



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 10:54 am GMT

PDB ID : 1XUP
Title : ENTEROCOCCUS CASSELIFLAVUS GLYCEROL KINASE COMPLEXED
WITH GLYCEROL
Authors : Yeh, J.I.; Charrier, V.; Paulo, J.; Hou, L.; Darbon, E.; Hol, W.G.J.; Deutscher,
J.
Deposited on : 2004-10-26
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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

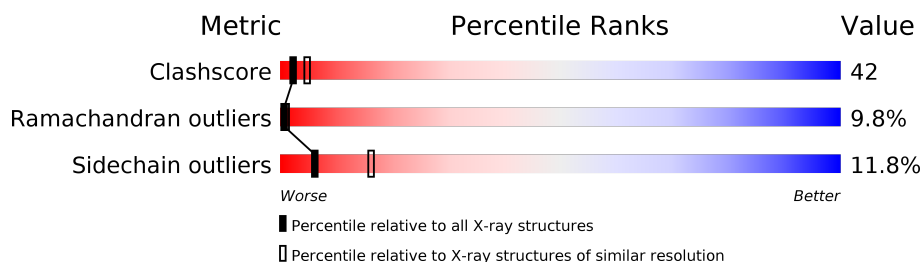
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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))
Clashscore	112137	4174 (2.80-2.72)
Ramachandran outliers	110173	4103 (2.80-2.72)
Sidechain outliers	110143	4106 (2.80-2.72)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	O	487	
1	X	487	

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
2	GOL	O	500	-	-	X	-
2	GOL	X	501	-	-	X	-

2 Entry composition [i](#)

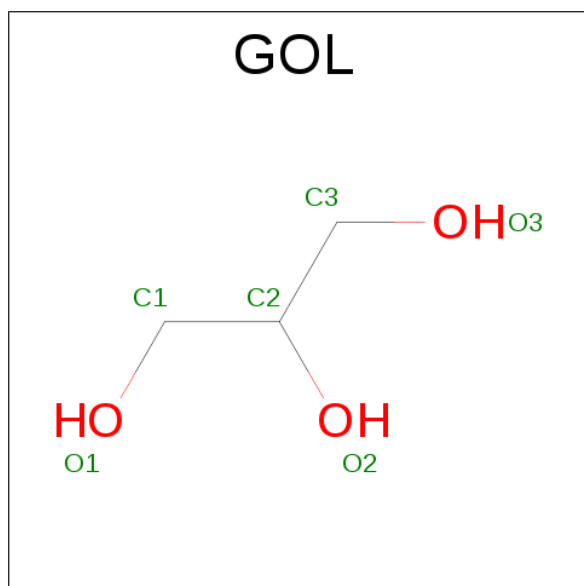
There are 2 unique types of molecules in this entry. The entry contains 7557 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Glycerol kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	O	487	Total	C	N	O	S	0	0	0
			3776	2392	629	741	14			
1	X	487	Total	C	N	O	S	0	0	0
			3769	2387	627	741	14			

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



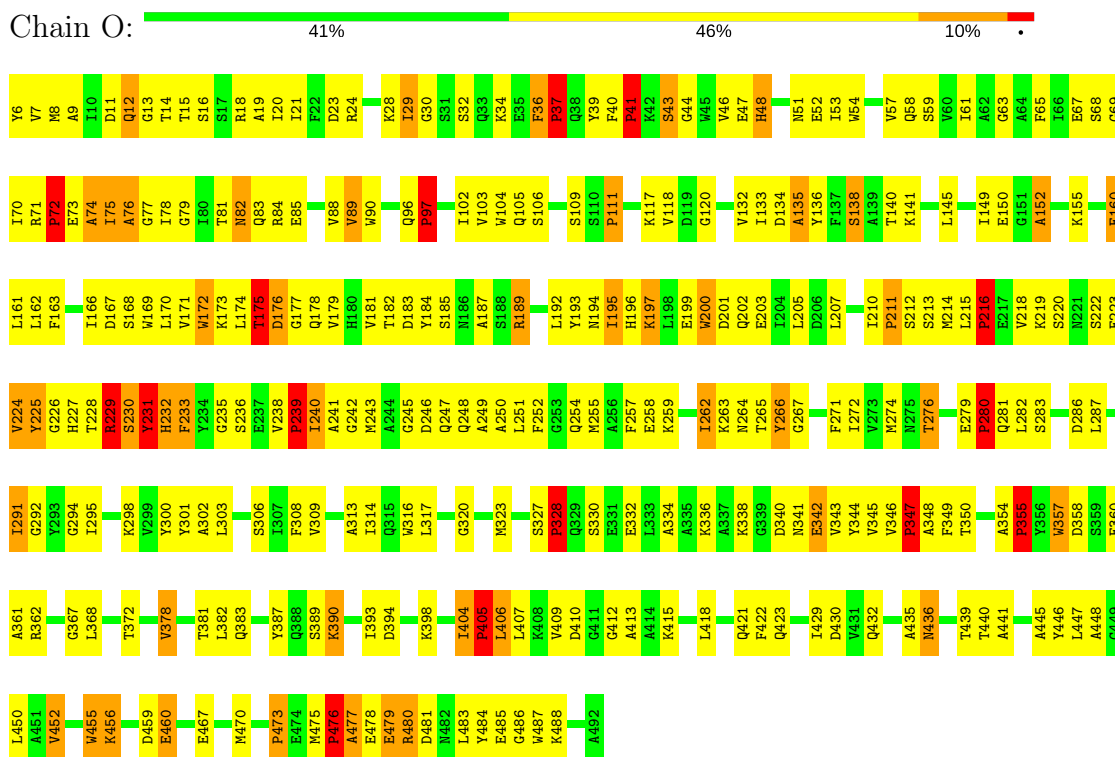
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	O	1	Total	C	O	0	0
			6	3	3		
2	X	1	Total	C	O	0	0
			6	3	3		

3 Residue-property plots

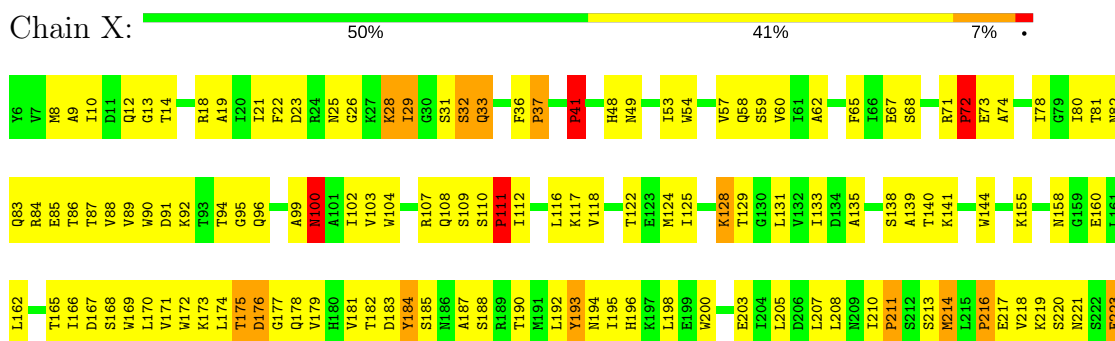
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

Note EDS was not executed.

• Molecule 1: Glycerol kinase



• Molecule 1: Glycerol kinase



V224	V225	G226	H227	T228	R229	F233	Y234	G235	S236	E237	V238	P239	I240	A241	M243	A244	G245	D246	Q247	Q248	M255	G260	M261	T262	K263	Y266	G267	T268	G269	F270	F271	T272	V273	M274	E278	E279	P280	Q281	L282	S283	D284	N285	D286	L287	L288	T289	T290	T291	G292	N296	G297	K298
V299	Y300	Y301	A302	L303	E304	F308	G311	S312	A313	I314	E325	T326	S327	P328	Q329	S330	E331	E332	L333	A334	A335	K336	A337	D340	V343	P347	A348	G354	P355	G367	T373	K374	E375	D376	F377	V378	R379	A380	Q383	A386	K390	I393	P405	L406	L407							
K408	V409	A414	D417	L418	L419	A424	D425	T426	L427	D430	T439	G443	A444	A445	Y446	L447	A448	G449	V452	G453	F454	N455	K456	D457	L458	D459	E460	L461	F471	T472	P473	E474	N475	P476	A477	R480	Q489	A492														

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	68.01Å 107.67Å 201.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.75	Depositor
% Data completeness (in resolution range)	87.0 (6.00-2.75)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	0.05	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.242 , 0.268	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7557	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

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	O	0.48	0/3855	1.08	23/5229 (0.4%)
1	X	0.43	0/3847	0.96	19/5218 (0.4%)
All	All	0.45	0/7702	1.02	42/10447 (0.4%)

There are no bond length outliers.

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	355	PRO	CA-N-CD	-18.62	85.44	111.50
1	O	405	PRO	CA-N-CD	-17.28	87.30	111.50
1	O	347	PRO	CA-N-CD	-16.64	88.20	111.50
1	O	111	PRO	CA-N-CD	-15.73	89.48	111.50
1	X	405	PRO	CA-N-CD	-14.63	91.01	111.50
1	O	280	PRO	CA-N-CD	-14.51	91.19	111.50
1	O	97	PRO	CA-N-CD	-14.22	91.58	111.50
1	X	211	PRO	CA-N-CD	-13.90	92.03	111.50
1	O	216	PRO	CA-N-CD	-13.08	93.19	111.50
1	X	72	PRO	CA-N-CD	-12.80	93.58	111.50
1	O	72	PRO	CA-N-CD	-12.75	93.65	111.50
1	O	473	PRO	CA-N-CD	-12.29	94.29	111.50
1	O	41	PRO	CA-N-CD	-12.08	94.59	111.50
1	X	239	PRO	CA-N-CD	-12.02	94.67	111.50
1	X	476	PRO	CA-N-CD	-11.86	94.90	111.50
1	X	41	PRO	CA-N-CD	-11.57	95.30	111.50
1	X	347	PRO	CA-N-CD	-11.26	95.74	111.50
1	X	37	PRO	CA-N-CD	-10.93	96.20	111.50
1	O	476	PRO	CA-N-CD	-10.64	96.61	111.50
1	X	111	PRO	CA-N-CD	-10.60	96.66	111.50
1	X	328	PRO	CA-N-CD	-10.48	96.83	111.50
1	X	216	PRO	CA-N-CD	-10.06	97.42	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	175	THR	C-N-CA	-9.36	98.31	121.70
1	O	211	PRO	CA-N-CD	-9.04	98.84	111.50
1	O	328	PRO	CA-N-CD	-8.85	99.12	111.50
1	O	37	PRO	CA-N-CD	-8.26	99.93	111.50
1	X	280	PRO	CA-N-CD	-8.21	100.01	111.50
1	X	355	PRO	CA-N-CD	-8.07	100.19	111.50
1	X	473	PRO	CA-N-CD	-7.64	100.80	111.50
1	X	33	GLN	CA-C-N	-6.95	101.92	117.20
1	X	33	GLN	CB-CA-C	5.98	122.36	110.40
1	X	32	SER	C-N-CA	-5.96	106.80	121.70
1	O	176	ASP	CA-C-N	-5.92	104.35	116.20
1	O	355	PRO	N-CD-CG	5.72	111.78	103.20
1	X	33	GLN	C-N-CA	5.58	135.64	121.70
1	O	405	PRO	N-CD-CG	5.48	111.42	103.20
1	O	355	PRO	N-CA-CB	5.35	109.72	103.30
1	X	33	GLN	O-C-N	5.27	131.13	122.70
1	O	239	PRO	CA-N-CD	-5.22	104.19	111.50
1	O	175	THR	CA-C-N	5.12	128.48	117.20
1	O	404	ILE	C-N-CD	-5.04	109.51	120.60
1	O	97	PRO	N-CD-CG	5.01	110.72	103.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	O	3776	0	3673	323	0
1	X	3769	0	3661	326	0
2	O	6	0	8	9	0
2	X	6	0	8	14	0
All	All	7557	0	7350	626	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 42.

All (626) 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:X:175:THR:HG21	1:X:179:VAL:CG1	1.41	1.50
1:X:175:THR:HB	1:X:227:HIS:CB	1.46	1.43
1:X:84:ARG:CG	2:X:501:GOL:H12	1.58	1.33
1:X:167:ASP:HA	1:X:243:MET:CE	1.60	1.31
1:X:32:SER:O	1:X:33:GLN:NE2	1.61	1.31
1:X:219:LYS:NZ	1:X:243:MET:HB3	1.47	1.30
1:O:84:ARG:CD	1:O:248:GLN:HE22	1.45	1.28
1:X:8:MET:HB3	1:X:78:ILE:CD1	1.63	1.28
1:X:167:ASP:CA	1:X:243:MET:HE1	1.63	1.27
1:O:29:ILE:CG2	1:O:67:GLU:HB2	1.66	1.24
1:X:176:ASP:HB3	1:X:235:GLY:O	1.37	1.24
1:O:177:GLY:O	1:O:228:THR:HB	1.35	1.24
1:O:84:ARG:HD2	1:O:248:GLN:NE2	1.53	1.23
1:O:175:THR:CG2	1:O:229:ARG:HG3	1.66	1.22
1:X:78:ILE:O	1:X:241:ALA:HB3	1.39	1.20
1:O:104:TRP:CZ2	2:O:500:GOL:C3	2.25	1.19
1:X:175:THR:HG21	1:X:179:VAL:HG12	1.18	1.15
1:X:8:MET:HB3	1:X:78:ILE:HD13	1.18	1.14
1:O:29:ILE:HG23	1:O:67:GLU:HB2	1.26	1.14
1:O:104:TRP:CZ2	2:O:500:GOL:H31	1.82	1.13
1:X:175:THR:HG21	1:X:179:VAL:HG11	1.21	1.09
1:X:178:GLN:HG3	1:X:229:ARG:HA	1.16	1.09
1:O:286:ASP:OD2	1:O:355:PRO:HB3	1.52	1.09
1:X:84:ARG:HG2	2:X:501:GOL:H12	1.09	1.08
1:X:227:HIS:O	1:X:237:GLU:HG3	1.50	1.08
1:O:104:TRP:CE2	2:O:500:GOL:H32	1.89	1.07
1:X:175:THR:CG2	1:X:179:VAL:CG1	2.34	1.06
1:X:78:ILE:C	1:X:241:ALA:HB3	1.77	1.05
1:X:219:LYS:HZ1	1:X:243:MET:HB3	0.88	1.04
1:O:175:THR:HG22	1:O:229:ARG:HG3	1.04	1.04
1:O:104:TRP:CZ2	2:O:500:GOL:H32	1.92	1.04
1:X:175:THR:CG2	1:X:179:VAL:HG11	1.87	1.04
1:X:175:THR:CB	1:X:227:HIS:CB	2.37	1.01
1:O:229:ARG:HD2	1:O:235:GLY:O	1.59	1.01
1:O:71:ARG:HB3	1:X:229:ARG:HH21	1.22	1.00
1:O:229:ARG:NH2	1:X:238:VAL:CB	2.24	1.00
1:O:175:THR:HG22	1:O:229:ARG:CG	1.91	1.00
1:O:229:ARG:HH22	1:X:238:VAL:CB	1.75	1.00
1:X:174:LEU:HD23	1:X:240:ILE:HD11	1.44	1.00
1:X:65:PHE:CE2	1:X:72:PRO:HD3	1.97	0.99
1:O:286:ASP:CB	1:O:355:PRO:HB3	1.93	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:23:ASP:OD1	1:O:29:ILE:HG13	1.63	0.99
1:O:177:GLY:C	1:O:228:THR:HB	1.82	0.98
1:X:176:ASP:OD2	1:X:229:ARG:HB2	1.63	0.97
1:X:178:GLN:HG3	1:X:229:ARG:CA	1.95	0.96
1:X:84:ARG:HG2	2:X:501:GOL:C1	1.95	0.96
1:X:82:ASN:ND2	1:X:243:MET:HE3	1.79	0.95
1:X:247:GLN:OE1	1:X:271:PHE:CE1	2.20	0.95
1:X:167:ASP:HA	1:X:243:MET:HE1	0.95	0.93
1:O:79:GLY:HA3	1:O:445:ALA:HA	1.51	0.93
1:O:282:LEU:HA	1:O:303:LEU:HD21	1.48	0.93
1:X:12:GLN:HE22	1:X:166:ILE:HD11	1.29	0.93
1:X:84:ARG:HG3	2:X:501:GOL:H12	1.49	0.91
1:X:219:LYS:HZ1	1:X:243:MET:CB	1.82	0.91
1:X:85:GLU:HG3	1:X:138:SER:HB2	1.52	0.91
1:O:251:LEU:HD21	1:O:292:GLY:HA2	1.50	0.91
1:X:82:ASN:OD1	1:X:243:MET:CG	2.18	0.91
1:O:104:TRP:CH2	2:O:500:GOL:H31	2.07	0.90
1:O:84:ARG:CD	1:O:248:GLN:NE2	2.23	0.90
1:O:78:ILE:HD12	1:O:240:ILE:HG12	1.52	0.89
1:X:29:ILE:HG22	1:X:29:ILE:O	1.70	0.89
1:O:286:ASP:CG	1:O:355:PRO:HB3	1.93	0.88
1:O:236:SER:H	1:X:236:SER:HA	1.39	0.88
1:X:178:GLN:HB3	1:X:228:THR:O	1.72	0.88
1:X:110:SER:HB2	1:X:111:PRO:HD2	1.55	0.87
1:O:84:ARG:HD2	1:O:248:GLN:HE22	0.73	0.87
1:X:280:PRO:HD3	1:X:301:TYR:CD2	2.09	0.87
1:X:8:MET:CB	1:X:78:ILE:HD13	2.04	0.86
1:X:155:LYS:HG3	1:X:160:GLU:OE1	1.74	0.86
1:O:71:ARG:HB3	1:X:229:ARG:NH2	1.90	0.86
1:X:104:TRP:CZ3	1:X:271:PHE:HZ	1.94	0.86
1:O:75:ILE:HD11	1:O:238:VAL:HG21	1.57	0.85
1:O:340:ASP:HB2	1:O:383:GLN:HG3	1.58	0.85
1:X:176:ASP:CB	1:X:235:GLY:O	2.23	0.85
1:X:178:GLN:CG	1:X:229:ARG:HA	2.05	0.85
1:O:236:SER:N	1:X:236:SER:HA	1.92	0.84
1:O:162:LEU:HA	1:O:214:MET:SD	2.18	0.84
1:X:86:THR:HB	1:X:166:ILE:HB	1.59	0.84
1:O:29:ILE:O	1:O:29:ILE:HG22	1.78	0.83
1:O:229:ARG:HD3	1:O:230:SER:H	1.42	0.83
1:O:90:TRP:CB	1:O:97:PRO:HG3	2.08	0.83
1:X:167:ASP:HA	1:X:243:MET:SD	2.17	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:82:ASN:OD1	1:X:243:MET:HG2	1.80	0.82
1:X:19:ALA:HB2	1:X:60:VAL:HG13	1.62	0.81
1:X:247:GLN:OE1	1:X:271:PHE:CD1	2.34	0.81
1:O:78:ILE:CD1	1:O:240:ILE:HG12	2.11	0.80
1:X:8:MET:CB	1:X:78:ILE:CD1	2.55	0.80
1:X:414:ALA:HB2	1:X:419:LEU:HD22	1.63	0.80
1:X:175:THR:CG2	1:X:179:VAL:HG12	2.07	0.80
1:O:104:TRP:CE2	2:O:500:GOL:C3	2.58	0.79
1:X:178:GLN:CG	1:X:229:ARG:HG3	2.13	0.79
1:O:229:ARG:HD3	1:O:230:SER:N	1.98	0.78
1:X:29:ILE:HD12	1:X:68:SER:OG	1.83	0.78
1:O:280:PRO:HD3	1:O:301:TYR:CG	2.19	0.78
1:X:78:ILE:O	1:X:241:ALA:CB	2.27	0.78
1:X:49:ASN:HA	1:X:100:ASN:OD1	1.83	0.78
1:X:29:ILE:HG21	1:X:67:GLU:HB3	1.66	0.78
1:X:183:ASP:OD2	1:X:244:ALA:HA	1.85	0.77
1:X:168:SER:O	1:X:171:VAL:HG22	1.84	0.77
1:X:18:ARG:CZ	1:X:33:GLN:OE1	2.32	0.77
1:O:71:ARG:CB	1:X:229:ARG:HH21	1.97	0.77
1:X:178:GLN:CB	1:X:228:THR:O	2.33	0.76
1:X:219:LYS:NZ	1:X:243:MET:CB	2.39	0.76
1:O:235:GLY:HA3	1:X:234:TYR:HD2	1.50	0.76
1:O:84:ARG:HD3	1:O:248:GLN:OE1	1.84	0.76
1:O:235:GLY:HA3	1:X:234:TYR:CD2	2.22	0.75
1:X:82:ASN:ND2	1:X:243:MET:CE	2.49	0.75
1:X:280:PRO:HG3	1:X:301:TYR:CE1	2.22	0.75
1:O:155:LYS:HB2	1:O:160:GLU:OE1	1.86	0.75
1:O:171:VAL:HG21	1:O:243:MET:SD	2.26	0.75
1:O:175:THR:HG21	1:O:236:SER:CB	2.16	0.75
1:O:28:LYS:O	1:O:29:ILE:HD13	1.86	0.75
1:O:291:ILE:H	1:O:291:ILE:HD13	1.52	0.74
1:O:286:ASP:OD2	1:O:355:PRO:CB	2.33	0.74
1:X:82:ASN:OD1	1:X:243:MET:CE	2.35	0.74
1:O:390:LYS:HE2	1:O:423:GLN:HG3	1.67	0.74
1:O:104:TRP:CE3	1:O:104:TRP:O	2.40	0.74
1:X:29:ILE:CD1	1:X:68:SER:HA	2.18	0.73
1:X:82:ASN:HD21	1:X:243:MET:HE3	1.51	0.73
1:O:29:ILE:HG23	1:O:67:GLU:CB	2.15	0.73
1:X:110:SER:HB2	1:X:111:PRO:CD	2.18	0.73
1:O:264:ASN:HB3	1:O:409:VAL:HG12	1.69	0.73
1:O:225:TYR:C	1:O:225:TYR:CD2	2.62	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:314:ILE:H	1:X:314:ILE:HD12	1.53	0.73
1:O:225:TYR:HD2	1:O:225:TYR:C	1.93	0.72
1:O:286:ASP:HB2	1:O:355:PRO:HB3	1.71	0.72
1:O:84:ARG:HG2	2:O:500:GOL:O2	1.90	0.72
1:O:280:PRO:HD3	1:O:301:TYR:CB	2.19	0.72
1:X:131:LEU:HA	1:X:288:LEU:HD22	1.72	0.72
1:O:229:ARG:HH11	1:O:236:SER:HB2	1.54	0.72
1:O:104:TRP:HE3	1:O:104:TRP:O	1.71	0.72
1:O:29:ILE:HG21	1:O:68:SER:OG	1.90	0.71
1:O:46:VAL:HB	1:O:106:SER:OG	1.91	0.71
1:O:138:SER:HA	1:O:141:LYS:HE2	1.73	0.70
1:O:175:THR:HG21	1:O:236:SER:HB2	1.73	0.70
1:X:272:ILE:N	1:X:272:ILE:HD12	2.06	0.70
1:O:28:LYS:NZ	1:O:28:LYS:HB3	2.07	0.70
1:O:78:ILE:HD12	1:O:240:ILE:CG1	2.22	0.70
1:X:285:ASN:O	1:X:286:ASP:HB2	1.91	0.70
1:O:229:ARG:CD	1:O:235:GLY:O	2.36	0.70
1:O:175:THR:HG21	1:O:229:ARG:HG3	1.68	0.70
1:X:430:ASP:OD1	1:X:473:PRO:CD	2.40	0.70
1:O:286:ASP:CB	1:O:355:PRO:CB	2.69	0.69
1:O:475:MET:HG2	1:O:476:PRO:HD3	1.73	0.69
1:O:29:ILE:HG22	1:O:67:GLU:HB2	1.69	0.69
1:X:29:ILE:CG2	1:X:67:GLU:HB3	2.23	0.69
1:O:195:ILE:O	1:O:195:ILE:HD13	1.92	0.69
1:X:178:GLN:HG2	1:X:229:ARG:HG3	1.75	0.69
1:O:283:SER:HB2	1:O:287:LEU:HB2	1.75	0.69
1:O:23:ASP:OD1	1:O:29:ILE:CG1	2.38	0.69
1:O:313:ALA:HB2	1:O:347:PRO:HG3	1.73	0.69
1:X:65:PHE:CZ	1:X:72:PRO:HD3	2.28	0.69
1:O:177:GLY:O	1:O:228:THR:CB	2.29	0.68
1:X:174:LEU:HD23	1:X:240:ILE:CD1	2.23	0.68
1:X:176:ASP:HB3	1:X:235:GLY:C	2.13	0.68
1:X:8:MET:HB3	1:X:78:ILE:HD11	1.68	0.68
1:X:9:ALA:HB2	1:X:445:ALA:HB2	1.74	0.68
1:O:236:SER:H	1:X:236:SER:CA	2.06	0.68
1:X:9:ALA:HB1	1:X:444:ALA:HB3	1.74	0.68
1:X:12:GLN:NE2	1:X:166:ILE:HD11	2.07	0.68
1:X:82:ASN:HD21	1:X:243:MET:CE	2.06	0.68
1:X:471:PHE:O	1:X:473:PRO:HD3	1.94	0.67
1:O:28:LYS:O	1:O:29:ILE:CD1	2.42	0.67
1:X:234:TYR:CD1	1:X:237:GLU:HB3	2.30	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:175:THR:HB	1:O:229:ARG:HB2	1.76	0.67
1:O:75:ILE:CD1	1:O:238:VAL:HG21	2.23	0.67
1:X:247:GLN:NE2	1:X:267:GLY:HA3	2.10	0.67
1:X:23:ASP:OD1	1:X:29:ILE:HD11	1.94	0.67
1:X:82:ASN:CG	1:X:243:MET:CE	2.63	0.66
1:X:329:GLN:HA	1:X:332:GLU:HB3	1.76	0.66
1:O:84:ARG:CD	1:O:248:GLN:OE1	2.43	0.66
1:O:179:VAL:HG13	1:O:181:VAL:HG13	1.77	0.66
1:O:262:ILE:HD13	1:O:262:ILE:H	1.60	0.66
1:X:226:GLY:HA2	1:X:240:ILE:HB	1.76	0.66
1:O:65:PHE:HD1	1:O:69:GLY:HA2	1.61	0.66
1:X:178:GLN:HG3	1:X:229:ARG:CG	2.26	0.66
1:O:54:TRP:HB2	1:O:169:TRP:HZ2	1.59	0.66
1:X:219:LYS:HZ2	1:X:243:MET:HB3	1.55	0.66
1:O:262:ILE:HG13	1:O:404:ILE:HG23	1.76	0.66
1:O:145:LEU:HD12	1:O:149:ILE:HD12	1.76	0.66
1:O:175:THR:CG2	1:O:229:ARG:CG	2.59	0.65
1:X:104:TRP:CZ3	1:X:271:PHE:CZ	2.82	0.65
1:X:82:ASN:OD1	1:X:243:MET:SD	2.53	0.65
1:X:175:THR:OG1	1:X:176:ASP:N	2.27	0.65
1:O:28:LYS:HB3	1:O:28:LYS:HZ3	1.61	0.65
1:X:95:GLY:HA2	1:X:172:TRP:HH2	1.60	0.65
1:X:178:GLN:HG3	1:X:229:ARG:CB	2.27	0.65
1:O:182:THR:HG22	1:O:183:ASP:H	1.60	0.65
1:O:291:ILE:N	1:O:291:ILE:HD13	2.12	0.65
1:X:18:ARG:NE	1:X:33:GLN:OE1	2.30	0.65
1:O:308:PHE:HD2	1:O:309:VAL:HG22	1.63	0.64
1:X:29:ILE:CD1	1:X:68:SER:CA	2.75	0.64
1:X:171:VAL:O	1:X:175:THR:HG23	1.97	0.64
1:X:129:THR:HA	1:X:195:ILE:HG22	1.80	0.64
1:X:82:ASN:OD1	1:X:243:MET:HE2	1.98	0.64
1:X:167:ASP:CB	1:X:243:MET:HE1	2.27	0.64
1:O:12:GLN:HB2	1:O:82:ASN:HA	1.80	0.63
1:O:84:ARG:O	1:O:85:GLU:HB2	1.97	0.63
1:X:449:GLY:HA3	1:X:455:TRP:CZ3	2.34	0.63
1:O:175:THR:HG21	1:O:236:SER:HB3	1.80	0.63
1:O:341:ASN:O	1:O:342:GLU:HG2	1.99	0.63
1:X:8:MET:HB3	1:X:78:ILE:CG1	2.26	0.63
1:O:78:ILE:HD12	1:O:239:PRO:O	1.99	0.63
1:X:175:THR:O	1:X:237:GLU:HA	1.99	0.62
1:O:65:PHE:CD1	1:O:69:GLY:HA2	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:296:ASN:HB3	1:X:298:LYS:NZ	2.14	0.62
1:O:378:VAL:O	1:O:381:THR:HG22	2.00	0.62
1:O:429:ILE:HG13	1:O:430:ASP:H	1.65	0.62
1:O:81:THR:HG22	1:O:246:ASP:HA	1.82	0.62
1:O:90:TRP:HB3	1:O:97:PRO:HG3	1.82	0.62
1:X:19:ALA:CB	1:X:60:VAL:HG13	2.30	0.62
1:X:18:ARG:HG2	1:X:33:GLN:HE22	1.64	0.61
1:O:176:ASP:OD1	1:O:177:GLY:N	2.33	0.61
1:O:229:ARG:CD	1:O:230:SER:H	2.11	0.61
1:O:161:LEU:HD23	1:O:161:LEU:H	1.65	0.61
1:O:184:TYR:CZ	1:O:220:SER:HA	2.35	0.61
1:X:247:GLN:OE1	1:X:271:PHE:CZ	2.53	0.61
1:O:184:TYR:CE1	1:O:220:SER:HA	2.36	0.61
1:O:436:ASN:HB3	1:O:439:THR:OG1	2.00	0.60
1:O:197:LYS:NZ	1:O:199:GLU:HB2	2.16	0.60
1:X:82:ASN:CG	1:X:243:MET:HE3	2.22	0.60
1:O:193:TYR:CE2	1:O:218:VAL:HB	2.36	0.60
1:X:78:ILE:H	1:X:241:ALA:HB2	1.65	0.60
1:O:406:LEU:HD22	1:O:432:GLN:NE2	2.17	0.60
1:O:83:GLN:HG2	1:O:166:ILE:HD12	1.84	0.60
1:X:102:ILE:HD12	1:X:102:ILE:N	2.17	0.60
1:O:72:PRO:HB2	1:X:229:ARG:NH1	2.16	0.60
1:X:32:SER:O	1:X:33:GLN:CD	2.39	0.60
1:O:330:SER:HB3	1:O:382:LEU:HD12	1.82	0.59
1:O:102:ILE:HD11	1:O:145:LEU:HD13	1.83	0.59
1:O:274:MET:CE	1:O:276:THR:HG23	2.32	0.59
1:O:104:TRP:NE1	2:O:500:GOL:H32	2.16	0.59
1:X:104:TRP:CD2	2:X:501:GOL:H32	2.37	0.59
1:X:29:ILE:CD1	1:X:68:SER:OG	2.50	0.59
1:X:57:VAL:O	1:X:60:VAL:HB	2.02	0.59
1:O:155:LYS:CB	1:O:160:GLU:OE1	2.50	0.59
1:O:70:ILE:HG21	1:O:74:ALA:HB3	1.85	0.59
1:O:14:THR:O	1:O:83:GLN:NE2	2.36	0.59
1:X:167:ASP:CG	1:X:243:MET:HE1	2.22	0.59
1:O:475:MET:HB3	1:O:476:PRO:HD2	1.85	0.58
1:X:340:ASP:HB2	1:X:383:GLN:HG3	1.85	0.58
1:X:234:TYR:OH	1:X:239:PRO:HD2	2.02	0.58
1:O:79:GLY:HA3	1:O:445:ALA:CA	2.30	0.58
1:X:266:TYR:CE1	1:X:409:VAL:HG21	2.38	0.58
1:X:18:ARG:CD	1:X:33:GLN:HE22	2.15	0.58
1:X:172:TRP:HA	1:X:179:VAL:CG1	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:166:ILE:HG12	1:O:170:LEU:HD23	1.84	0.58
1:O:456:LYS:H	1:O:456:LYS:HD3	1.68	0.58
1:O:79:GLY:CA	1:O:445:ALA:HA	2.31	0.58
1:O:72:PRO:CD	1:X:229:ARG:HH22	2.17	0.58
1:X:335:ALA:HA	1:X:379:ARG:HH11	1.68	0.58
1:O:90:TRP:CA	1:O:97:PRO:HG3	2.34	0.58
1:O:231:TYR:O	1:O:232:HIS:HB3	2.03	0.57
1:O:46:VAL:O	1:O:103:VAL:HG22	2.04	0.57
1:O:84:ARG:HH11	1:O:84:ARG:HG3	1.69	0.57
1:O:257:PHE:HA	1:O:294:GLY:HA2	1.86	0.57
1:O:382:LEU:HD22	1:O:383:GLN:HE21	1.69	0.57
1:X:95:GLY:HA2	1:X:172:TRP:CH2	2.39	0.57
1:O:267:GLY:HA2	1:O:413:ALA:HB3	1.87	0.57
1:X:220:SER:C	1:X:221:ASN:HD22	2.08	0.57
1:O:228:THR:HG22	1:O:228:THR:O	2.04	0.57
1:O:407:LEU:H	1:O:407:LEU:HD23	1.70	0.57
1:O:90:TRP:HA	1:O:97:PRO:HG3	1.86	0.57
1:X:65:PHE:CD2	1:X:72:PRO:HD3	2.39	0.57
1:O:286:ASP:HB2	1:O:355:PRO:CB	2.34	0.56
1:O:340:ASP:HB2	1:O:383:GLN:CG	2.32	0.56
1:X:23:ASP:OD1	1:X:29:ILE:CD1	2.52	0.56
1:X:33:GLN:HA	1:X:33:GLN:NE2	2.20	0.56
1:O:327:SER:OG	1:O:328:PRO:HD2	2.05	0.56
1:X:285:ASN:O	1:X:286:ASP:CB	2.53	0.56
1:O:193:TYR:OH	1:O:218:VAL:HB	2.05	0.56
1:O:327:SER:OG	1:O:328:PRO:CD	2.54	0.56
1:O:54:TRP:HB2	1:O:169:TRP:CZ2	2.40	0.56
1:O:171:VAL:CG2	1:O:243:MET:SD	2.93	0.56
1:X:430:ASP:OD1	1:X:473:PRO:CG	2.53	0.56
1:O:229:ARG:HD3	1:O:230:SER:HA	1.88	0.56
1:O:84:ARG:NE	1:O:248:GLN:NE2	2.54	0.56
1:O:90:TRP:O	1:O:161:LEU:HA	2.05	0.56
1:X:158:ASN:OD1	1:X:160:GLU:HG3	2.05	0.55
1:X:224:VAL:HA	1:X:240:ILE:O	2.06	0.55
1:X:23:ASP:OD1	1:X:29:ILE:HG13	2.05	0.55
1:X:335:ALA:HA	1:X:379:ARG:NH1	2.21	0.55
1:X:240:ILE:CG2	1:X:241:ALA:N	2.70	0.55
1:X:48:HIS:HB3	1:X:103:VAL:HG13	1.89	0.55
1:O:53:ILE:O	1:O:57:VAL:HG23	2.06	0.55
1:X:28:LYS:N	1:X:28:LYS:HD3	2.21	0.55
1:O:29:ILE:HG21	1:O:68:SER:H	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:286:ASP:HB3	1:O:355:PRO:HA	1.88	0.55
1:X:280:PRO:HD3	1:X:301:TYR:CG	2.42	0.55
1:X:29:ILE:HD11	1:X:68:SER:HA	1.89	0.55
1:X:292:GLY:O	1:X:300:TYR:HB2	2.06	0.54
1:O:231:TYR:O	1:O:232:HIS:CB	2.56	0.54
1:O:79:GLY:HA2	1:O:241:ALA:O	2.07	0.54
1:X:235:GLY:O	1:X:236:SER:HB2	2.08	0.54
1:X:23:ASP:OD1	1:X:29:ILE:CG1	2.55	0.54
1:X:21:ILE:HG21	1:X:67:GLU:HB2	1.90	0.54
1:X:424:ALA:HB1	1:X:430:ASP:HA	1.90	0.54
1:O:168:SER:O	1:O:172:TRP:HB2	2.08	0.54
1:O:58:GLN:CG	1:X:59:SER:HA	2.36	0.54
1:O:227:HIS:NE2	1:O:240:ILE:HD12	2.22	0.54
1:O:75:ILE:HG13	1:O:76:ALA:H	1.72	0.54
1:O:84:ARG:NE	1:O:248:GLN:HE22	1.98	0.54
1:X:110:SER:CB	1:X:111:PRO:CD	2.86	0.54
1:X:28:LYS:HD3	1:X:28:LYS:H	1.73	0.54
1:X:71:ARG:O	1:X:73:GLU:N	2.39	0.54
1:O:210:ILE:HD12	1:O:213:SER:OG	2.08	0.54
1:O:78:ILE:HB	1:O:240:ILE:HA	1.89	0.54
1:X:326:THR:O	1:X:328:PRO:N	2.41	0.54
1:X:333:LEU:HA	1:X:336:LYS:HE3	1.90	0.54
1:X:443:GLY:O	1:X:447:LEU:HG	2.08	0.54
1:O:20:ILE:HD11	1:O:28:LYS:HZ3	1.72	0.54
1:O:224:VAL:HG22	1:O:447:LEU:O	2.08	0.53
1:X:172:TRP:HD1	1:X:179:VAL:O	1.91	0.53
1:X:234:TYR:CG	1:X:237:GLU:HB3	2.43	0.53
1:X:104:TRP:HZ3	1:X:271:PHE:HZ	1.53	0.53
1:X:18:ARG:CG	1:X:33:GLN:HE22	2.20	0.53
1:O:456:LYS:HE3	1:O:460:GLU:OE2	2.08	0.53
1:O:39:TYR:O	1:O:46:VAL:HG13	2.08	0.53
1:O:28:LYS:O	1:O:29:ILE:CG1	2.57	0.53
1:X:139:ALA:HB1	1:X:192:LEU:HD13	1.90	0.53
1:X:195:ILE:O	1:X:198:LEU:HD12	2.08	0.53
1:X:408:LYS:NZ	1:X:408:LYS:HB3	2.23	0.53
1:X:128:LYS:HB3	1:X:194:ASN:HD21	1.73	0.53
1:X:272:ILE:HG12	1:X:393:ILE:HG12	1.91	0.53
1:O:178:GLN:HG3	1:O:179:VAL:H	1.74	0.53
1:X:168:SER:O	1:X:171:VAL:CG2	2.55	0.53
1:X:243:MET:HG2	1:X:244:ALA:N	2.24	0.53
1:O:83:GLN:HG2	1:O:166:ILE:CD1	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:197:LYS:HZ2	1:O:199:GLU:HB2	1.73	0.53
1:O:344:TYR:HE2	1:O:486:GLY:HA3	1.74	0.53
1:O:185:SER:HB3	1:O:248:GLN:HG2	1.91	0.52
1:X:176:ASP:OD2	1:X:234:TYR:O	2.27	0.52
1:X:425:ASP:HB3	1:X:477:ALA:HB2	1.91	0.52
1:O:485:GLU:HG2	1:O:488:LYS:HE2	1.91	0.52
1:O:6:TYR:CD2	1:O:21:ILE:HD11	2.44	0.52
1:X:117:LYS:HG3	1:X:118:VAL:HG13	1.91	0.52
1:X:475:MET:HB2	1:X:476:PRO:HD2	1.91	0.52
1:O:225:TYR:CD2	1:O:226:GLY:O	2.62	0.52
1:O:229:ARG:HD3	1:O:230:SER:CA	2.39	0.52
1:X:255:MET:O	1:X:261:MET:SD	2.68	0.52
1:O:29:ILE:O	1:O:29:ILE:CG2	2.51	0.52
1:X:280:PRO:HD3	1:X:301:TYR:CE2	2.44	0.52
1:X:452:VAL:HG12	1:X:452:VAL:O	2.09	0.52
1:O:197:LYS:O	1:O:199:GLU:HG3	2.09	0.52
1:X:128:LYS:HB3	1:X:194:ASN:ND2	2.24	0.52
1:O:72:PRO:N	1:X:229:ARG:NH2	2.58	0.52
1:O:286:ASP:HB2	1:O:355:PRO:HG3	1.92	0.52
1:X:190:THR:HB	1:X:193:TYR:HB2	1.91	0.52
1:O:314:ILE:HG12	1:O:381:THR:HG21	1.91	0.52
1:X:104:TRP:CE3	2:X:501:GOL:H31	2.45	0.52
1:O:134:ASP:O	1:O:136:TYR:N	2.43	0.52
1:O:28:LYS:O	1:O:29:ILE:HG12	2.10	0.52
1:X:29:ILE:HD13	1:X:68:SER:HA	1.91	0.52
1:X:175:THR:O	1:X:237:GLU:CA	2.58	0.52
1:O:229:ARG:HH11	1:O:236:SER:CB	2.21	0.51
1:O:196:HIS:CE1	1:O:280:PRO:HB2	2.46	0.51
1:O:84:ARG:NH1	1:O:189:ARG:HG2	2.25	0.51
1:O:11:ASP:HA	1:O:81:THR:HB	1.93	0.51
1:O:84:ARG:NH1	1:O:84:ARG:HG3	2.25	0.51
1:O:9:ALA:O	1:O:19:ALA:HB1	2.11	0.51
1:X:112:ILE:N	1:X:112:ILE:HD12	2.25	0.51
1:X:90:TRP:HH2	1:X:168:SER:HB2	1.74	0.51
1:X:183:ASP:HB3	1:X:219:LYS:HE2	1.92	0.51
1:X:223:GLU:HG2	1:X:224:VAL:N	2.26	0.51
1:O:230:SER:HB3	1:O:233:PHE:O	2.11	0.51
1:O:272:ILE:HD12	1:O:272:ILE:N	2.26	0.51
1:O:29:ILE:CG2	1:O:68:SER:H	2.24	0.51
1:O:40:PHE:HA	1:O:46:VAL:HG22	1.92	0.51
1:O:47:GLU:HA	1:O:103:VAL:HG13	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:185:SER:HA	1:O:291:ILE:HD11	1.92	0.51
1:O:432:GLN:HB3	1:O:470:MET:HG2	1.93	0.50
1:X:54:TRP:CZ2	1:X:173:LYS:HB2	2.46	0.50
1:O:233:PHE:N	1:O:233:PHE:CD1	2.79	0.50
1:O:223:GLU:OE1	1:O:242:GLY:O	2.28	0.50
1:O:84:ARG:CD	1:O:248:GLN:CD	2.79	0.50
1:O:72:PRO:HB2	1:X:229:ARG:HH12	1.76	0.50
1:X:343:VAL:HA	1:X:367:GLY:O	2.11	0.50
1:O:18:ARG:O	1:O:19:ALA:HB3	2.11	0.50
1:O:235:GLY:HA2	1:X:236:SER:H	1.75	0.50
1:X:217:GLU:OE1	1:X:225:TYR:OH	2.30	0.50
1:O:262:ILE:N	1:O:262:ILE:HD13	2.26	0.50
1:O:265:THR:HG23	1:O:410:ASP:O	2.11	0.50
1:O:58:GLN:HG2	1:X:59:SER:HA	1.93	0.50
1:X:141:LYS:O	1:X:144:TRP:HB3	2.11	0.50
1:X:226:GLY:O	1:X:227:HIS:CB	2.59	0.50
1:O:274:MET:HE2	1:O:276:THR:HG23	1.93	0.50
1:X:90:TRP:CH2	1:X:168:SER:HB2	2.47	0.50
1:X:455:TRP:CD1	1:X:461:LEU:HD11	2.47	0.50
1:X:58:GLN:OE1	1:X:58:GLN:HA	2.11	0.50
1:O:187:ALA:HB1	1:O:193:TYR:CG	2.47	0.50
1:X:18:ARG:HD3	1:X:33:GLN:NE2	2.26	0.50
1:X:181:VAL:HB	1:X:219:LYS:HD3	1.93	0.50
1:X:273:VAL:HG23	1:X:304:GLU:HB2	1.94	0.50
1:X:414:ALA:CB	1:X:419:LEU:HD22	2.37	0.50
1:X:54:TRP:CZ3	1:X:170:LEU:HA	2.47	0.50
1:O:29:ILE:HG21	1:O:68:SER:N	2.27	0.50
1:O:72:PRO:N	1:X:229:ARG:HH22	2.10	0.50
1:X:167:ASP:N	1:X:243:MET:HE1	2.21	0.50
1:X:308:PHE:H	1:X:308:PHE:HD1	1.59	0.50
1:X:224:VAL:HA	1:X:241:ALA:HA	1.94	0.49
1:X:174:LEU:CD2	1:X:240:ILE:HD11	2.31	0.49
1:X:175:THR:OG1	1:X:177:GLY:N	2.45	0.49
1:X:171:VAL:HG23	1:X:172:TRP:N	2.27	0.49
1:X:192:LEU:O	1:X:200:TRP:HA	2.12	0.49
1:X:234:TYR:O	1:X:237:GLU:HB2	2.12	0.49
1:O:346:VAL:O	1:O:348:ALA:N	2.45	0.49
1:O:192:LEU:CA	1:O:205:LEU:HD21	2.43	0.49
1:O:214:MET:O	1:O:216:PRO:HD2	2.13	0.49
1:O:266:TYR:HE2	1:O:423:GLN:HE22	1.61	0.49
1:X:220:SER:C	1:X:221:ASN:ND2	2.66	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:234:TYR:C	1:X:237:GLU:HB2	2.33	0.49
1:O:173:LYS:HG3	1:X:71:ARG:HG3	1.95	0.49
1:O:196:HIS:CE1	1:O:280:PRO:CB	2.96	0.49
1:O:196:HIS:HE1	1:O:280:PRO:HB2	1.78	0.49
1:O:229:ARG:CG	1:O:230:SER:N	2.74	0.49
1:O:345:VAL:O	1:O:347:PRO:CD	2.61	0.49
1:X:280:PRO:HG3	1:X:301:TYR:CD1	2.48	0.48
1:O:298:LYS:HG3	1:O:300:TYR:HE1	1.78	0.48
1:X:18:ARG:CD	1:X:33:GLN:NE2	2.76	0.48
1:X:176:ASP:OD2	1:X:235:GLY:HA3	2.13	0.48
1:O:59:SER:O	1:O:63:GLY:HA3	2.14	0.48
1:X:198:LEU:HD21	1:X:299:VAL:HG11	1.95	0.48
1:X:184:TYR:O	1:X:291:ILE:HD12	2.13	0.48
1:O:279:GLU:O	1:O:281:GLN:N	2.46	0.48
1:O:280:PRO:HD3	1:O:301:TYR:CD2	2.48	0.48
1:O:274:MET:HE1	1:O:276:THR:HG23	1.94	0.48
1:O:286:ASP:HB3	1:O:355:PRO:CA	2.43	0.48
1:O:298:LYS:HG3	1:O:300:TYR:CE1	2.48	0.48
1:X:171:VAL:O	1:X:175:THR:CG2	2.59	0.48
1:X:240:ILE:HG23	1:X:241:ALA:N	2.29	0.48
1:X:183:ASP:HB3	1:X:219:LYS:CE	2.43	0.48
1:O:224:VAL:HG22	1:O:448:ALA:HA	1.95	0.48
1:O:240:ILE:HG22	1:O:241:ALA:N	2.28	0.47
1:O:389:SER:O	1:O:393:ILE:HG12	2.13	0.47
1:X:19:ALA:HB2	1:X:60:VAL:HG22	1.97	0.47
1:X:205:LEU:HB3	1:X:210:ILE:HB	1.96	0.47
1:X:29:ILE:O	1:X:29:ILE:CG2	2.44	0.47
1:O:229:ARG:CD	1:O:230:SER:N	2.70	0.47
1:O:73:GLU:HG2	1:O:73:GLU:O	2.14	0.47
1:O:235:GLY:CA	1:X:234:TYR:HD2	2.23	0.47
1:X:84:ARG:HG2	2:X:501:GOL:O2	2.12	0.47
1:X:10:ILE:HG21	1:X:60:VAL:CG1	2.43	0.47
1:O:9:ALA:HA	1:O:445:ALA:HB2	1.96	0.47
1:O:20:ILE:HG21	1:O:30:GLY:HA3	1.96	0.47
1:O:192:LEU:HA	1:O:205:LEU:HD21	1.95	0.47
1:O:316:TRP:HB2	1:O:349:PHE:HZ	1.79	0.47
1:X:176:ASP:HB2	1:X:229:ARG:CZ	2.44	0.47
1:X:84:ARG:HG2	2:X:501:GOL:C2	2.43	0.47
1:X:8:MET:CB	1:X:78:ILE:HD11	2.39	0.47
1:X:181:VAL:CG2	1:X:219:LYS:HD3	2.45	0.47
1:X:247:GLN:HE21	1:X:267:GLY:HA3	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:264:ASN:O	1:O:409:VAL:HA	2.15	0.47
1:O:192:LEU:O	1:O:205:LEU:HD21	2.15	0.46
1:O:452:VAL:HG22	1:O:452:VAL:O	2.15	0.46
1:X:272:ILE:N	1:X:272:ILE:CD1	2.74	0.46
1:X:296:ASN:HB3	1:X:298:LYS:HZ3	1.79	0.46
1:O:227:HIS:HB3	1:O:228:THR:H	1.47	0.46
1:O:82:ASN:HB2	1:O:166:ILE:HD13	1.97	0.46
1:X:314:ILE:HG13	1:X:330:SER:OG	2.16	0.46
1:O:195:ILE:HD13	1:O:195:ILE:C	2.35	0.46
1:O:201:ASP:O	1:O:205:LEU:HD13	2.15	0.46
1:O:193:TYR:CZ	1:O:218:VAL:HB	2.51	0.46
1:O:44:GLY:O	1:O:106:SER:HB3	2.15	0.46
1:X:53:ILE:O	1:X:57:VAL:HG23	2.16	0.46
1:O:18:ARG:HA	1:O:32:SER:O	2.15	0.46
1:X:224:VAL:HG13	1:X:225:TYR:N	2.31	0.46
1:O:485:GLU:O	1:O:488:LYS:HG2	2.15	0.46
1:O:266:TYR:HE2	1:O:423:GLN:NE2	2.13	0.46
1:O:72:PRO:HA	1:O:75:ILE:HG12	1.98	0.46
1:X:104:TRP:CB	2:X:501:GOL:H11	2.45	0.46
1:O:193:TYR:O	1:O:194:ASN:HB2	2.16	0.46
1:O:28:LYS:C	1:O:29:ILE:HG12	2.36	0.46
1:O:343:VAL:HA	1:O:367:GLY:HA3	1.96	0.46
1:X:296:ASN:HB3	1:X:298:LYS:HZ2	1.77	0.46
1:X:78:ILE:N	1:X:241:ALA:CB	2.78	0.46
1:O:387:TYR:HB3	1:O:487:TRP:HZ2	1.80	0.46
1:X:287:LEU:HD22	1:X:287:LEU:H	1.80	0.46
1:O:8:MET:HB2	1:O:78:ILE:HA	1.97	0.46
1:X:178:GLN:HB2	1:X:228:THR:O	2.15	0.46
1:X:104:TRP:CD2	2:X:501:GOL:C3	2.99	0.46
1:O:233:PHE:HB2	1:X:234:TYR:CD2	2.50	0.45
1:X:175:THR:HG21	1:X:179:VAL:CB	2.35	0.45
1:X:455:TRP:HB3	1:X:461:LEU:HD21	1.97	0.45
1:O:456:LYS:NZ	1:O:460:GLU:CD	2.70	0.45
1:O:238:VAL:O	1:O:239:PRO:O	2.34	0.45
1:O:429:ILE:HG13	1:O:430:ASP:N	2.29	0.45
1:O:152:ALA:HB1	1:O:155:LYS:HD2	1.98	0.45
1:O:258:GLU:HG2	1:O:259:LYS:H	1.81	0.45
1:X:171:VAL:HG21	1:X:181:VAL:HG22	1.98	0.45
1:X:188:SER:OG	1:X:290:THR:HA	2.16	0.45
1:X:62:ALA:O	1:X:65:PHE:HD1	2.00	0.45
1:O:475:MET:CB	1:O:476:PRO:CD	2.95	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:247:GLN:HE21	1:O:271:PHE:HB2	1.81	0.45
1:O:34:LYS:HB2	1:O:34:LYS:NZ	2.31	0.45
1:O:8:MET:SD	1:O:21:ILE:HB	2.57	0.45
1:O:286:ASP:HB2	1:O:355:PRO:CG	2.47	0.45
1:O:90:TRP:HB2	1:O:97:PRO:HG3	1.97	0.45
1:X:234:TYR:CA	1:X:237:GLU:HB2	2.47	0.45
1:X:89:VAL:HG13	1:X:162:LEU:O	2.17	0.45
1:X:185:SER:HB3	1:X:248:GLN:OE1	2.16	0.45
1:O:263:LYS:HD2	1:O:264:ASN:N	2.31	0.44
1:O:48:HIS:ND1	1:O:48:HIS:O	2.50	0.44
1:O:9:ALA:HB1	1:O:441:ALA:HB1	1.98	0.44
1:X:81:THR:HB	1:X:246:ASP:HB3	1.99	0.44
1:O:13:GLY:O	1:O:83:GLN:HB3	2.18	0.44
1:O:254:GLN:HE21	1:O:263:LYS:HD3	1.82	0.44
1:O:88:VAL:HG12	1:O:89:VAL:N	2.33	0.44
1:X:208:LEU:N	1:X:208:LEU:HD22	2.32	0.44
1:X:262:ILE:HG22	1:X:263:LYS:N	2.32	0.44
1:O:247:GLN:HG3	1:O:271:PHE:CD1	2.53	0.44
1:O:481:ASP:O	1:O:484:TYR:HB3	2.18	0.44
1:X:234:TYR:CZ	1:X:239:PRO:HD2	2.53	0.44
1:O:357:TRP:O	1:O:358:ASP:HB2	2.17	0.44
1:X:430:ASP:OD1	1:X:473:PRO:HD3	2.16	0.44
1:O:167:ASP:O	1:O:171:VAL:HG23	2.16	0.44
1:O:250:ALA:HB2	1:O:440:THR:HG23	2.00	0.44
1:O:344:TYR:OH	1:O:483:LEU:HB3	2.17	0.44
1:X:193:TYR:OH	1:X:218:VAL:HG22	2.18	0.44
1:X:336:LYS:HG3	1:X:337:ALA:H	1.83	0.44
1:O:7:VAL:CG2	1:O:455:TRP:HH2	2.31	0.44
1:X:131:LEU:HD22	1:X:288:LEU:HD13	1.98	0.44
1:X:393:ILE:HG21	1:X:407:LEU:HD21	1.99	0.44
1:O:182:THR:HG22	1:O:183:ASP:N	2.30	0.44
1:O:446:TYR:O	1:O:450:LEU:HD13	2.17	0.44
1:O:456:LYS:HB2	1:O:456:LYS:NZ	2.33	0.44
1:X:280:PRO:CD	1:X:301:TYR:CE2	3.01	0.44
1:X:326:THR:O	1:X:327:SER:C	2.57	0.43
1:X:78:ILE:H	1:X:241:ALA:CB	2.30	0.43
1:O:382:LEU:HD23	1:O:382:LEU:C	2.39	0.43
1:X:29:ILE:HD13	1:X:67:GLU:C	2.38	0.43
1:O:249:ALA:HA	1:O:252:PHE:CE2	2.53	0.43
1:O:36:PHE:HD2	1:O:52:GLU:HG3	1.84	0.43
1:X:174:LEU:O	1:X:237:GLU:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:80:ILE:HB	1:X:243:MET:HA	1.99	0.43
1:O:479:GLU:O	1:O:481:ASP:N	2.51	0.43
1:X:172:TRP:HA	1:X:179:VAL:HG12	2.00	0.43
1:X:325:GLU:HG3	1:X:326:THR:N	2.34	0.43
1:O:200:TRP:CZ3	1:O:212:SER:HB3	2.53	0.43
1:O:368:LEU:H	1:O:368:LEU:HD22	1.83	0.43
1:X:18:ARG:HD3	1:X:31:SER:HB3	2.00	0.43
1:O:14:THR:HG21	1:O:105:GLN:NE2	2.33	0.43
1:X:475:MET:O	1:X:477:ALA:N	2.50	0.43
1:O:171:VAL:HG11	1:O:225:TYR:OH	2.18	0.43
1:O:276:THR:OG1	1:O:302:ALA:HA	2.19	0.43
1:O:36:PHE:CD2	1:O:52:GLU:HG3	2.54	0.43
1:X:104:TRP:CZ3	2:X:501:GOL:H31	2.53	0.43
1:X:78:ILE:N	1:X:241:ALA:HB2	2.31	0.42
1:X:425:ASP:HB3	1:X:477:ALA:CB	2.49	0.42
1:O:263:LYS:O	1:O:272:ILE:HG23	2.19	0.42
1:X:104:TRP:CE2	2:X:501:GOL:H32	2.55	0.42
1:X:83:GLN:O	1:X:166:ILE:HG21	2.18	0.42
1:X:390:LYS:HE2	1:X:427:LEU:HD13	2.01	0.42
1:O:394:ASP:O	1:O:398:LYS:HG2	2.20	0.42
1:X:167:ASP:OD2	1:X:243:MET:CE	2.68	0.42
1:X:19:ALA:HB2	1:X:60:VAL:CG1	2.43	0.42
1:O:135:ALA:O	1:O:140:THR:HB	2.18	0.42
1:O:163:PHE:CE2	1:O:214:MET:HB2	2.55	0.42
1:X:22:PHE:CD1	1:X:22:PHE:N	2.88	0.42
1:X:84:ARG:HG3	2:X:501:GOL:C1	2.35	0.42
1:X:110:SER:OG	1:X:135:ALA:HB2	2.20	0.42
1:X:221:ASN:ND2	1:X:221:ASN:N	2.67	0.42
1:X:13:GLY:HA2	1:X:53:ILE:HG12	2.02	0.42
1:X:102:ILE:CD1	1:X:102:ILE:N	2.82	0.42
1:O:240:ILE:CG2	1:O:241:ALA:N	2.83	0.42
1:X:133:ILE:H	1:X:133:ILE:HD12	1.85	0.42
1:X:234:TYR:CB	1:X:237:GLU:HB3	2.50	0.42
1:X:271:PHE:C	1:X:272:ILE:HD12	2.40	0.42
1:X:91:ASP:HB2	1:X:94:THR:HB	2.02	0.42
1:O:77:GLY:HA2	1:O:448:ALA:HB3	2.02	0.42
1:X:207:LEU:HB3	1:X:208:LEU:HD22	2.01	0.42
1:X:374:LYS:HA	1:X:374:LYS:HE3	2.02	0.42
1:O:412:GLY:HA2	1:O:415:LYS:NZ	2.35	0.42
1:O:456:LYS:HZ2	1:O:460:GLU:CD	2.23	0.42
1:X:386:ALA:O	1:X:390:LYS:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:224:VAL:HA	1:O:241:ALA:HB2	2.01	0.41
1:O:291:ILE:N	1:O:291:ILE:CD1	2.83	0.41
1:X:234:TYR:CE1	1:X:239:PRO:HD3	2.54	0.41
1:X:167:ASP:CA	1:X:243:MET:CE	2.48	0.41
1:O:344:TYR:CE2	1:O:486:GLY:HA3	2.54	0.41
1:O:387:TYR:HA	1:O:390:LYS:HB2	2.03	0.41
1:X:104:TRP:HB2	2:X:501:GOL:H11	2.01	0.41
1:X:62:ALA:HB1	1:X:71:ARG:NH2	2.35	0.41
1:X:274:MET:O	1:X:302:ALA:HB1	2.21	0.41
1:X:373:THR:O	1:X:376:ASP:HB2	2.20	0.41
1:O:232:HIS:CD2	1:O:232:HIS:O	2.74	0.41
1:O:84:ARG:HD3	1:O:245:GLY:HA3	2.02	0.41
1:X:187:ALA:O	1:X:188:SER:HB2	2.20	0.41
1:X:194:ASN:O	1:X:198:LEU:N	2.54	0.41
1:X:475:MET:HB2	1:X:476:PRO:CD	2.50	0.41
1:O:350:THR:HG22	1:O:362:ARG:HH21	1.86	0.41
1:O:418:LEU:HD12	1:O:421:GLN:HE21	1.86	0.41
1:X:8:MET:O	1:X:78:ILE:HG23	2.21	0.41
1:X:446:TYR:HA	1:X:455:TRP:CZ3	2.56	0.41
1:O:477:ALA:O	1:O:479:GLU:N	2.54	0.41
1:X:107:ARG:NH1	1:X:135:ALA:HB3	2.36	0.41
1:X:226:GLY:CA	1:X:240:ILE:HB	2.47	0.41
1:O:205:LEU:C	1:O:207:LEU:H	2.24	0.41
1:O:229:ARG:NH2	1:X:238:VAL:CA	2.82	0.41
1:O:225:TYR:N	1:O:240:ILE:O	2.53	0.41
1:O:358:ASP:HB3	1:O:361:ALA:HB3	2.03	0.41
1:X:88:VAL:HG11	1:X:169:TRP:HE3	1.86	0.41
1:X:175:THR:HG1	1:X:178:GLN:H	1.69	0.41
1:X:296:ASN:O	1:X:298:LYS:N	2.53	0.41
1:O:196:HIS:HE1	1:O:280:PRO:O	2.04	0.40
1:O:219:LYS:HE2	1:O:223:GLU:HB2	2.03	0.40
1:O:475:MET:HG2	1:O:476:PRO:CD	2.48	0.40
1:X:122:THR:O	1:X:125:ILE:HB	2.22	0.40
1:X:87:THR:HA	1:X:165:THR:HA	2.03	0.40
1:X:336:LYS:HG3	1:X:337:ALA:N	2.36	0.40
1:O:235:GLY:HA3	1:X:234:TYR:CB	2.51	0.40
1:O:480:ARG:HG3	1:O:481:ASP:H	1.85	0.40
1:X:167:ASP:CB	1:X:182:THR:HA	2.51	0.40
1:X:175:THR:HG22	1:X:179:VAL:HG11	1.94	0.40
1:O:132:VAL:O	1:O:134:ASP:N	2.53	0.40
1:O:225:TYR:CD2	1:O:225:TYR:O	2.74	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:78:ILE:HD13	1:O:240:ILE:HG12	1.99	0.40
1:O:43:SER:HB3	1:O:362:ARG:NH1	2.36	0.40
1:X:162:LEU:CD1	1:X:214:MET:HB2	2.52	0.40
1:X:234:TYR:OH	1:X:239:PRO:CD	2.69	0.40
1:O:193:TYR:HE2	1:O:218:VAL:HB	1.83	0.40
1:O:314:ILE:HG12	1:O:381:THR:CG2	2.51	0.40
1:X:235:GLY:O	1:X:236:SER:CB	2.69	0.40
1:O:102:ILE:HG21	1:O:141:LYS:HD2	2.03	0.40
1:O:84:ARG:HG3	2:O:500:GOL:H12	2.03	0.40
1:X:65:PHE:CZ	1:X:72:PRO:CD	3.02	0.40
1:X:82:ASN:OD1	1:X:243:MET:HG3	2.17	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	O	485/487 (100%)	330 (68%)	103 (21%)	52 (11%)	0	1
1	X	485/487 (100%)	330 (68%)	112 (23%)	43 (9%)	1	1
All	All	970/974 (100%)	660 (68%)	215 (22%)	95 (10%)	1	1

All (95) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	O	24	ARG
1	O	117	LYS
1	O	135	ALA
1	O	138	SER
1	O	203	GLU
1	O	229	ARG
1	O	239	PRO

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Mol	Chain	Res	Type
1	O	240	ILE
1	O	479	GLU
1	O	480	ARG
1	X	176	ASP
1	X	225	TYR
1	X	227	HIS
1	X	313	ALA
1	O	16	SER
1	O	29	ILE
1	O	75	ILE
1	O	118	VAL
1	O	120	GLY
1	O	202	GLN
1	O	222	SER
1	O	230	SER
1	O	231	TYR
1	O	295	ILE
1	O	334	ALA
1	O	354	ALA
1	O	477	ALA
1	X	14	THR
1	X	224	VAL
1	X	267	GLY
1	X	311	GLY
1	X	327	SER
1	X	330	SER
1	X	348	ALA
1	X	454	PHE
1	X	459	ASP
1	O	323	MET
1	O	347	PRO
1	O	357	TRP
1	O	478	GLU
1	X	92	LYS
1	X	203	GLU
1	X	260	GLY
1	O	15	THR
1	O	43	SER
1	O	61	ILE
1	O	74	ALA
1	O	160	GLU
1	O	232	HIS

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Mol	Chain	Res	Type
1	O	332	GLU
1	O	338	LYS
1	O	372	THR
1	O	405	PRO
1	O	435	ALA
1	O	460	GLU
1	X	41	PRO
1	X	72	PRO
1	X	74	ALA
1	X	99	ALA
1	X	108	GLN
1	X	116	LEU
1	X	128	LYS
1	X	214	MET
1	X	238	VAL
1	X	284	ASP
1	X	457	ASP
1	X	489	GLN
1	O	37	PRO
1	O	76	ALA
1	O	133	ILE
1	O	150	GLU
1	O	152	ALA
1	O	197	LYS
1	O	224	VAL
1	O	436	ASN
1	X	25	ASN
1	X	100	ASN
1	X	280	PRO
1	X	335	ALA
1	X	340	ASP
1	X	380	ALA
1	X	414	ALA
1	X	417	ASP
1	O	41	PRO
1	O	342	GLU
1	O	452	VAL
1	X	29	ILE
1	X	286	ASP
1	X	354	ALA
1	O	378	VAL
1	X	476	PRO

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Mol	Chain	Res	Type
1	X	269	GLY
1	X	378	VAL
1	O	320	GLY
1	X	26	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	O	395/395 (100%)	345 (87%)	50 (13%)	5	13
1	X	393/395 (100%)	350 (89%)	43 (11%)	7	20
All	All	788/790 (100%)	695 (88%)	93 (12%)	6	16

All (93) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	12	GLN
1	O	36	PHE
1	O	37	PRO
1	O	41	PRO
1	O	48	HIS
1	O	51	ASN
1	O	72	PRO
1	O	82	ASN
1	O	89	VAL
1	O	96	GLN
1	O	97	PRO
1	O	109	SER
1	O	111	PRO
1	O	172	TRP
1	O	174	LEU
1	O	175	THR
1	O	189	ARG
1	O	195	ILE
1	O	200	TRP

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Mol	Chain	Res	Type
1	O	211	PRO
1	O	215	LEU
1	O	216	PRO
1	O	225	TYR
1	O	229	ARG
1	O	231	TYR
1	O	233	PHE
1	O	239	PRO
1	O	255	MET
1	O	262	ILE
1	O	266	TYR
1	O	276	THR
1	O	280	PRO
1	O	291	ILE
1	O	306	SER
1	O	317	LEU
1	O	328	PRO
1	O	336	LYS
1	O	347	PRO
1	O	355	PRO
1	O	360	GLU
1	O	390	LYS
1	O	405	PRO
1	O	406	LEU
1	O	422	PHE
1	O	455	TRP
1	O	456	LYS
1	O	459	ASP
1	O	467	GLU
1	O	473	PRO
1	O	476	PRO
1	X	28	LYS
1	X	36	PHE
1	X	37	PRO
1	X	41	PRO
1	X	72	PRO
1	X	96	GLN
1	X	100	ASN
1	X	109	SER
1	X	111	PRO
1	X	124	MET
1	X	140	THR

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Mol	Chain	Res	Type
1	X	175	THR
1	X	184	TYR
1	X	193	TYR
1	X	196	HIS
1	X	211	PRO
1	X	213	SER
1	X	216	PRO
1	X	223	GLU
1	X	224	VAL
1	X	233	PHE
1	X	234	TYR
1	X	237	GLU
1	X	239	PRO
1	X	263	LYS
1	X	278	GLU
1	X	280	PRO
1	X	282	LEU
1	X	287	LEU
1	X	326	THR
1	X	328	PRO
1	X	347	PRO
1	X	355	PRO
1	X	374	LYS
1	X	405	PRO
1	X	406	LEU
1	X	425	ASP
1	X	430	ASP
1	X	439	THR
1	X	454	PHE
1	X	473	PRO
1	X	476	PRO
1	X	480	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	O	96	GLN
1	O	105	GLN
1	O	148	ASN
1	O	196	HIS
1	O	202	GLN
1	O	232	HIS

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Mol	Chain	Res	Type
1	O	247	GLN
1	O	254	GLN
1	O	421	GLN
1	O	423	GLN
1	O	482	ASN
1	X	12	GLN
1	X	108	GLN
1	X	202	GLN
1	X	209	ASN
1	X	221	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	O	500	-	5,5,5	0.91	0	5,5,5	0.84	0
2	GOL	X	501	-	5,5,5	0.90	0	5,5,5	0.85	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	O	500	-	-	0/4/4/4	0/0/0/0
2	GOL	X	501	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	O	500	GOL	9	0
2	X	501	GOL	14	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.