
1:B:42:MET:HE1	1:B:45:TYR:CD2	2.54	0.43
1:C:183:GLN:HB2	1:C:268:GLY:HA3	2.01	0.43
1:C:230:ASP:OD2	1:C:257:PRO:CG	2.67	0.43
1:A:208:ILE:HA	1:A:211:VAL:HG23	2.01	0.42
1:B:160:THR:O	1:B:253:TRP:CD1	2.72	0.42
1:C:52:LEU:HB2	1:C:130:ILE:HG21	2.01	0.42
1:C:55:VAL:HG13	1:C:157:ILE:HB	2.01	0.42
1:D:189:ILE:CD1	1:D:205:VAL:HG12	2.46	0.42
1:D:201:THR:HG22	1:D:201:THR:O	2.19	0.42
1:A:208:ILE:HA	1:A:211:VAL:CG2	2.49	0.42
1:A:263:LEU:O	1:A:267:LEU:HD22	2.19	0.42
1:B:37:PHE:HZ	1:B:114:VAL:C	2.27	0.42
1:A:42:MET:HE2	1:C:184:LEU:CD2	2.49	0.42
1:B:50:PHE:CZ	1:D:212:ILE:HG23	2.54	0.42
1:B:148:VAL:HA	1:B:155:ALA:HB2	2.01	0.42
1:D:175:GLU:HB3	1:D:260:ALA:HB3	2.00	0.42
1:A:71:ASN:O	1:A:211:VAL:HA	2.19	0.42
1:A:163:PRO:O	1:A:165:HIS:N	2.53	0.42
1:B:219:MET:HE2	1:B:219:MET:HB3	1.79	0.42
1:C:60:LEU:HD21	1:C:137:ALA:O	2.20	0.42
1:C:63:LYS:O	1:C:64:TYR:HD1	2.02	0.42
1:D:130:ILE:HD12	1:D:130:ILE:HA	1.90	0.42
1:D:205:VAL:HA	1:D:208:ILE:CG2	2.50	0.42
1:C:38:LEU:HD12	1:C:38:LEU:H	1.85	0.42
1:C:104:LEU:HD21	1:C:266:TYR:HE1	1.84	0.42
1:C:178:LEU:HB3	1:C:225:ILE:HG22	2.00	0.42
1:D:120:PHE:CE1	1:D:232:PRO:HD3	2.55	0.42
1:B:266:TYR:O	1:B:270:ILE:HG13	2.18	0.42
1:C:67:TYR:O	1:C:68:LEU:C	2.63	0.42
1:D:112:PHE:HB3	1:D:113:PRO:HD3	2.01	0.42
1:A:37:PHE:CD1	1:A:37:PHE:C	2.98	0.42
1:A:219:MET:CB	1:D:57:HIS:HD1	2.27	0.42
1:A:72:LEU:HB3	1:A:211:VAL:HG13	2.02	0.42
1:A:85:ALA:HB3	1:A:91:ALA:HB2	2.01	0.42
1:A:120:PHE:CD2	1:A:228:SER:HA	2.55	0.42
1:B:162:LEU:HD13	1:B:253:TRP:CZ3	2.55	0.42
1:B:223:TYR:C	1:B:225:ILE:N	2.78	0.42
1:C:71:ASN:H	1:C:71:ASN:HD22	1.68	0.42
1:A:94:ASN:C	1:A:96:ALA:H	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:227:PRO:HD3	1:B:261:PRO:HG2	2.01	0.42
1:D:36:GLU:O	1:D:115:TYR:HE1	2.02	0.42
1:D:165:HIS:CE1	1:D:166:MET:HG2	2.55	0.42
1:A:85:ALA:HB1	1:A:90:GLY:O	2.19	0.42
1:A:109:TRP:C	1:A:111:LYS:N	2.78	0.42
1:A:159:ALA:HB1	1:A:234:ARG:CZ	2.50	0.41
1:A:198:LEU:HD21	1:D:200:GLY:H	1.85	0.41
1:B:73:GLY:CA	1:D:212:ILE:HD11	2.45	0.41
1:D:58:MET:HG3	1:D:66:SER:O	2.20	0.41
1:D:117:LEU:HD23	1:D:117:LEU:HA	1.80	0.41
1:D:238:PHE:HD1	1:D:243:GLY:C	2.27	0.41
1:A:208:ILE:O	1:A:208:ILE:HG23	2.19	0.41
1:B:41:PHE:CE2	1:B:121:LEU:HB2	2.55	0.41
1:B:272:TYR:O	1:B:275:PHE:HD1	2.02	0.41
1:A:189:ILE:O	1:A:196:PRO:HB2	2.20	0.41
1:B:76:PHE:CE1	1:D:208:ILE:HG12	2.55	0.41
1:C:231:LEU:N	1:C:232:PRO:CD	2.83	0.41
1:D:76:PHE:HZ	1:D:208:ILE:HD13	1.85	0.41
1:A:179:THR:HG21	1:A:261:PRO:O	2.21	0.41
1:B:85:ALA:CB	1:B:91:ALA:HA	2.50	0.41
1:D:68:LEU:HD23	1:D:68:LEU:HA	1.90	0.41
1:D:249:ASN:C	1:D:251:GLU:H	2.28	0.41
1:C:63:LYS:HB2	1:C:63:LYS:HE2	1.67	0.41
1:C:142:SER:OG	1:C:142:SER:O	2.37	0.41
1:D:174:ASN:O	1:D:174:ASN:ND2	2.53	0.41
1:A:45:TYR:CD1	1:A:45:TYR:C	2.97	0.41
1:B:41:PHE:HA	1:B:119:GLN:OE1	2.20	0.41
1:B:128:ALA:C	1:B:130:ILE:N	2.79	0.41
1:B:250:GLY:O	1:B:251:GLU:C	2.64	0.41
1:A:44:THR:CG2	1:A:123:SER:HB3	2.50	0.41
1:A:212:ILE:HD11	1:D:76:PHE:HB3	2.01	0.41
1:B:75:GLY:HA2	1:B:78:VAL:HG12	2.02	0.41
1:C:102:CYS:SG	1:C:112:PHE:HB2	2.61	0.41
1:A:121:LEU:HD13	1:A:125:LEU:CD2	2.45	0.41
1:A:166:MET:CE	1:A:220:ASN:HB3	2.49	0.41
1:A:177:TRP:CZ3	1:D:129:THR:OG1	2.73	0.41
1:C:42:MET:O	1:C:46:VAL:N	2.46	0.41
1:C:207:GLY:O	1:C:211:VAL:HG13	2.21	0.41
1:C:234:ARG:NH1	1:C:246:VAL:O	2.53	0.41
1:A:58:MET:HG3	1:A:59:VAL:N	2.36	0.41
1:A:236:PHE:O	1:A:239:ILE:HB	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:GLU:HB3	1:B:119:GLN:CG	2.51	0.41
1:B:103:ALA:HB2	1:B:266:TYR:HD1	1.86	0.41
1:B:118:GLY:O	1:B:119:GLN:NE2	2.54	0.41
1:B:142:SER:HB2	1:B:154:THR:HG21	2.02	0.41
1:B:233:PRO:O	1:B:237:THR:HG23	2.20	0.41
1:C:33:MET:CE	1:C:111:LYS:HD2	2.41	0.41
1:C:55:VAL:HA	1:C:70:VAL:HG22	2.03	0.41
1:C:83:HIS:NE2	1:C:203:ALA:HB3	2.36	0.41
1:C:148:VAL:CG2	1:C:242:TRP:HD1	2.34	0.41
1:C:174:ASN:O	1:C:178:LEU:HG	2.21	0.41
1:C:277:GLY:O	1:C:278:SER:C	2.63	0.41
1:D:76:PHE:CZ	1:D:208:ILE:HD13	2.56	0.41
1:D:148:VAL:CG2	1:D:155:ALA:HB3	2.44	0.41
1:D:267:LEU:O	1:D:267:LEU:HD23	2.20	0.41
1:A:76:PHE:HB2	1:C:212:ILE:HG13	2.03	0.41
1:A:114:VAL:H	1:A:114:VAL:HG22	1.49	0.41
1:B:175:GLU:OE2	1:B:225:ILE:HA	2.20	0.41
1:D:50:PHE:HB3	1:D:77:GLY:HA3	2.03	0.41
1:D:96:ALA:HB2	1:D:227:PRO:CD	2.40	0.41
1:D:136:THR:OG1	1:D:136:THR:O	2.37	0.41
1:A:177:TRP:HZ3	1:D:129:THR:OG1	2.03	0.40
1:A:202:GLU:HG2	1:A:203:ALA:N	2.36	0.40
1:A:213:ILE:HD12	1:A:213:ILE:HG23	1.88	0.40
1:B:62:LYS:HA	1:B:65:GLY:O	2.20	0.40
1:B:219:MET:O	1:B:219:MET:HE3	2.21	0.40
1:C:85:ALA:O	1:C:87:ARG:N	2.54	0.40
1:C:238:PHE:HB2	1:C:246:VAL:HG21	2.03	0.40
1:A:80:MET:HG2	1:C:185:CYS:SG	2.61	0.40
1:A:160:THR:HG21	1:A:224:ALA:HB2	2.03	0.40
1:B:76:PHE:HE1	1:B:204:LEU:HD12	1.87	0.40
1:B:165:HIS:ND1	1:C:137:ALA:HA	2.37	0.40
1:B:231:LEU:HA	1:B:234:ARG:HB3	2.04	0.40
1:C:32:LYS:HG3	1:C:34:VAL:HG22	2.02	0.40
1:C:158:PHE:HE2	1:C:236:PHE:CE2	2.39	0.40
1:B:272:TYR:CE1	1:B:275:PHE:CE1	3.09	0.40
1:C:63:LYS:C	1:C:64:TYR:HD1	2.28	0.40
1:C:96:ALA:CB	1:C:227:PRO:HD2	2.39	0.40
1:C:162:LEU:HD11	1:C:250:GLY:CA	2.50	0.40
1:D:174:ASN:CG	1:D:220:ASN:HD22	2.30	0.40
1:D:226:ASN:OD1	1:D:229:ARG:HB3	2.20	0.40
1:A:60:LEU:HD22	1:C:219:MET:SD	2.61	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:ALA:HB1	1:B:266:TYR:HD1	1.86	0.40
1:C:162:LEU:HA	1:C:163:PRO:HD3	1.76	0.40
1:A:254:TRP:CD1	1:A:255:TRP:H	2.39	0.40
1:A:270:ILE:O	1:A:274:VAL:HB	2.22	0.40
1:B:96:ALA:HB2	1:B:227:PRO:HD3	2.04	0.40
1:B:124:PHE:CE1	1:B:236:PHE:HD1	2.39	0.40
1:D:232:PRO:HG2	1:D:233:PRO:HD3	2.03	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	250/342 (73%)	185 (74%)	60 (24%)	5 (2%)	6	32
1	B	247/342 (72%)	176 (71%)	66 (27%)	5 (2%)	6	32
1	C	247/342 (72%)	174 (70%)	67 (27%)	6 (2%)	4	29
1	D	247/342 (72%)	189 (76%)	55 (22%)	3 (1%)	10	40
All	All	991/1368 (72%)	724 (73%)	248 (25%)	19 (2%)	6	33

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	95	ALA
1	A	86	GLY
1	C	86	GLY
1	A	95	ALA
1	B	254	TRP
1	C	240	ALA
1	A	32	LYS
1	A	110	ARG

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Mol	Chain	Res	Type
1	B	221	THR
1	C	101	ASN
1	C	225	ILE
1	A	87	ARG
1	B	196	PRO
1	C	88	ILE
1	D	56	ALA
1	B	88	ILE
1	B	225	ILE
1	D	196	PRO
1	D	69	GLY

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	195/278 (70%)	195 (100%)	0	100	100
1	B	189/278 (68%)	189 (100%)	0	100	100
1	C	191/278 (69%)	191 (100%)	0	100	100
1	D	187/278 (67%)	186 (100%)	1 (0%)	81	80
All	All	762/1112 (68%)	761 (100%)	1 (0%)	88	88

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	60	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	145	GLN
1	B	174	ASN
1	B	220	ASN
1	B	226	ASN

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Mol	Chain	Res	Type
1	B	252	ASN
1	C	71	ASN
1	D	195	ASN
1	D	226	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 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	$\# Z > 2$
2	GOL	A	401	-	5,5,5	1.60	1 (20%)	5,5,5	0.85	0
2	GOL	C	400	-	5,5,5	1.79	2 (40%)	5,5,5	0.71	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	A	401	-	-	1/4/4/4	-
2	GOL	C	400	-	-	3/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	GOL	C3-C2	2.87	1.62	1.51
2	C	400	GOL	C3-C2	2.58	1.61	1.51
2	C	400	GOL	C1-C2	2.57	1.61	1.51

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

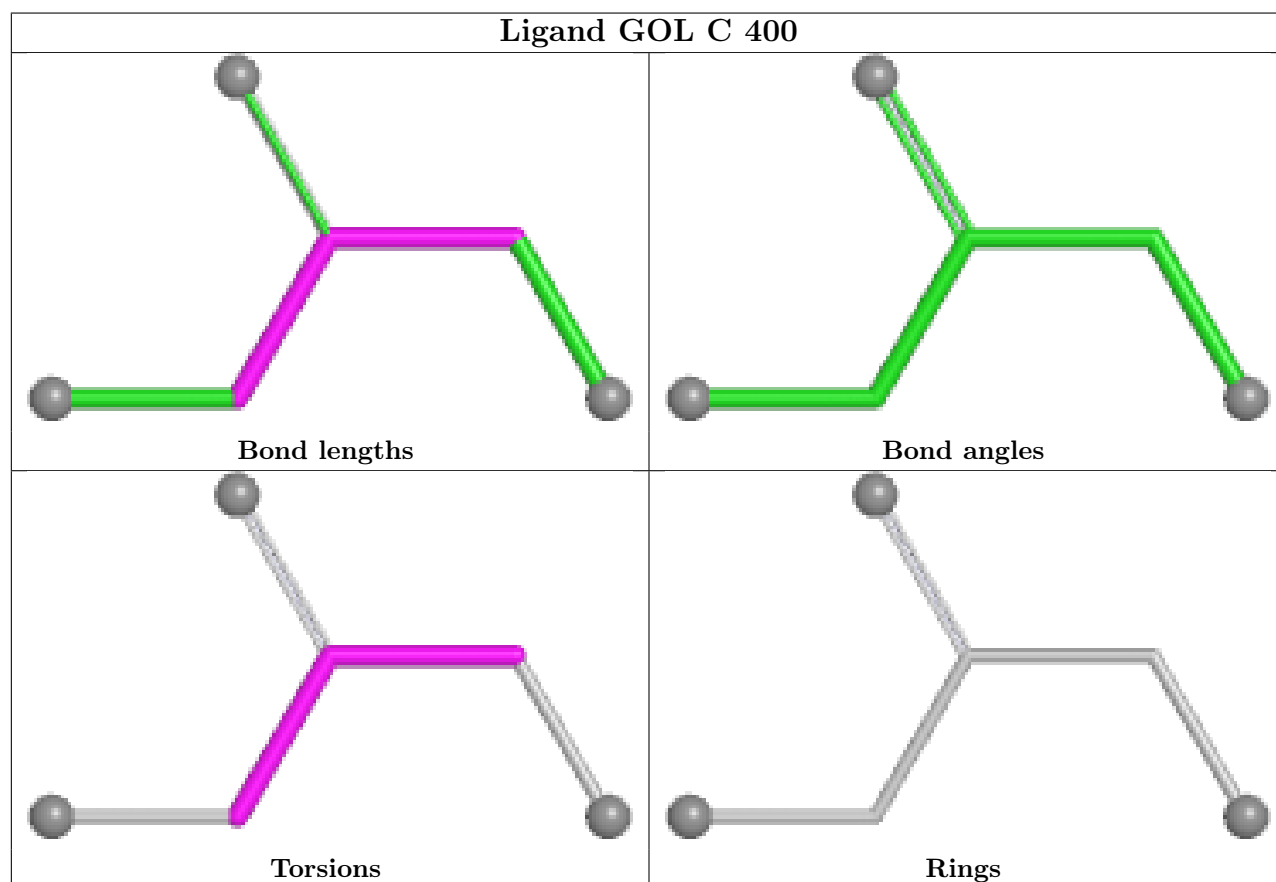
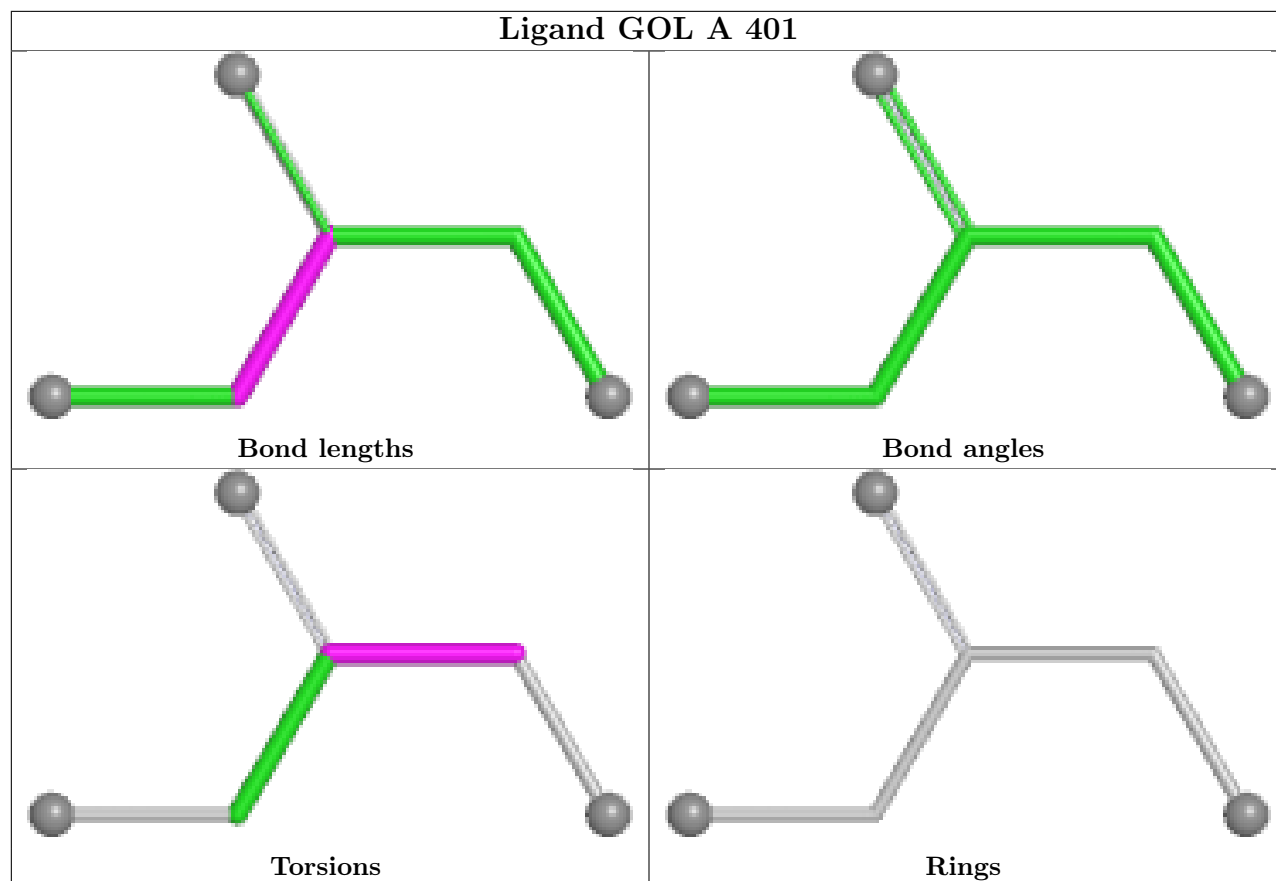
Mol	Chain	Res	Type	Atoms
2	C	400	GOL	C1-C2-C3-O3
2	C	400	GOL	O2-C2-C3-O3
2	A	401	GOL	O1-C1-C2-O2
2	C	400	GOL	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	GOL	1	0
2	C	400	GOL	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	252/342 (73%)	0.42	15 (5%) 27 19	17, 71, 132, 174	0
1	B	249/342 (72%)	1.16	41 (16%) 4 6	60, 147, 218, 244	0
1	C	249/342 (72%)	0.05	7 (2%) 55 34	8, 55, 121, 166	0
1	D	249/342 (72%)	1.22	51 (20%) 2 3	74, 153, 211, 252	0
All	All	999/1368 (73%)	0.71	114 (11%) 10 11	8, 102, 201, 252	0

All (114) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	88	ILE	9.6
1	D	101	ASN	8.3
1	D	92	HIS	8.2
1	A	89	SER	7.1
1	D	88	ILE	6.0
1	D	89	SER	5.8
1	B	88	ILE	5.7
1	B	134	PHE	5.7
1	B	132	SER	5.6
1	D	148	VAL	5.6
1	D	87	ARG	5.5
1	B	278	SER	5.3
1	D	218	GLY	5.1
1	D	91	ALA	4.7
1	D	153	ALA	4.7
1	A	86	GLY	4.7
1	D	106	ARG	4.5
1	D	86	GLY	4.3
1	D	224	ALA	4.2
1	D	220	ASN	4.2
1	D	97	VAL	4.2

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Mol	Chain	Res	Type	RSRZ
1	C	89	SER	4.1
1	B	190	THR	4.1
1	D	96	ALA	4.0
1	B	238	PHE	3.9
1	B	92	HIS	3.9
1	B	241	GLY	3.9
1	A	224	ALA	3.8
1	B	277	GLY	3.7
1	B	131	TYR	3.7
1	D	39	ALA	3.6
1	A	87	ARG	3.6
1	D	270	ILE	3.5
1	B	157	ILE	3.5
1	D	161	TYR	3.5
1	B	135	TYR	3.4
1	D	149	THR	3.4
1	B	94	ASN	3.4
1	D	200	GLY	3.4
1	B	166	MET	3.4
1	A	218	GLY	3.3
1	B	130	ILE	3.2
1	B	242	TRP	3.2
1	B	111	LYS	3.2
1	B	86	GLY	3.2
1	C	153	ALA	3.1
1	B	239	ILE	3.1
1	D	105	GLY	3.1
1	B	156	GLY	3.0
1	D	180	GLY	3.0
1	B	263	LEU	3.0
1	B	89	SER	3.0
1	A	90	GLY	2.9
1	D	266	TYR	2.9
1	D	252	ASN	2.9
1	D	90	GLY	2.8
1	D	274	VAL	2.8
1	D	95	ALA	2.8
1	D	85	ALA	2.7
1	A	249	ASN	2.7
1	D	226	ASN	2.7
1	D	178	LEU	2.7
1	A	167	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	200	GLY	2.6
1	A	263	LEU	2.6
1	D	269	GLY	2.6
1	C	88	ILE	2.6
1	B	224	ALA	2.6
1	B	133	LEU	2.5
1	B	167	THR	2.5
1	D	37	PHE	2.5
1	D	254	TRP	2.5
1	C	86	GLY	2.5
1	A	275	PHE	2.4
1	D	249	ASN	2.4
1	B	237	THR	2.4
1	B	108	PRO	2.4
1	D	278	SER	2.4
1	B	30	GLN	2.3
1	A	184	LEU	2.3
1	B	162	LEU	2.3
1	A	101	ASN	2.3
1	D	118	GLY	2.3
1	D	255	TRP	2.2
1	D	185	CYS	2.2
1	C	47	MET	2.2
1	D	94	ASN	2.2
1	D	151	PRO	2.2
1	B	99	PHE	2.2
1	B	103	ALA	2.2
1	B	114	VAL	2.2
1	A	186	LEU	2.2
1	D	135	TYR	2.2
1	D	167	THR	2.2
1	B	195	ASN	2.2
1	A	182	LEU	2.2
1	B	146	LEU	2.2
1	D	263	LEU	2.2
1	B	57	HIS	2.1
1	C	31	ARG	2.1
1	D	114	VAL	2.1
1	B	104	LEU	2.1
1	D	219	MET	2.1
1	D	267	LEU	2.1
1	B	154	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	106	ARG	2.1
1	B	62	LYS	2.1
1	B	101	ASN	2.1
1	D	107	VAL	2.1
1	B	39	ALA	2.0
1	D	93	MET	2.0
1	D	171	GLY	2.0
1	D	48	MET	2.0
1	D	82	VAL	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

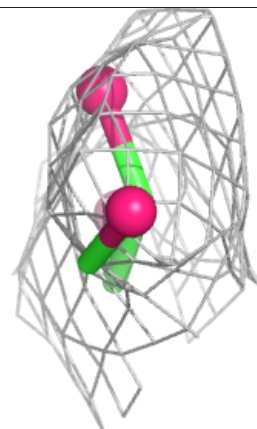
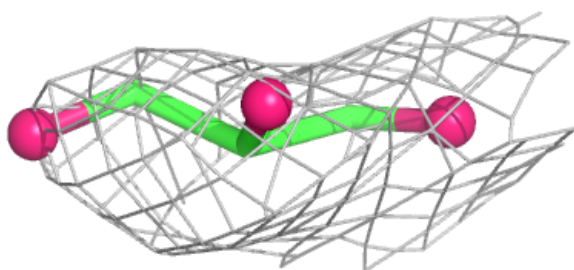
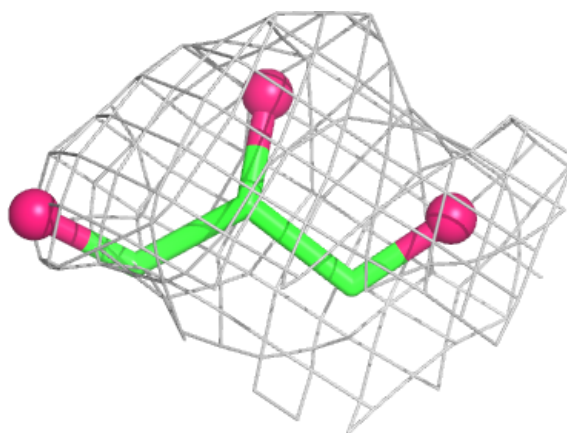
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GOL	A	401	6/6	0.89	0.15	69,73,76,82	0
2	GOL	C	400	6/6	0.94	0.19	23,29,48,54	0

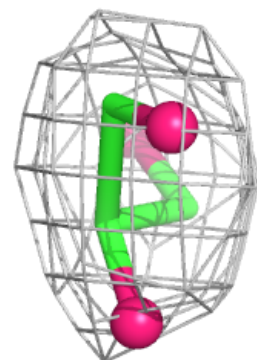
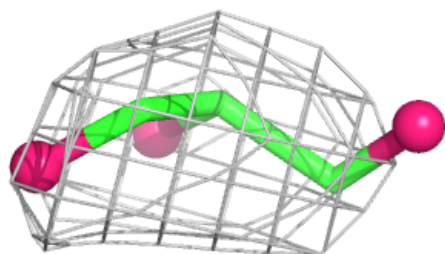
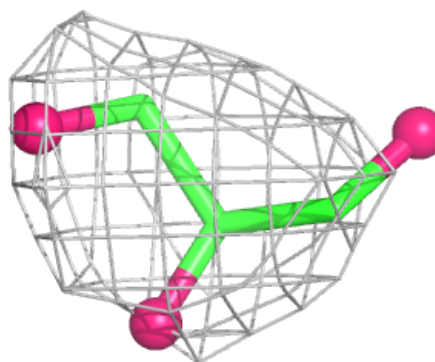
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around GOL A 401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around GOL C 400:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers

There are no such residues in this entry.