Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2023 – 08:43 AM EDT

PDB ID	:	2OEN
Title	:	Structural mechanism for the fine-tuning of CcpA function by the small molecule effectors glucose-6-phosphate and fructose-1,6-bisphosphate
Authors	:	Schumacher, M.A.; Seidel, G.; Hillen, W.; Brennan, R.G.
Deposited on	:	2006-12-30
Resolution	:	3.17 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:

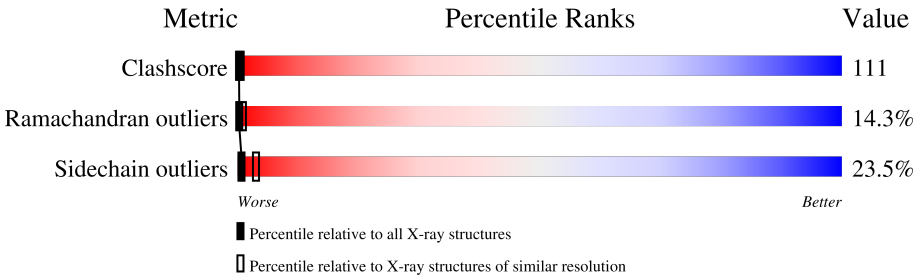
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.17 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	141614	1599 (3.20-3.16)
Ramachandran outliers	138981	1574 (3.20-3.16)
Sidechain outliers	138945	1573 (3.20-3.16)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	G	280	9% 65% 22%
2	L	88	11% 56% 27% 5%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 2773 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 Catabolite control protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	G	275	2141	1349	356	428	8	0	0	0

- Molecule 2 is a protein called Phosphocarrier protein HPr.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
2	L	87	632	386	104	138	1	3	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	46	SEP	SER	modified residue	UNP O69250

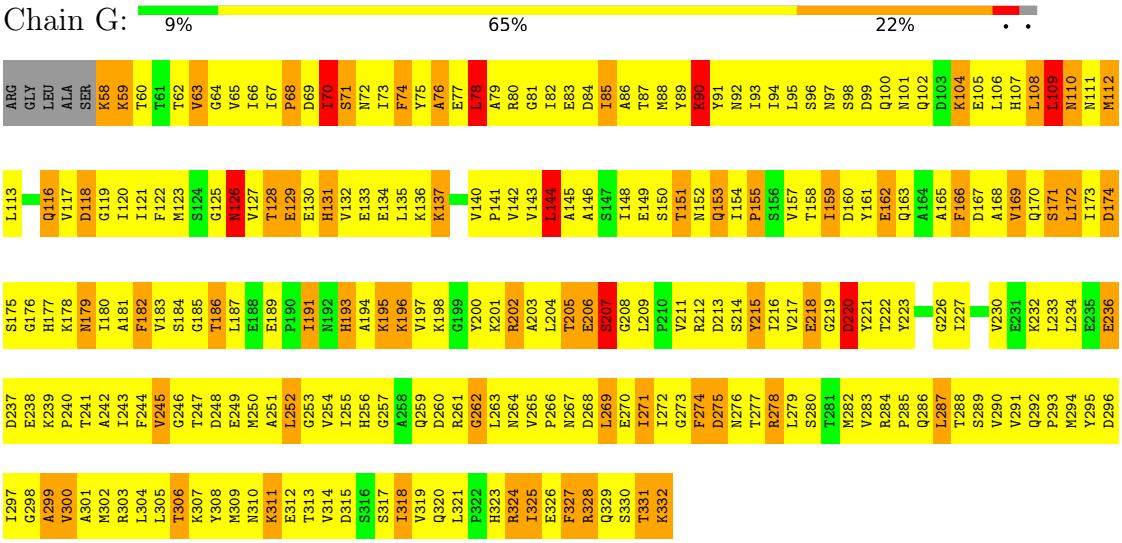
3 Residue-property plots (i)

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

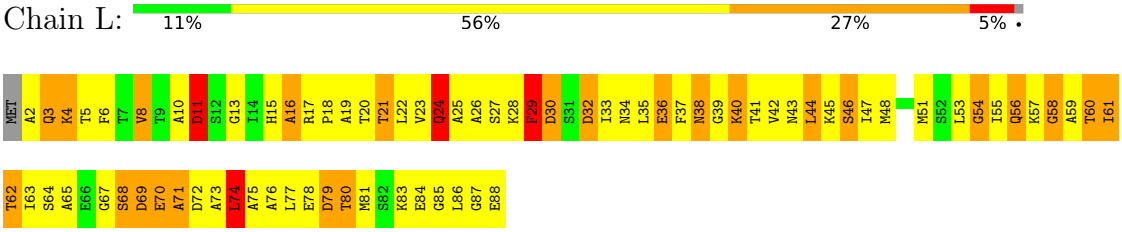
• Molecule 1: Catabolite control protein

Chain G:



• Molecule 2: Phosphocarrier protein HPr

Chain L:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	69.33Å 69.33Å 229.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	66.37 – 3.17	Depositor
% Data completeness (in resolution range)	98.9 (66.37-3.17)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.278 , 0.318	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2773	wwPDB-VP
Average B, all atoms (Å^2)	78.0	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: SEP

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	G	0.75	0/2174	1.02	6/2945 (0.2%)
2	L	0.79	0/625	1.06	2/839 (0.2%)
All	All	0.76	0/2799	1.03	8/3784 (0.2%)

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
2	L	0	1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L	74	LEU	CA-CB-CG	6.10	129.33	115.30
2	L	29	PHE	N-CA-C	5.59	126.09	111.00
1	G	151	THR	N-CA-C	5.32	125.37	111.00
1	G	71	SER	N-CA-C	-5.29	96.73	111.00
1	G	128	THR	N-CA-C	5.25	125.17	111.00
1	G	78	LEU	CA-CB-CG	-5.24	103.25	115.30
1	G	269	LEU	CA-CB-CG	5.17	127.18	115.30
1	G	207	SER	N-CA-C	-5.06	97.33	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	L	29	PHE	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	2141	0	2147	466	1
2	L	632	0	624	158	0
All	All	2773	0	2771	615	1

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 111.

All (615) 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:G:293:PRO:HB2	1:G:296:ASP:HB2	1.25	1.14
1:G:288:THR:HG23	1:G:327:PHE:HA	1.24	1.10
2:L:8:VAL:HG13	2:L:58:GLY:H	1.17	1.09
1:G:58:LYS:HE3	1:G:58:LYS:HA	1.34	1.07
2:L:4:LYS:HB3	2:L:63:ILE:HD12	1.37	1.04
2:L:4:LYS:HB2	2:L:74:LEU:HD11	1.40	1.03
1:G:255:ILE:O	1:G:259:GLN:HG3	1.62	1.00
2:L:53:LEU:HB2	2:L:55:ILE:HD11	1.44	1.00
1:G:264:ASN:HB2	1:G:267:ASN:HB2	1.45	0.98
1:G:67:ILE:HD11	1:G:75:TYR:HB3	1.46	0.98
2:L:21:THR:O	2:L:24:GLN:HB2	1.64	0.97
1:G:101:ASN:HB3	1:G:104:LYS:HG3	1.45	0.96
2:L:81:MET:HE2	2:L:87:GLY:H	1.29	0.94
1:G:104:LYS:HA	1:G:104:LYS:HZ3	1.30	0.94
2:L:19:ALA:O	2:L:23:VAL:HG23	1.67	0.94
1:G:293:PRO:CB	1:G:296:ASP:HB2	2.00	0.92
2:L:77:LEU:HA	2:L:80:THR:HB	1.48	0.91
1:G:292:GLN:NE2	1:G:294:MET:HE1	1.86	0.90
1:G:95:LEU:HG	1:G:96:SER:N	1.84	0.90
2:L:34:ASN:HB2	2:L:64:SER:HB2	1.51	0.90
1:G:70:ILE:HD11	1:G:97:ASN:HD21	1.34	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:159:ILE:HD13	1:G:160:ASP:H	1.36	0.89
2:L:4:LYS:HB2	2:L:74:LEU:CD1	2.03	0.89
1:G:104:LYS:HA	1:G:104:LYS:NZ	1.88	0.88
2:L:4:LYS:HG2	2:L:6:PHE:CE1	2.09	0.88
1:G:161:TYR:CD2	1:G:191:ILE:HD11	2.09	0.87
1:G:78:LEU:HD13	1:G:123:MET:CE	2.06	0.86
2:L:67:GLY:O	2:L:69:ASP:N	2.09	0.86
1:G:194:ALA:O	1:G:195:LYS:HD2	1.76	0.86
2:L:4:LYS:HG2	2:L:6:PHE:HE1	1.41	0.86
2:L:4:LYS:HG3	2:L:5:THR:H	1.40	0.85
1:G:128:THR:O	1:G:131:HIS:HB2	1.77	0.85
1:G:256:HIS:HA	1:G:259:GLN:OE1	1.77	0.85
1:G:158:THR:O	1:G:320:GLN:HA	1.75	0.85
1:G:144:LEU:HG	1:G:154:ILE:HD13	1.58	0.84
1:G:266:PRO:HB2	1:G:270:GLU:OE2	1.78	0.84
1:G:252:LEU:HG	1:G:283:VAL:HG11	1.59	0.84
1:G:288:THR:HG23	1:G:327:PHE:CA	2.07	0.84
1:G:218:GLU:O	1:G:218:GLU:HG2	1.77	0.84
1:G:173:ILE:HA	1:G:177:HIS:HB2	1.60	0.83
2:L:4:LYS:HB3	2:L:63:ILE:CD1	2.08	0.83
1:G:177:HIS:HB3	1:G:180:ILE:HD11	1.62	0.82
2:L:53:LEU:CB	2:L:55:ILE:HD11	2.09	0.82
1:G:264:ASN:HB3	1:G:267:ASN:HD22	1.42	0.82
2:L:4:LYS:CB	2:L:63:ILE:HD12	2.09	0.81
1:G:101:ASN:CB	1:G:104:LYS:HG3	2.10	0.81
1:G:287:LEU:HD22	1:G:288:THR:N	1.96	0.81
1:G:154:ILE:HD12	1:G:154:ILE:O	1.80	0.81
1:G:189:GLU:HB3	1:G:191:ILE:HG22	1.63	0.80
2:L:24:GLN:HE21	2:L:24:GLN:N	1.79	0.80
2:L:35:LEU:O	2:L:41:THR:HG23	1.81	0.80
1:G:122:PHE:HE1	1:G:127:VAL:HG22	1.47	0.80
1:G:293:PRO:HB2	1:G:296:ASP:CB	2.09	0.80
2:L:11:ASP:HA	2:L:57:LYS:HB2	1.64	0.79
1:G:252:LEU:HG	1:G:283:VAL:CG1	2.12	0.79
2:L:23:VAL:HG21	2:L:47:ILE:HD12	1.64	0.79
1:G:137:LYS:HA	1:G:137:LYS:HE3	1.63	0.78
1:G:264:ASN:O	1:G:268:ASP:N	2.14	0.78
1:G:144:LEU:HD23	1:G:144:LEU:H	1.48	0.78
1:G:272:ILE:HG22	1:G:273:GLY:H	1.48	0.78
2:L:79:ASP:O	2:L:83:LYS:HB2	1.84	0.78
2:L:24:GLN:O	2:L:27:SER:HB2	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:36:GLU:HB3	2:L:62:THR:OG1	1.85	0.77
2:L:47:ILE:HG23	2:L:48:MET:N	1.99	0.77
2:L:8:VAL:CG1	2:L:58:GLY:H	1.95	0.76
1:G:227:ILE:HG12	1:G:253:GLY:O	1.86	0.76
1:G:318:ILE:HD13	1:G:318:ILE:H	1.50	0.76
2:L:47:ILE:HG23	2:L:48:MET:H	1.51	0.76
1:G:264:ASN:HB3	1:G:267:ASN:ND2	2.00	0.75
1:G:66:ILE:HD11	1:G:108:LEU:HB3	1.66	0.75
1:G:191:ILE:HD13	1:G:191:ILE:O	1.85	0.75
1:G:288:THR:CG2	1:G:327:PHE:HA	2.12	0.75
2:L:36:GLU:HG2	2:L:41:THR:OG1	1.86	0.75
1:G:263:LEU:HA	1:G:268:ASP:OD1	1.87	0.75
2:L:81:MET:HE2	2:L:87:GLY:N	2.01	0.75
1:G:78:LEU:HD13	1:G:123:MET:HE1	1.69	0.74
1:G:155:PRO:HG3	1:G:317:SER:OG	1.87	0.74
1:G:101:ASN:O	1:G:105:GLU:HG3	1.87	0.74
1:G:275:ASP:HB3	1:G:277:THR:HG23	1.67	0.74
1:G:272:ILE:HG22	1:G:273:GLY:N	2.02	0.74
1:G:216:ILE:O	1:G:216:ILE:HG13	1.86	0.74
1:G:319:VAL:HG12	1:G:320:GLN:N	2.01	0.73
2:L:42:VAL:HG23	2:L:53:LEU:HD11	1.68	0.73
1:G:109:LEU:O	1:G:111:ASN:N	2.21	0.73
1:G:128:THR:HB	1:G:131:HIS:CE1	2.23	0.73
1:G:58:LYS:HE3	1:G:58:LYS:CA	2.14	0.73
1:G:79:ALA:O	1:G:82:ILE:N	2.22	0.73
1:G:101:ASN:HB3	1:G:104:LYS:CG	2.17	0.73
1:G:110:ASN:HA	1:G:113:LEU:HD12	1.70	0.72
1:G:174:ASP:C	1:G:176:GLY:H	1.91	0.72
1:G:230:VAL:HG21	1:G:254:VAL:HA	1.69	0.72
1:G:234:LEU:CD2	1:G:239:LYS:HG3	2.19	0.72
2:L:81:MET:HE2	2:L:86:LEU:HB3	1.71	0.72
1:G:169:VAL:HG21	1:G:200:TYR:HA	1.71	0.72
1:G:201:LYS:O	1:G:204:LEU:HB3	1.90	0.71
1:G:218:GLU:O	1:G:218:GLU:CG	2.37	0.71
1:G:151:THR:HB	1:G:153:GLN:HG3	1.71	0.71
1:G:130:GLU:O	1:G:133:GLU:N	2.23	0.71
1:G:102:GLN:HG3	1:G:106:LEU:HD23	1.72	0.71
1:G:137:LYS:HE3	1:G:137:LYS:CA	2.19	0.71
2:L:81:MET:HB2	2:L:86:LEU:HB2	1.71	0.71
1:G:58:LYS:HA	1:G:58:LYS:CE	2.13	0.70
1:G:125:GLY:O	1:G:189:GLU:HG2	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:212:ARG:O	1:G:214:SER:N	2.22	0.70
1:G:182:PHE:HB3	1:G:216:ILE:HG22	1.73	0.70
1:G:304:LEU:HD13	2:L:48:MET:CE	2.22	0.70
1:G:110:ASN:O	1:G:113:LEU:HB2	1.91	0.70
1:G:295:TYR:O	1:G:298:GLY:N	2.24	0.70
2:L:17:ARG:O	2:L:21:THR:N	2.24	0.70
1:G:166:PHE:CG	1:G:203:ALA:HB2	2.27	0.70
1:G:277:THR:OG1	1:G:279:LEU:HD12	1.92	0.70
1:G:135:LEU:HD22	1:G:142:VAL:HG11	1.74	0.70
1:G:234:LEU:HD23	1:G:239:LYS:HG3	1.74	0.69
1:G:89:TYR:HD1	1:G:306:THR:HG21	1.57	0.69
1:G:172:LEU:HD22	1:G:177:HIS:CD2	2.27	0.69
1:G:67:ILE:CD1	1:G:75:TYR:HB3	2.20	0.69
1:G:180:ILE:CG2	1:G:181:ALA:N	2.54	0.69
2:L:34:ASN:CB	2:L:64:SER:HB2	2.21	0.69
2:L:55:ILE:HD12	2:L:55:ILE:N	2.07	0.69
1:G:310:ASN:O	1:G:312:GLU:HG3	1.91	0.69
1:G:255:ILE:O	1:G:259:GLN:CG	2.41	0.69
2:L:77:LEU:HA	2:L:80:THR:CB	2.23	0.69
1:G:255:ILE:C	1:G:257:GLY:H	1.93	0.68
1:G:76:ALA:O	1:G:78:LEU:N	2.25	0.68
2:L:77:LEU:O	2:L:80:THR:HG22	1.92	0.68
1:G:63:VAL:HG22	1:G:91:TYR:HD2	1.59	0.68
1:G:78:LEU:HD13	1:G:123:MET:HE3	1.74	0.68
1:G:81:GLY:HA3	1:G:298:GLY:HA3	1.75	0.68
1:G:288:THR:HA	1:G:328:ARG:H	1.57	0.68
1:G:62:THR:HG23	1:G:92:ASN:HB2	1.74	0.68
1:G:319:VAL:HG12	1:G:320:GLN:H	1.58	0.68
1:G:165:ALA:HB2	1:G:196:LYS:HA	1.75	0.67
1:G:264:ASN:CB	1:G:267:ASN:HB2	2.22	0.67
2:L:84:GLU:HB2	2:L:86:LEU:HD13	1.73	0.67
1:G:107:HIS:O	1:G:109:LEU:N	2.26	0.67
2:L:47:ILE:CG2	2:L:48:MET:H	2.08	0.67
1:G:159:ILE:CD1	1:G:323:HIS:HB3	2.25	0.67
1:G:166:PHE:CD2	1:G:203:ALA:HB2	2.29	0.67
2:L:2:ALA:O	2:L:3:GLN:HB3	1.94	0.67
1:G:93:ILE:HD12	1:G:93:ILE:O	1.93	0.67
2:L:38:ASN:O	2:L:40:LYS:N	2.28	0.67
1:G:121:ILE:HG23	1:G:143:VAL:HG13	1.77	0.67
1:G:264:ASN:HB2	1:G:267:ASN:CB	2.23	0.67
1:G:133:GLU:O	1:G:137:LYS:HD2	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:128:THR:HB	1:G:131:HIS:ND1	2.10	0.66
1:G:304:LEU:HD13	2:L:48:MET:HE1	1.77	0.66
2:L:24:GLN:O	2:L:27:SER:N	2.27	0.66
1:G:154:ILE:O	1:G:155:PRO:O	2.13	0.66
1:G:173:ILE:HA	1:G:177:HIS:CB	2.26	0.66
1:G:227:ILE:CG1	1:G:253:GLY:O	2.43	0.66
1:G:247:THR:HB	1:G:250:MET:HG3	1.76	0.66
2:L:81:MET:HB2	2:L:86:LEU:CB	2.24	0.66
1:G:165:ALA:O	1:G:169:VAL:HG23	1.96	0.66
1:G:292:GLN:HE21	1:G:294:MET:HE1	1.58	0.66
2:L:24:GLN:HE21	2:L:24:GLN:CA	2.06	0.66
1:G:66:ILE:HG23	1:G:98:SER:HB2	1.77	0.65
1:G:159:ILE:CD1	1:G:160:ASP:H	2.08	0.65
1:G:230:VAL:HG22	1:G:254:VAL:HG22	1.78	0.65
2:L:6:PHE:O	2:L:61:ILE:N	2.27	0.65
1:G:143:VAL:HG13	1:G:143:VAL:O	1.95	0.65
2:L:10:ALA:HB2	2:L:85:GLY:O	1.97	0.65
2:L:36:GLU:HA	2:L:41:THR:OG1	1.97	0.65
1:G:64:GLY:HA3	1:G:112:MET:HG3	1.79	0.65
1:G:132:VAL:O	1:G:136:LYS:N	2.24	0.64
1:G:146:ALA:N	1:G:158:THR:HG22	2.12	0.64
2:L:88:GLU:O	2:L:88:GLU:OE1	2.14	0.64
2:L:33:ILE:O	2:L:34:ASN:ND2	2.30	0.64
1:G:127:VAL:HG21	1:G:144:LEU:HD13	1.78	0.64
1:G:217:VAL:HG12	1:G:233:LEU:HD12	1.79	0.64
1:G:73:ILE:HD13	1:G:279:LEU:HD11	1.79	0.64
1:G:266:PRO:HA	1:G:269:LEU:O	1.97	0.64
2:L:84:GLU:HB2	2:L:86:LEU:CD1	2.28	0.64
1:G:238:GLU:HA	1:G:238:GLU:OE1	1.98	0.64
2:L:6:PHE:CE1	2:L:63:ILE:HD11	2.32	0.63
1:G:252:LEU:CG	1:G:283:VAL:HG11	2.28	0.63
1:G:154:ILE:O	1:G:154:ILE:CD1	2.47	0.63
1:G:255:ILE:HG22	1:G:259:GLN:CD	2.19	0.63
1:G:151:THR:HB	1:G:153:GLN:CG	2.28	0.63
1:G:159:ILE:O	1:G:161:TYR:CD1	2.52	0.63
1:G:205:THR:HG22	1:G:211:VAL:HG21	1.81	0.63
1:G:146:ALA:CA	1:G:158:THR:HG22	2.29	0.63
1:G:80:ARG:HE	1:G:84:ASP:CG	2.01	0.63
1:G:285:PRO:HB2	1:G:329:GLN:HB2	1.81	0.63
1:G:259:GLN:NE2	1:G:285:PRO:HD2	2.14	0.62
1:G:67:ILE:HD11	1:G:75:TYR:CB	2.26	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:33:ILE:HA	2:L:64:SER:O	1.98	0.62
1:G:111:ASN:O	1:G:112:MET:C	2.36	0.62
1:G:206:GLU:O	1:G:206:GLU:HG2	1.97	0.62
1:G:247:THR:CB	1:G:250:MET:HG3	2.28	0.62
1:G:76:ALA:C	1:G:78:LEU:H	2.03	0.62
1:G:280:SER:O	1:G:328:ARG:HD3	2.00	0.62
1:G:62:THR:O	1:G:117:VAL:HB	1.98	0.62
1:G:73:ILE:O	1:G:76:ALA:HB3	2.00	0.62
1:G:78:LEU:HG	1:G:294:MET:O	2.00	0.62
1:G:174:ASP:C	1:G:176:GLY:N	2.52	0.62
2:L:35:LEU:C	2:L:41:THR:HG23	2.19	0.62
1:G:180:ILE:HG23	1:G:181:ALA:H	1.64	0.62
1:G:146:ALA:HB2	1:G:297:ILE:HG21	1.82	0.61
1:G:178:LYS:HG3	1:G:179:ASN:H	1.65	0.61
1:G:227:ILE:HA	1:G:253:GLY:O	2.00	0.61
1:G:265:VAL:HG13	1:G:269:LEU:O	2.00	0.61
1:G:309:MET:C	1:G:310:ASN:HD22	2.03	0.61
1:G:173:ILE:CA	1:G:177:HIS:HB2	2.30	0.61
2:L:74:LEU:O	2:L:78:GLU:HG3	2.00	0.61
2:L:76:ALA:O	2:L:80:THR:HB	2.01	0.61
1:G:252:LEU:CD1	1:G:283:VAL:HG11	2.30	0.61
1:G:90:LYS:HE3	1:G:90:LYS:O	1.99	0.60
1:G:271:ILE:CG2	1:G:272:ILE:N	2.64	0.60
2:L:47:ILE:CG2	2:L:48:MET:N	2.63	0.60
1:G:180:ILE:O	1:G:215:TYR:CD2	2.54	0.60
2:L:11:ASP:HA	2:L:57:LYS:CB	2.29	0.60
1:G:178:LYS:HG2	1:G:241:THR:HG21	1.82	0.60
1:G:226:GLY:O	1:G:230:VAL:HG23	2.02	0.60
1:G:135:LEU:HD22	1:G:142:VAL:HG21	1.84	0.60
1:G:303:ARG:O	1:G:307:LYS:HG3	2.01	0.60
2:L:3:GLN:O	2:L:74:LEU:HD21	2.02	0.60
2:L:29:PHE:CD1	2:L:73:ALA:HB2	2.36	0.60
1:G:66:ILE:O	1:G:66:ILE:HG22	2.01	0.60
1:G:154:ILE:O	1:G:155:PRO:C	2.37	0.60
1:G:158:THR:HB	1:G:161:TYR:HE1	1.67	0.60
1:G:182:PHE:CB	1:G:216:ILE:HG22	2.31	0.60
1:G:186:THR:HG21	1:G:189:GLU:HG3	1.84	0.60
2:L:75:ALA:O	2:L:79:ASP:HB2	2.01	0.60
1:G:283:VAL:HG23	1:G:286:GLN:HA	1.83	0.59
1:G:165:ALA:CB	1:G:196:LYS:HA	2.32	0.59
1:G:289:SER:OG	1:G:290:VAL:N	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:81:MET:HB2	2:L:86:LEU:HD22	1.83	0.59
1:G:205:THR:OG1	1:G:206:GLU:N	2.34	0.59
2:L:21:THR:HG22	2:L:22:LEU:HD12	1.83	0.59
1:G:89:TYR:HE1	1:G:303:ARG:NH1	2.01	0.59
1:G:135:LEU:CD2	1:G:142:VAL:HG11	2.32	0.59
1:G:146:ALA:HA	1:G:158:THR:HG22	1.84	0.59
1:G:149:GLU:OE2	1:G:151:THR:OG1	2.18	0.58
1:G:236:GLU:HG3	1:G:237:ASP:N	2.17	0.58
2:L:77:LEU:O	2:L:80:THR:N	2.37	0.58
1:G:159:ILE:HD13	1:G:160:ASP:N	2.14	0.58
1:G:186:THR:HG22	1:G:189:GLU:H	1.69	0.58
1:G:159:ILE:HD11	1:G:323:HIS:HB3	1.85	0.58
1:G:184:SER:O	1:G:218:GLU:HA	2.04	0.58
1:G:128:THR:HG23	1:G:129:GLU:OE1	2.04	0.58
1:G:272:ILE:CG2	1:G:273:GLY:H	2.15	0.58
1:G:166:PHE:CD1	1:G:166:PHE:C	2.77	0.58
1:G:310:ASN:O	1:G:311:LYS:C	2.41	0.58
2:L:40:LYS:O	2:L:41:THR:OG1	2.18	0.58
1:G:255:ILE:C	1:G:257:GLY:N	2.58	0.57
1:G:277:THR:O	1:G:279:LEU:N	2.36	0.57
2:L:81:MET:CB	2:L:86:LEU:HB2	2.33	0.57
1:G:183:VAL:O	1:G:245:VAL:HG13	2.04	0.57
1:G:273:GLY:C	1:G:289:SER:OG	2.43	0.57
2:L:77:LEU:CA	2:L:80:THR:HB	2.29	0.57
1:G:291:VAL:HB	1:G:324:ARG:HD3	1.87	0.57
2:L:4:LYS:CG	2:L:5:THR:H	2.14	0.57
1:G:183:VAL:O	1:G:245:VAL:CG1	2.52	0.57
1:G:293:PRO:CG	1:G:296:ASP:HB2	2.35	0.57
2:L:6:PHE:O	2:L:60:THR:HA	2.05	0.57
2:L:21:THR:HG21	2:L:84:GLU:OE2	2.04	0.57
1:G:144:LEU:HG	1:G:154:ILE:CD1	2.33	0.57
1:G:287:LEU:HD11	1:G:289:SER:HB2	1.86	0.57
2:L:8:VAL:HG13	2:L:58:GLY:N	2.02	0.57
1:G:76:ALA:C	1:G:78:LEU:N	2.58	0.57
1:G:230:VAL:O	1:G:234:LEU:HB2	2.05	0.57
1:G:250:MET:O	1:G:254:VAL:HG23	2.04	0.56
1:G:256:HIS:CA	1:G:259:GLN:OE1	2.50	0.56
1:G:222:THR:O	1:G:250:MET:HG2	2.06	0.56
1:G:324:ARG:HG2	1:G:325:ILE:N	2.20	0.56
1:G:79:ALA:O	1:G:80:ARG:C	2.43	0.56
1:G:80:ARG:NE	1:G:84:ASP:OD1	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:204:LEU:HD12	1:G:209:LEU:HD13	1.87	0.56
1:G:266:PRO:CB	1:G:270:GLU:OE2	2.51	0.56
1:G:227:ILE:CA	1:G:253:GLY:O	2.54	0.55
1:G:319:VAL:CG1	1:G:320:GLN:N	2.69	0.55
1:G:104:LYS:NZ	1:G:104:LYS:CA	2.68	0.55
1:G:102:GLN:O	1:G:106:LEU:HB2	2.07	0.55
1:G:151:THR:C	1:G:153:GLN:H	2.09	0.55
1:G:182:PHE:O	1:G:216:ILE:HA	2.06	0.55
2:L:80:THR:CG2	2:L:81:MET:N	2.69	0.55
1:G:80:ARG:HG3	1:G:295:TYR:CE2	2.41	0.55
2:L:3:GLN:CA	2:L:74:LEU:HD22	2.37	0.55
1:G:127:VAL:HG11	1:G:144:LEU:HD11	1.89	0.54
1:G:178:LYS:CG	1:G:241:THR:HG21	2.37	0.54
2:L:15:HIS:O	2:L:16:ALA:O	2.25	0.54
2:L:81:MET:O	2:L:86:LEU:HB2	2.07	0.54
1:G:272:ILE:CG2	1:G:273:GLY:N	2.70	0.54
1:G:329:GLN:C	1:G:331:THR:H	2.11	0.54
2:L:21:THR:HG22	2:L:22:LEU:N	2.22	0.54
1:G:74:PHE:C	1:G:74:PHE:CD2	2.81	0.54
1:G:251:ALA:HB1	1:G:287:LEU:HG	1.88	0.54
2:L:16:ALA:HB3	2:L:18:PRO:HD2	1.90	0.54
1:G:80:ARG:HH21	1:G:84:ASP:CG	2.10	0.54
1:G:85:ILE:HD11	2:L:20:THR:HG23	1.89	0.54
1:G:263:LEU:CA	1:G:268:ASP:OD1	2.56	0.54
2:L:36:GLU:HA	2:L:41:THR:HG1	1.73	0.54
1:G:107:HIS:O	1:G:108:LEU:C	2.45	0.54
1:G:134:GLU:OE2	1:G:134:GLU:N	2.41	0.54
1:G:137:LYS:HE3	1:G:137:LYS:N	2.22	0.54
1:G:165:ALA:O	1:G:169:VAL:CG2	2.55	0.54
1:G:183:VAL:O	1:G:245:VAL:HA	2.07	0.54
1:G:117:VAL:HG23	1:G:119:GLY:O	2.08	0.54
1:G:143:VAL:O	1:G:144:LEU:C	2.45	0.54
1:G:180:ILE:HG22	1:G:181:ALA:N	2.23	0.54
1:G:300:VAL:HG12	1:G:300:VAL:O	2.08	0.54
1:G:232:LYS:O	1:G:232:LYS:HG2	2.07	0.54
2:L:43:ASN:HD21	2:L:46:SEP:HB3	1.73	0.54
2:L:65:ALA:HB1	2:L:70:GLU:HB3	1.90	0.54
1:G:152:ASN:HD21	1:G:318:ILE:HG13	1.73	0.53
2:L:6:PHE:CZ	2:L:78:GLU:HG2	2.43	0.53
2:L:24:GLN:O	2:L:25:ALA:C	2.47	0.53
1:G:161:TYR:CE2	1:G:191:ILE:HD11	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:318:ILE:O	1:G:318:ILE:HG12	2.08	0.53
1:G:275:ASP:OD2	1:G:294:MET:HE1	2.08	0.53
2:L:17:ARG:N	2:L:18:PRO:CD	2.72	0.53
1:G:80:ARG:O	1:G:81:GLY:C	2.44	0.53
1:G:95:LEU:CG	1:G:96:SER:N	2.64	0.53
1:G:80:ARG:HG3	1:G:295:TYR:HE2	1.73	0.53
1:G:80:ARG:O	1:G:84:ASP:HB2	2.08	0.53
1:G:152:ASN:ND2	1:G:318:ILE:HG13	2.24	0.53
1:G:234:LEU:HB3	1:G:261:ARG:HH21	1.74	0.53
1:G:189:GLU:C	1:G:191:ILE:H	2.09	0.53
1:G:248:ASP:HB2	1:G:275:ASP:HB2	1.91	0.53
2:L:24:GLN:CA	2:L:24:GLN:NE2	2.71	0.53
1:G:86:ALA:HB2	1:G:302:MET:CE	2.38	0.53
1:G:123:MET:HG2	1:G:145:ALA:O	2.09	0.53
1:G:247:THR:HB	1:G:250:MET:HB2	1.91	0.53
1:G:304:LEU:HD13	2:L:48:MET:HE2	1.91	0.52
1:G:201:LYS:HG2	1:G:211:VAL:CG1	2.40	0.52
1:G:234:LEU:HB3	1:G:261:ARG:NH2	2.24	0.52
1:G:328:ARG:O	1:G:329:GLN:OE1	2.27	0.52
1:G:318:ILE:HD13	1:G:318:ILE:N	2.19	0.52
1:G:63:VAL:HG22	1:G:91:TYR:CD2	2.43	0.52
1:G:122:PHE:CE1	1:G:127:VAL:HG22	2.36	0.52
2:L:8:VAL:HG13	2:L:8:VAL:O	2.10	0.52
2:L:29:PHE:CE1	2:L:73:ALA:HA	2.45	0.52
1:G:155:PRO:HA	1:G:317:SER:O	2.09	0.52
1:G:172:LEU:HD22	1:G:242:ALA:CB	2.39	0.52
1:G:310:ASN:HD22	1:G:310:ASN:N	2.05	0.52
2:L:33:ILE:HD12	2:L:45:LYS:CG	2.39	0.52
2:L:73:ALA:C	2:L:75:ALA:N	2.62	0.52
2:L:25:ALA:HB3	2:L:77:LEU:HD21	1.92	0.51
1:G:76:ALA:O	1:G:79:ALA:N	2.41	0.51
1:G:104:LYS:O	1:G:108:LEU:HB2	2.10	0.51
2:L:19:ALA:O	2:L:23:VAL:CG2	2.52	0.51
1:G:166:PHE:CD1	1:G:203:ALA:HB2	2.46	0.51
1:G:168:ALA:HB3	1:G:244:PHE:CE1	2.46	0.51
1:G:221:TYR:O	1:G:247:THR:HG21	2.10	0.51
1:G:74:PHE:C	1:G:74:PHE:HD2	2.14	0.51
1:G:94:ILE:HG22	1:G:94:ILE:O	2.11	0.51
1:G:101:ASN:HB3	1:G:104:LYS:HB2	1.93	0.51
1:G:223:TYR:CD2	1:G:253:GLY:HA2	2.45	0.51
2:L:19:ALA:C	2:L:21:THR:N	2.62	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:191:ILE:O	1:G:191:ILE:CD1	2.57	0.51
1:G:308:TYR:CE2	1:G:314:VAL:HG21	2.46	0.51
1:G:59:LYS:HA	1:G:118:ASP:OD1	2.10	0.51
1:G:327:PHE:CD1	1:G:327:PHE:N	2.74	0.51
2:L:3:GLN:HA	2:L:74:LEU:HD22	1.92	0.51
1:G:227:ILE:HG23	1:G:257:GLY:HA2	1.92	0.51
1:G:271:ILE:HG22	1:G:272:ILE:N	2.25	0.51
2:L:33:ILE:HG22	2:L:44:LEU:HB2	1.92	0.50
1:G:319:VAL:CG1	1:G:320:GLN:H	2.24	0.50
1:G:126:ASN:C	1:G:126:ASN:HD22	2.14	0.50
1:G:274:PHE:CE1	1:G:290:VAL:HG11	2.46	0.50
1:G:283:VAL:HG23	1:G:285:PRO:O	2.11	0.50
1:G:297:ILE:O	1:G:301:ALA:HB2	2.11	0.50
1:G:166:PHE:HD1	1:G:167:ASP:N	2.09	0.50
1:G:132:VAL:HG12	1:G:136:LYS:HG3	1.93	0.50
1:G:70:ILE:HD12	1:G:70:ILE:H	1.76	0.50
1:G:327:PHE:H	1:G:327:PHE:HD1	1.57	0.50
1:G:70:ILE:HD11	1:G:97:ASN:ND2	2.16	0.50
2:L:77:LEU:HA	2:L:80:THR:CG2	2.42	0.50
1:G:187:LEU:O	1:G:193:HIS:HB3	2.10	0.50
2:L:77:LEU:HD23	2:L:80:THR:HG21	1.93	0.50
1:G:106:LEU:HD11	1:G:130:GLU:OE2	2.11	0.49
1:G:113:LEU:CD2	1:G:120:ILE:HD11	2.43	0.49
1:G:111:ASN:C	1:G:113:LEU:N	2.64	0.49
1:G:117:VAL:HG23	1:G:117:VAL:O	2.12	0.49
1:G:177:HIS:CE1	1:G:241:THR:O	2.66	0.49
1:G:189:GLU:C	1:G:191:ILE:N	2.65	0.49
2:L:16:ALA:O	2:L:19:ALA:HB3	2.12	0.49
1:G:177:HIS:ND1	1:G:241:THR:HB	2.26	0.49
1:G:205:THR:O	1:G:207:SER:N	2.44	0.49
1:G:292:GLN:NE2	1:G:294:MET:CE	2.69	0.49
1:G:119:GLY:O	1:G:120:ILE:HG13	2.12	0.49
1:G:154:ILE:C	1:G:155:PRO:O	2.49	0.49
1:G:184:SER:O	1:G:218:GLU:HB2	2.12	0.49
1:G:273:GLY:O	1:G:290:VAL:HG23	2.12	0.49
1:G:288:THR:OG1	1:G:328:ARG:N	2.45	0.49
1:G:170:GLN:OE1	1:G:174:ASP:OD1	2.30	0.49
1:G:247:THR:HB	1:G:250:MET:CG	2.43	0.49
1:G:264:ASN:CB	1:G:267:ASN:HD22	2.17	0.49
1:G:135:LEU:CD2	1:G:142:VAL:HG21	2.43	0.49
1:G:206:GLU:O	1:G:207:SER:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:226:GLY:O	1:G:254:VAL:HG22	2.13	0.49
1:G:304:LEU:CD1	2:L:48:MET:HE1	2.43	0.49
2:L:11:ASP:OD2	2:L:11:ASP:N	2.43	0.49
2:L:73:ALA:O	2:L:75:ALA:N	2.46	0.49
1:G:112:MET:O	1:G:117:VAL:HG13	2.13	0.48
2:L:43:ASN:OD1	2:L:45:LYS:HB2	2.13	0.48
1:G:121:ILE:HG23	1:G:143:VAL:CG1	2.43	0.48
1:G:174:ASP:O	1:G:176:GLY:N	2.42	0.48
1:G:89:TYR:CD1	1:G:306:THR:HG21	2.43	0.48
1:G:130:GLU:O	1:G:132:VAL:N	2.47	0.48
1:G:86:ALA:HB2	1:G:302:MET:HE3	1.95	0.48
1:G:283:VAL:O	1:G:286:GLN:HA	2.13	0.48
2:L:43:ASN:HB2	2:L:45:LYS:HE3	1.95	0.48
1:G:89:TYR:CE1	1:G:303:ARG:HD2	2.49	0.48
2:L:69:ASP:CG	2:L:69:ASP:O	2.51	0.48
1:G:201:LYS:HG2	1:G:211:VAL:HG11	1.96	0.48
1:G:244:PHE:O	1:G:245:VAL:HG22	2.12	0.48
1:G:300:VAL:HG13	2:L:48:MET:HE3	1.96	0.48
1:G:303:ARG:HG2	2:L:48:MET:HG3	1.96	0.48
1:G:310:ASN:N	1:G:310:ASN:ND2	2.62	0.48
1:G:113:LEU:HD21	1:G:120:ILE:HD11	1.95	0.48
1:G:166:PHE:O	1:G:169:VAL:HG23	2.13	0.48
1:G:149:GLU:CD	1:G:149:GLU:O	2.52	0.48
2:L:8:VAL:HG11	2:L:56:GLN:O	2.13	0.48
1:G:151:THR:C	1:G:153:GLN:N	2.67	0.47
1:G:206:GLU:O	1:G:207:SER:CB	2.62	0.47
1:G:177:HIS:CE1	1:G:241:THR:HB	2.49	0.47
1:G:177:HIS:NE2	1:G:270:GLU:HB2	2.29	0.47
2:L:53:LEU:HB2	2:L:55:ILE:CD1	2.29	0.47
1:G:117:VAL:O	1:G:117:VAL:CG2	2.63	0.47
1:G:204:LEU:O	1:G:209:LEU:HD12	2.12	0.47
1:G:230:VAL:CG2	1:G:254:VAL:HG22	2.42	0.47
1:G:276:ASN:CB	1:G:291:VAL:HG22	2.43	0.47
1:G:305:LEU:O	1:G:309:MET:HG3	2.13	0.47
1:G:201:LYS:O	1:G:205:THR:HG23	2.14	0.47
1:G:73:ILE:HD13	1:G:279:LEU:CD1	2.42	0.47
1:G:172:LEU:O	1:G:175:SER:HB3	2.15	0.47
1:G:259:GLN:HE22	1:G:285:PRO:HD2	1.79	0.47
1:G:301:ALA:O	1:G:304:LEU:HB3	2.14	0.47
2:L:32:ASP:HA	2:L:45:LYS:NZ	2.29	0.47
1:G:194:ALA:O	1:G:198:LYS:HG3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:302:MET:O	1:G:306:THR:OG1	2.32	0.47
1:G:165:ALA:HB2	1:G:196:LYS:HG3	1.97	0.47
2:L:35:LEU:O	2:L:41:THR:HA	2.15	0.47
1:G:130:GLU:O	1:G:131:HIS:C	2.53	0.47
1:G:141:PRO:HB2	1:G:305:LEU:CD1	2.45	0.47
1:G:239:LYS:HA	1:G:240:PRO:HD3	1.60	0.47
1:G:244:PHE:C	1:G:245:VAL:HG22	2.36	0.47
1:G:182:PHE:HZ	1:G:196:LYS:HB3	1.79	0.46
1:G:223:TYR:CZ	1:G:227:ILE:HD11	2.49	0.46
1:G:274:PHE:HD1	1:G:275:ASP:H	1.62	0.46
2:L:46:SEP:O3P	2:L:47:ILE:HG22	2.14	0.46
2:L:67:GLY:H	2:L:70:GLU:HG2	1.80	0.46
1:G:109:LEU:O	1:G:110:ASN:C	2.53	0.46
1:G:230:VAL:CG2	1:G:254:VAL:HG13	2.45	0.46
1:G:300:VAL:HG13	2:L:48:MET:HG2	1.97	0.46
1:G:66:ILE:CD1	1:G:108:LEU:HB3	2.41	0.46
1:G:277:THR:O	1:G:278:ARG:C	2.54	0.46
2:L:55:ILE:N	2:L:55:ILE:CD1	2.76	0.46
1:G:167:ASP:O	1:G:171:SER:HB2	2.14	0.46
1:G:181:ALA:HB3	1:G:243:ILE:HG12	1.98	0.46
1:G:287:LEU:HD22	1:G:287:LEU:C	2.33	0.46
2:L:70:GLU:HB2	2:L:71:ALA:H	1.53	0.46
2:L:19:ALA:C	2:L:21:THR:H	2.17	0.46
1:G:78:LEU:O	1:G:82:ILE:HG12	2.16	0.46
1:G:303:ARG:HG2	2:L:47:ILE:CG2	2.46	0.46
1:G:72:ASN:OD1	1:G:74:PHE:HB3	2.16	0.46
1:G:118:ASP:O	1:G:309:MET:SD	2.74	0.45
1:G:101:ASN:HB3	1:G:104:LYS:CB	2.45	0.45
1:G:172:LEU:O	1:G:177:HIS:HB2	2.17	0.45
1:G:223:TYR:OH	1:G:256:HIS:HB2	2.16	0.45
2:L:29:PHE:CE1	2:L:73:ALA:CA	2.99	0.45
1:G:70:ILE:HD12	1:G:70:ILE:N	2.31	0.45
1:G:287:LEU:O	1:G:328:ARG:HD2	2.16	0.45
2:L:6:PHE:HZ	2:L:78:GLU:HG2	1.80	0.45
1:G:303:ARG:HA	1:G:306:THR:OG1	2.16	0.45
2:L:4:LYS:CD	2:L:78:GLU:OE2	2.64	0.45
1:G:170:GLN:HB2	1:G:203:ALA:HB1	1.97	0.45
1:G:220:ASP:HB2	1:G:221:TYR:H	1.69	0.45
1:G:244:PHE:C	1:G:245:VAL:CG2	2.84	0.45
1:G:247:THR:OG1	1:G:250:MET:CE	2.64	0.45
1:G:305:LEU:HG	1:G:309:MET:HE2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:17:ARG:C	2:L:19:ALA:N	2.69	0.45
2:L:80:THR:HG22	2:L:81:MET:N	2.31	0.45
1:G:95:LEU:HG	1:G:96:SER:H	1.73	0.45
1:G:151:THR:CB	1:G:153:GLN:HG3	2.43	0.45
1:G:272:ILE:HG23	1:G:288:THR:O	2.17	0.45
1:G:144:LEU:H	1:G:144:LEU:CD2	2.22	0.45
1:G:286:GLN:HB2	1:G:329:GLN:HG2	1.98	0.45
1:G:135:LEU:HD23	1:G:135:LEU:HA	1.82	0.45
1:G:271:ILE:HB	1:G:330:SER:HB2	1.99	0.45
2:L:4:LYS:HG3	2:L:5:THR:N	2.20	0.45
2:L:33:ILE:HD12	2:L:45:LYS:HG2	1.98	0.45
1:G:79:ALA:O	1:G:83:GLU:N	2.49	0.45
1:G:226:GLY:O	1:G:230:VAL:CG2	2.63	0.45
1:G:152:ASN:ND2	1:G:318:ILE:HG21	2.32	0.44
1:G:172:LEU:CD1	1:G:242:ALA:HB1	2.47	0.44
2:L:33:ILE:HD12	2:L:45:LYS:HD3	1.98	0.44
1:G:274:PHE:O	1:G:275:ASP:HB2	2.17	0.44
1:G:255:ILE:HD11	1:G:330:SER:HB2	1.98	0.44
2:L:47:ILE:O	2:L:48:MET:C	2.55	0.44
1:G:93:ILE:H	1:G:93:ILE:HG13	1.61	0.44
1:G:182:PHE:CE2	1:G:244:PHE:CD2	3.06	0.44
1:G:215:TYR:HD1	1:G:215:TYR:HA	1.61	0.44
1:G:255:ILE:HG22	1:G:259:GLN:NE2	2.32	0.44
1:G:60:THR:N	1:G:118:ASP:OD1	2.47	0.44
1:G:183:VAL:HB	1:G:245:VAL:HG13	1.99	0.44
1:G:247:THR:HB	1:G:250:MET:CB	2.48	0.44
1:G:292:GLN:HB3	1:G:294:MET:HE2	1.98	0.44
2:L:16:ALA:CB	2:L:18:PRO:HD2	2.46	0.44
2:L:77:LEU:C	2:L:80:THR:H	2.20	0.44
1:G:170:GLN:C	1:G:172:LEU:H	2.19	0.44
2:L:3:GLN:HB2	2:L:63:ILE:O	2.18	0.44
1:G:89:TYR:HE1	1:G:303:ARG:HD2	1.83	0.44
1:G:291:VAL:HG21	1:G:326:GLU:HG2	2.00	0.44
1:G:310:ASN:O	1:G:312:GLU:N	2.50	0.44
1:G:184:SER:O	1:G:218:GLU:CA	2.66	0.44
1:G:328:ARG:HH11	1:G:328:ARG:HG3	1.82	0.44
1:G:119:GLY:C	1:G:120:ILE:HG13	2.38	0.44
1:G:162:GLU:O	1:G:165:ALA:HB3	2.18	0.44
1:G:177:HIS:HD1	1:G:241:THR:HB	1.83	0.43
2:L:42:VAL:O	2:L:43:ASN:C	2.56	0.43
1:G:70:ILE:H	1:G:70:ILE:CD1	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:128:THR:CG2	1:G:129:GLU:N	2.81	0.43
1:G:299:ALA:O	1:G:301:ALA:N	2.51	0.43
1:G:159:ILE:CD1	1:G:321:LEU:O	2.65	0.43
1:G:255:ILE:HG22	1:G:259:GLN:OE1	2.18	0.43
2:L:81:MET:HB2	2:L:86:LEU:CD2	2.48	0.43
1:G:109:LEU:HD22	1:G:113:LEU:HD11	1.99	0.43
1:G:127:VAL:HG21	1:G:144:LEU:CD1	2.45	0.43
1:G:132:VAL:O	1:G:135:LEU:HB2	2.19	0.43
1:G:157:VAL:O	1:G:158:THR:CG2	2.67	0.43
1:G:325:ILE:HG21	1:G:327:PHE:CE2	2.54	0.43
2:L:33:ILE:HG22	2:L:34:ASN:N	2.33	0.43
1:G:109:LEU:O	1:G:112:MET:N	2.51	0.43
1:G:143:VAL:O	1:G:144:LEU:O	2.37	0.43
1:G:255:ILE:HD11	1:G:330:SER:CB	2.48	0.43
2:L:44:LEU:HD23	2:L:44:LEU:HA	1.61	0.43
1:G:69:ASP:OD2	1:G:71:SER:HB2	2.19	0.43
1:G:195:LYS:O	1:G:198:LYS:HB2	2.18	0.43
1:G:270:GLU:OE2	1:G:332:LYS:N	2.52	0.43
2:L:22:LEU:C	2:L:24:GLN:N	2.71	0.43
1:G:64:GLY:HA3	1:G:112:MET:CE	2.48	0.43
1:G:292:GLN:HB3	1:G:294:MET:CE	2.49	0.43
1:G:303:ARG:CA	1:G:306:THR:OG1	2.66	0.43
1:G:60:THR:OG1	1:G:116:GLN:O	2.21	0.43
1:G:200:TYR:O	1:G:204:LEU:HB2	2.19	0.43
1:G:298:GLY:O	1:G:299:ALA:C	2.56	0.43
2:L:6:PHE:N	2:L:61:ILE:O	2.33	0.43
2:L:35:LEU:HD11	2:L:61:ILE:CG2	2.49	0.43
1:G:246:GLY:O	1:G:274:PHE:CB	2.67	0.43
1:G:202:ARG:O	1:G:206:GLU:HB3	2.18	0.42
1:G:272:ILE:HA	1:G:288:THR:O	2.19	0.42
1:G:90:LYS:O	1:G:90:LYS:CE	2.67	0.42
1:G:212:ARG:C	1:G:214:SER:H	2.15	0.42
1:G:249:GLU:C	1:G:251:ALA:H	2.19	0.42
1:G:276:ASN:ND2	1:G:291:VAL:HG22	2.34	0.42
1:G:305:LEU:HG	1:G:309:MET:SD	2.59	0.42
1:G:87:THR:O	1:G:88:MET:C	2.58	0.42
1:G:120:ILE:O	1:G:142:VAL:HA	2.19	0.42
1:G:197:VAL:O	1:G:198:LYS:C	2.58	0.42
1:G:202:ARG:O	1:G:202:ARG:HG2	2.17	0.42
1:G:298:GLY:O	1:G:301:ALA:HB3	2.20	0.42
1:G:107:HIS:C	1:G:109:LEU:N	2.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:175:SER:O	1:G:176:GLY:C	2.56	0.42
1:G:262:GLY:C	1:G:263:LEU:HD12	2.40	0.42
2:L:15:HIS:O	2:L:16:ALA:C	2.58	0.42
2:L:29:PHE:CE1	2:L:73:ALA:N	2.88	0.42
1:G:166:PHE:C	1:G:166:PHE:HD1	2.22	0.42
2:L:17:ARG:N	2:L:18:PRO:HD2	2.35	0.42
2:L:21:THR:CG2	2:L:84:GLU:OE2	2.67	0.42
1:G:288:THR:CA	1:G:328:ARG:H	2.26	0.42
1:G:64:GLY:HA3	1:G:112:MET:CG	2.47	0.42
1:G:172:LEU:HD22	1:G:242:ALA:HB2	2.00	0.42
2:L:84:GLU:O	2:L:86:LEU:HD12	2.20	0.42
1:G:166:PHE:CE2	1:G:203:ALA:HB2	2.54	0.42
1:G:271:ILE:N	1:G:271:ILE:CD1	2.83	0.42
1:G:324:ARG:HE	1:G:326:GLU:HG2	1.84	0.42
2:L:21:THR:O	2:L:24:GLN:CB	2.51	0.42
2:L:53:LEU:O	2:L:54:GLY:C	2.59	0.42
1:G:185:GLY:HA2	1:G:219:GLY:O	2.20	0.41
1:G:288:THR:HG23	1:G:327:PHE:CB	2.49	0.41
1:G:172:LEU:CD2	1:G:177:HIS:CD2	3.01	0.41
2:L:17:ARG:O	2:L:19:ALA:N	2.53	0.41
1:G:82:ILE:O	1:G:83:GLU:C	2.59	0.41
1:G:166:PHE:CD2	1:G:202:ARG:CZ	3.03	0.41
1:G:113:LEU:HD21	1:G:120:ILE:CD1	2.49	0.41
1:G:144:LEU:CD2	1:G:144:LEU:N	2.81	0.41
1:G:179:ASN:OD1	1:G:179:ASN:N	2.52	0.41
1:G:85:ILE:C	1:G:87:THR:N	2.74	0.41
1:G:143:VAL:O	1:G:143:VAL:HG22	2.19	0.41
1:G:67:ILE:HG13	1:G:68:PRO:HD2	2.02	0.41
1:G:128:THR:O	1:G:129:GLU:C	2.59	0.41
1:G:178:LYS:CG	1:G:241:THR:CG2	2.98	0.41
1:G:305:LEU:HG	1:G:309:MET:CE	2.51	0.41
1:G:325:ILE:HG22	1:G:327:PHE:CE1	2.55	0.41
2:L:67:GLY:N	2:L:70:GLU:HG2	2.36	0.41
1:G:172:LEU:CD2	1:G:242:ALA:HB1	2.51	0.41
1:G:180:ILE:HG22	1:G:200:TYR:HE2	1.85	0.41
1:G:249:GLU:O	1:G:249:GLU:HG3	2.20	0.41
2:L:80:THR:HG22	2:L:81:MET:H	1.86	0.41
1:G:255:ILE:O	1:G:257:GLY:N	2.54	0.41
1:G:262:GLY:O	1:G:263:LEU:HG	2.21	0.41
1:G:287:LEU:CD1	1:G:289:SER:HB2	2.50	0.41
1:G:318:ILE:N	1:G:318:ILE:CD1	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:34:ASN:HB2	2:L:64:SER:CB	2.36	0.41
2:L:35:LEU:HD11	2:L:61:ILE:HG22	2.02	0.41
2:L:53:LEU:C	2:L:55:ILE:HD12	2.41	0.41
1:G:102:GLN:OE1	1:G:131:HIS:HE1	2.03	0.41
1:G:151:THR:O	1:G:153:GLN:N	2.53	0.41
2:L:37:PHE:CD1	2:L:38:ASN:HB3	2.57	0.41
1:G:137:LYS:CA	1:G:137:LYS:CE	2.95	0.40
1:G:172:LEU:O	1:G:177:HIS:CD2	2.75	0.40
2:L:23:VAL:HG13	2:L:46:SEP:C	2.51	0.40
2:L:24:GLN:O	2:L:27:SER:CB	2.63	0.40
1:G:80:ARG:NH2	1:G:84:ASP:OD2	2.52	0.40
2:L:77:LEU:O	2:L:80:THR:CG2	2.64	0.40
2:L:4:LYS:HD2	2:L:78:GLU:OE2	2.20	0.40
2:L:25:ALA:O	2:L:26:ALA:C	2.59	0.40
2:L:63:ILE:H	2:L:63:ILE:HG13	1.63	0.40
1:G:159:ILE:CD1	1:G:160:ASP:N	2.79	0.40
1:G:292:GLN:CG	1:G:294:MET:HE2	2.51	0.40
2:L:54:GLY:C	2:L:55:ILE:HD12	2.42	0.40
1:G:104:LYS:HA	1:G:104:LYS:HZ2	1.81	0.40
1:G:189:GLU:CB	1:G:191:ILE:HG22	2.44	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:94:ILE:CD1	1:G:94:ILE:CD1[8_665]	1.71	0.49

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	G	273/280 (98%)	164 (60%)	77 (28%)	32 (12%)	0 1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	L	84/88 (96%)	47 (56%)	18 (21%)	19 (23%)	0 0
All	All	357/368 (97%)	211 (59%)	95 (27%)	51 (14%)	0 1

All (51) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	100	GLN
1	G	108	LEU
1	G	109	LEU
1	G	110	ASN
1	G	131	HIS
1	G	150	SER
1	G	206	GLU
1	G	207	SER
1	G	208	GLY
1	G	213	ASP
1	G	220	ASP
1	G	278	ARG
1	G	299	ALA
1	G	311	LYS
2	L	3	GLN
2	L	16	ALA
2	L	28	LYS
2	L	29	PHE
2	L	30	ASP
2	L	59	ALA
2	L	68	SER
2	L	70	GLU
2	L	71	ALA
1	G	77	GLU
1	G	116	GLN
1	G	118	ASP
1	G	144	LEU
1	G	186	THR
1	G	275	ASP
2	L	13	GLY
2	L	38	ASN
2	L	39	GLY
2	L	54	GLY
2	L	74	LEU
1	G	68	PRO
1	G	99	ASP

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Mol	Chain	Res	Type
1	G	129	GLU
1	G	155	PRO
1	G	262	GLY
1	G	282	MET
2	L	11	ASP
2	L	24	GLN
1	G	76	ALA
1	G	90	LYS
1	G	126	ASN
2	L	40	LYS
1	G	300	VAL
1	G	315	ASP
2	L	8	VAL
1	G	70	ILE
2	L	58	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	G	241/244 (99%)	187 (78%)	54 (22%)	1 4
2	L	66/67 (98%)	48 (73%)	18 (27%)	0 1
All	All	307/311 (99%)	235 (76%)	72 (24%)	1 3

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	58	LYS
1	G	59	LYS
1	G	63	VAL
1	G	65	VAL
1	G	70	ILE
1	G	74	PHE
1	G	78	LEU
1	G	85	ILE

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Mol	Chain	Res	Type
1	G	90	LYS
1	G	104	LYS
1	G	109	LEU
1	G	112	MET
1	G	126	ASN
1	G	137	LYS
1	G	140	VAL
1	G	144	LEU
1	G	148	ILE
1	G	153	GLN
1	G	159	ILE
1	G	162	GLU
1	G	163	GLN
1	G	166	PHE
1	G	169	VAL
1	G	171	SER
1	G	172	LEU
1	G	174	ASP
1	G	179	ASN
1	G	182	PHE
1	G	191	ILE
1	G	193	HIS
1	G	195	LYS
1	G	196	LYS
1	G	202	ARG
1	G	205	THR
1	G	215	TYR
1	G	218	GLU
1	G	220	ASP
1	G	236	GLU
1	G	245	VAL
1	G	252	LEU
1	G	260	ASP
1	G	271	ILE
1	G	274	PHE
1	G	284	ARG
1	G	287	LEU
1	G	306	THR
1	G	313	THR
1	G	318	ILE
1	G	324	ARG
1	G	325	ILE

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Mol	Chain	Res	Type
1	G	327	PHE
1	G	328	ARG
1	G	331	THR
1	G	332	LYS
2	L	4	LYS
2	L	11	ASP
2	L	21	THR
2	L	24	GLN
2	L	30	ASP
2	L	32	ASP
2	L	36	GLU
2	L	44	LEU
2	L	51	MET
2	L	56	GLN
2	L	60	THR
2	L	61	ILE
2	L	62	THR
2	L	68	SER
2	L	69	ASP
2	L	72	ASP
2	L	79	ASP
2	L	80	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	92	ASN
1	G	126	ASN
1	G	152	ASN
1	G	153	GLN
1	G	163	GLN
1	G	256	HIS
1	G	267	ASN
1	G	292	GLN
1	G	310	ASN
2	L	24	GLN
2	L	56	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	SEP	L	46	2	8,9,10	1.08	0	8,12,14	2.56	2 (25%)

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	SEP	L	46	2	-	4/5/8/10	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L	46	SEP	OG-CB-CA	6.26	114.23	108.14
2	L	46	SEP	O3P-P-O1P	2.46	120.29	110.68

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	L	46	SEP	CB-OG-P-O2P
2	L	46	SEP	CB-OG-P-O3P
2	L	46	SEP	CA-CB-OG-P
2	L	46	SEP	N-CA-CB-OG

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L	46	SEP	3	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

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.