Full wwPDB X-ray Structure Validation Report (i)

Oct 18, 2023 – 03:55 PM EDT

PDB ID	:	2AHO
Title	:	Structure of the archaeal initiation factor eIF2 alpha-gamma heterodimer from Sulfolobus solfataricus complexed with GDPNP
Authors	:	Yatime, L.; Mechulam, Y.; Blanquet, S.; Schmitt, E.
Deposited on	:	2005-07-28
Resolution	:	3.00 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

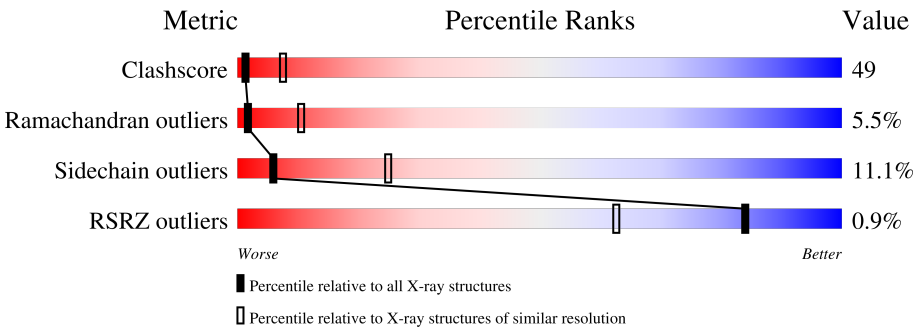
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.00 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	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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

Mol	Chain	Length	Quality of chain
1	A	414	37% 50% 9% • •
2	B	266	2% 26% 58% 12% • •

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 5253 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 Translation initiation factor 2 gamma subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	401	3102	1991	525	574	12	0	0	0

- Molecule 2 is a protein called Translation initiation factor 2 alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	259	2075	1326	354	393	2	0	0	0

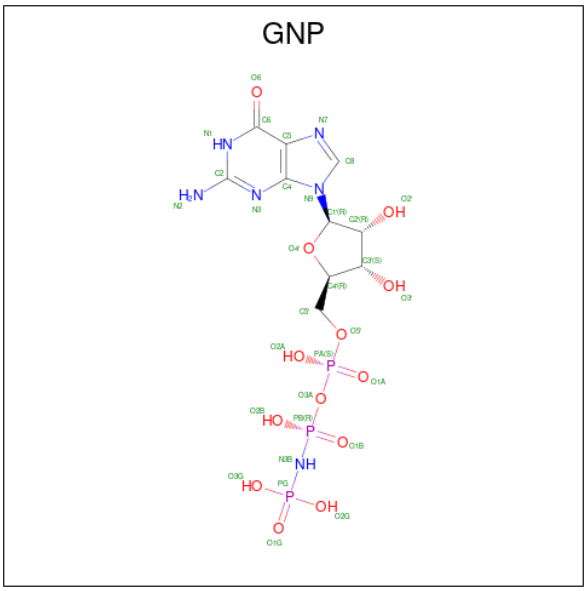
- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
3	A	1	1	1	0	0

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
4	A	1	1	1	0	0

- Molecule 5 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
5	A	1	32	10	6	13	3	0	0

- Molecule 6 is water.

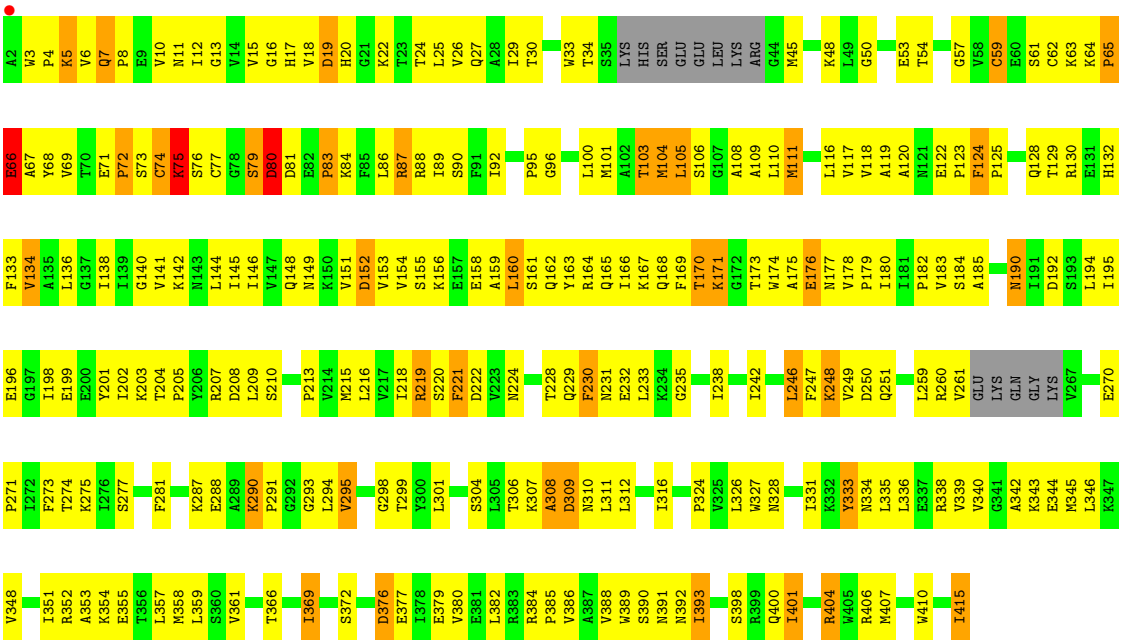
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	30	30	30	0	0
			Total	O		
6	B	12	12	12	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

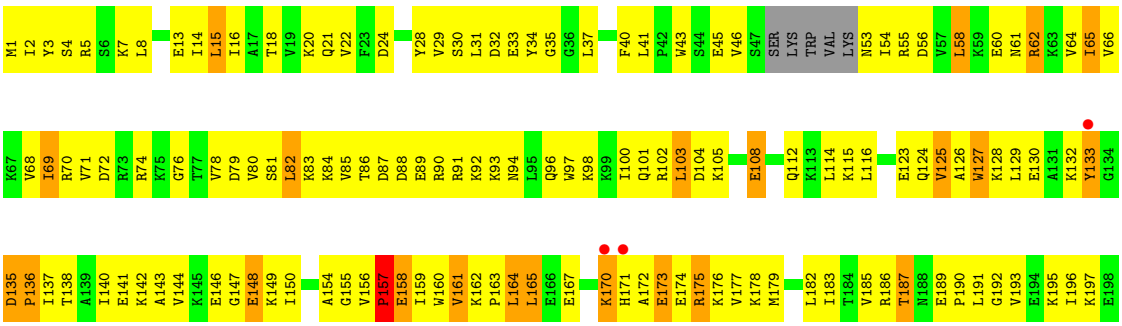
• Molecule 1: Translation initiation factor 2 gamma subunit

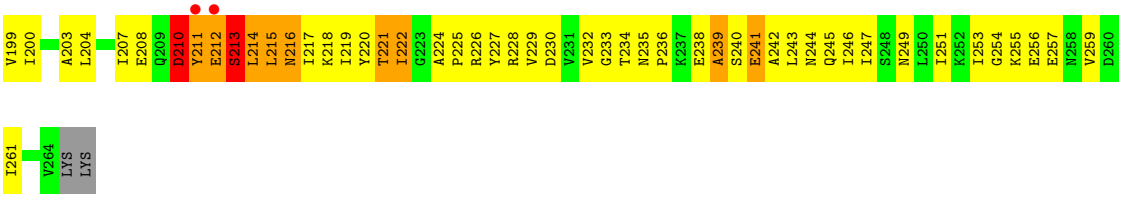
Chain A: 37% 50% 9%



• Molecule 2: Translation initiation factor 2 alpha subunit

Chain B: 2% 26% 58% 12%




V199
I200
A203
L204
I207
E208
Q209
D210
Y211
E212
S213
L214
L215
N216
I217
K218
I219
Y220
T221
I222
G223
A224
P225
R226
Y227
R228
V229
D230
V231
V232
G233
T234
N235
P236
K237
E238
A239
S240
E241
A242
L243
N244
Q245
I246
I247
S248
N249
L250
I251
K252
I253
G254
K255
E256
E257
N258
V259
D260

I261
V264
LYS
LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	39.60Å 112.90Å 194.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.00 – 3.00 38.80 – 3.00	Depositor EDS
% Data completeness (in resolution range)	92.6 (12.00-3.00) 96.0 (38.80-3.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	3.41 (at 3.01Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.224 , 0.291 0.240 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	56.2	Xtriage
Anisotropy	0.693	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 58.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	5253	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.66% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, GNP

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	0.45	0/3158	0.80	3/4279 (0.1%)
2	B	0.42	0/2102	0.80	8/2830 (0.3%)
All	All	0.44	0/5260	0.80	11/7109 (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	B	0	2

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	213	SER	CA-C-N	-12.02	90.75	117.20
1	A	80	ASP	N-CA-C	10.21	138.58	111.00
2	B	213	SER	N-CA-C	9.09	135.53	111.00
2	B	212	GLU	C-N-CA	-7.75	102.32	121.70
2	B	212	GLU	N-CA-C	7.40	130.98	111.00
2	B	213	SER	O-C-N	6.44	133.01	122.70
2	B	213	SER	C-N-CA	6.26	137.35	121.70
2	B	215	LEU	N-CA-C	5.53	125.93	111.00
1	A	79	SER	N-CA-C	5.25	125.18	111.00
1	A	105	LEU	CA-CB-CG	5.14	127.11	115.30
2	B	213	SER	CA-C-O	5.04	130.68	120.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	211	TYR	Sidechain
2	B	213	SER	Mainchain

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	3102	0	3217	293	0
2	B	2075	0	2183	244	0
3	A	1	0	0	0	0
4	A	1	0	0	0	0
5	A	32	0	13	2	0
6	A	30	0	0	3	0
6	B	12	0	0	0	0
All	All	5253	0	5413	522	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 (522) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:CYS:SG	1:A:83:PRO:HG3	1.84	1.17
2:B:212:GLU:HG2	2:B:213:SER:N	1.65	1.08
2:B:177:VAL:HG21	2:B:236:PRO:HG3	1.36	1.06
1:A:138:ILE:HD11	1:A:336:LEU:HD21	1.47	0.96
1:A:274:THR:HG22	1:A:275:LYS:H	1.28	0.95
1:A:221:PHE:HD2	1:A:222:ASP:H	1.06	0.94
1:A:11:ASN:ND2	1:A:293:GLY:H	1.65	0.94
2:B:211:TYR:HD1	2:B:245:GLN:NE2	1.66	0.93
2:B:114:LEU:O	2:B:116:LEU:HG	1.71	0.91
1:A:5:LYS:HE2	1:A:5:LYS:H	1.33	0.91
1:A:229:GLN:HB3	1:A:231:ASN:HD22	1.36	0.89
1:A:404:ARG:HD3	1:A:406:ARG:NH2	1.87	0.89
1:A:5:LYS:H	1:A:5:LYS:CE	1.86	0.89
1:A:11:ASN:HD21	1:A:293:GLY:H	1.15	0.88
2:B:224:ALA:HB3	2:B:225:PRO:HD3	1.55	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:170:LYS:HE3	2:B:173:GLU:HG3	1.56	0.87
1:A:120:ALA:HA	1:A:162:GLN:HE22	1.39	0.87
1:A:207:ARG:HE	1:A:291:PRO:HB2	1.40	0.87
2:B:124:GLN:NE2	2:B:160:TRP:HE1	1.73	0.86
1:A:24:THR:HG22	1:A:185:ALA:HB1	1.56	0.86
1:A:339:VAL:HG11	1:A:401:ILE:HD11	1.57	0.86
1:A:306:THR:HG22	1:A:311:LEU:CD1	2.05	0.85
1:A:218:ILE:HD11	1:A:294:LEU:HD11	1.56	0.85
2:B:172:ALA:HB1	2:B:176:LYS:NZ	1.92	0.85
2:B:219:ILE:HD12	2:B:229:VAL:HG12	1.59	0.85
1:A:5:LYS:HE2	1:A:5:LYS:N	1.91	0.84
1:A:176:GLU:HG3	1:A:177:ASN:H	1.41	0.84
2:B:155:GLY:O	2:B:157:PRO:HD3	1.79	0.82
1:A:124:PHE:HB3	1:A:125:PRO:HD3	1.58	0.82
1:A:306:THR:HG22	1:A:311:LEU:HD11	1.60	0.82
1:A:154:VAL:HG21	1:A:159:ALA:HB2	1.62	0.81
1:A:274:THR:HG22	1:A:275:LYS:N	1.96	0.81
1:A:248:LYS:NZ	1:A:288:GLU:HB3	1.95	0.81
1:A:11:ASN:HD21	1:A:293:GLY:N	1.78	0.81
1:A:30:THR:HG22	1:A:54:THR:HB	1.61	0.80
2:B:179:MET:SD	2:B:239:ALA:HB1	2.21	0.80
2:B:187:THR:HG22	2:B:189:GLU:HG2	1.62	0.80
1:A:179:PRO:HG2	1:A:201:TYR:CE2	2.18	0.79
2:B:172:ALA:HB1	2:B:176:LYS:HZ2	1.45	0.79
2:B:192:GLY:O	2:B:196:ILE:HG13	1.82	0.78
1:A:17:HIS:ND1	1:A:128:GLN:HB2	1.97	0.78
1:A:218:ILE:HG13	1:A:219:ARG:HG2	1.63	0.78
1:A:96:GLY:O	1:A:128:GLN:HG2	1.82	0.78
2:B:127:TRP:HE3	2:B:127:TRP:HA	1.49	0.77
1:A:233:LEU:HD11	2:B:227:TYR:HE2	1.50	0.77
1:A:248:LYS:HZ3	1:A:288:GLU:HB3	1.50	0.76
2:B:127:TRP:HA	2:B:127:TRP:CE3	2.18	0.76
2:B:212:GLU:CG	2:B:213:SER:N	2.38	0.76
1:A:339:VAL:HG23	1:A:339:VAL:O	1.85	0.76
1:A:161:SER:O	1:A:164:ARG:HB2	1.86	0.75
2:B:62:ARG:HB2	2:B:62:ARG:HH11	1.50	0.75
1:A:205:PRO:HD2	1:A:207:ARG:HH12	1.51	0.75
2:B:69:ILE:HG22	2:B:70:ARG:HG3	1.68	0.74
2:B:105:LYS:NZ	2:B:234:THR:HG21	2.01	0.74
2:B:124:GLN:HE21	2:B:160:TRP:HE1	1.34	0.74
2:B:102:ARG:HD2	2:B:137:ILE:HD11	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:GLN:HE22	1:A:290:LYS:H	1.36	0.73
2:B:148:GLU:HB3	2:B:165:LEU:HD11	1.70	0.73
2:B:214:LEU:O	2:B:214:LEU:HD23	1.88	0.73
2:B:7:LYS:HG3	2:B:8:LEU:HG	1.70	0.73
2:B:46:VAL:HA	2:B:82:LEU:CD1	2.18	0.73
1:A:207:ARG:HE	1:A:291:PRO:CB	2.00	0.73
1:A:3:TRP:CD2	1:A:72:PRO:HG3	2.23	0.72
1:A:339:VAL:HG12	1:A:348:VAL:HG22	1.69	0.72
2:B:215:LEU:HB2	2:B:233:GLY:HA2	1.70	0.72
2:B:224:ALA:HB3	2:B:225:PRO:CD	2.20	0.72
2:B:86:THR:HG22	2:B:88:ASP:H	1.55	0.72
2:B:97:TRP:HA	2:B:100:ILE:HG22	1.72	0.72
1:A:346:LEU:HD11	1:A:401:ILE:HD13	1.72	0.71
2:B:60:GLU:HG3	2:B:61:ASN:ND2	2.06	0.71
2:B:160:TRP:O	2:B:163:PRO:HD2	1.88	0.71
1:A:87:ARG:HD2	1:A:199:GLU:OE2	1.90	0.71
1:A:259:LEU:HD12	1:A:260:ARG:H	1.55	0.70
1:A:74:CYS:SG	1:A:83:PRO:CG	2.75	0.70
1:A:195:ILE:O	1:A:199:GLU:HB2	1.90	0.70
2:B:159:ILE:N	2:B:159:ILE:HD12	2.07	0.70
1:A:120:ALA:HA	1:A:162:GLN:NE2	2.05	0.69
1:A:308:ALA:O	1:A:309:ASP:OD2	2.11	0.69
1:A:274:THR:HG21	1:A:299:THR:HB	1.74	0.69
2:B:182:LEU:HD21	2:B:228:ARG:HH21	1.56	0.69
1:A:24:THR:HG22	1:A:185:ALA:CB	2.23	0.69
2:B:163:PRO:O	2:B:167:GLU:HB2	1.92	0.69
1:A:166:ILE:O	1:A:170:THR:HG22	1.93	0.69
1:A:68:TYR:HE1	1:A:196:GLU:HG3	1.57	0.68
1:A:176:GLU:HG3	1:A:177:ASN:N	2.08	0.68
2:B:220:TYR:OH	2:B:228:ARG:HD2	1.94	0.68
1:A:221:PHE:HD2	1:A:222:ASP:N	1.85	0.68
2:B:222:ILE:HD13	2:B:222:ILE:O	1.93	0.68
1:A:233:LEU:HD21	2:B:221:THR:HG21	1.74	0.68
2:B:182:LEU:HD21	2:B:228:ARG:NH2	2.09	0.68
2:B:238:GLU:HA	2:B:241:GLU:HG3	1.76	0.68
1:A:22:LYS:O	1:A:26:VAL:HG23	1.94	0.67
1:A:307:LYS:O	1:A:308:ALA:O	2.13	0.67
1:A:205:PRO:HD2	1:A:207:ARG:NH1	2.08	0.67
1:A:242:ILE:HD11	1:A:247:PHE:CD1	2.31	0.66
2:B:179:MET:HG3	2:B:239:ALA:HA	1.77	0.66
1:A:144:LEU:HD12	1:A:145:ILE:H	1.58	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:254:GLY:C	2:B:256:GLU:H	1.97	0.66
1:A:59:CYS:HB2	1:A:74:CYS:SG	2.36	0.65
2:B:46:VAL:HA	2:B:82:LEU:HD11	1.78	0.65
1:A:233:LEU:HD21	2:B:221:THR:CG2	2.25	0.65
1:A:220:SER:HB2	1:A:306:THR:HB	1.78	0.65
2:B:215:LEU:HB3	2:B:232:VAL:O	1.97	0.65
1:A:238:ILE:HG21	1:A:316:ILE:HD11	1.77	0.65
1:A:109:ALA:C	1:A:110:LEU:HD12	2.17	0.65
1:A:124:PHE:CB	1:A:125:PRO:HD3	2.26	0.65
1:A:274:THR:CG2	1:A:275:LYS:H	2.06	0.65
1:A:176:GLU:CG	1:A:177:ASN:H	2.08	0.64
1:A:154:VAL:CG2	1:A:159:ALA:HB2	2.27	0.64
1:A:249:VAL:O	1:A:250:ASP:HB2	1.97	0.64
1:A:352:ARG:HG3	1:A:352:ARG:HH11	1.63	0.64
2:B:234:THR:O	2:B:236:PRO:HD3	1.97	0.64
1:A:306:THR:HG22	1:A:311:LEU:HD12	1.78	0.64
1:A:406:ARG:HG3	1:A:406:ARG:HH11	1.63	0.64
1:A:156:LYS:HD2	1:A:156:LYS:N	2.13	0.63
1:A:307:LYS:HD2	2:B:224:ALA:CB	2.27	0.63
1:A:53:GLU:OE2	1:A:88:ARG:NH1	2.30	0.63
1:A:34:THR:HG21	1:A:50:GLY:HA3	1.80	0.63
2:B:191:LEU:HD12	2:B:191:LEU:N	2.13	0.63
1:A:155:SER:HB3	1:A:158:GLU:HG3	1.82	0.62
2:B:212:GLU:HG2	2:B:213:SER:CB	2.29	0.62
1:A:218:ILE:HD11	1:A:294:LEU:CD1	2.28	0.62
1:A:207:ARG:HG2	1:A:291:PRO:HB2	1.81	0.62
1:A:324:PRO:HD2	1:A:388:VAL:O	1.98	0.62
2:B:158:GLU:OE1	2:B:158:GLU:N	2.32	0.62
1:A:87:ARG:HD3	1:A:89:ILE:CG2	2.29	0.62
1:A:242:ILE:HD11	1:A:247:PHE:HD1	1.65	0.62
2:B:123:GLU:HA	2:B:127:TRP:CD1	2.35	0.62
1:A:248:LYS:HZ3	1:A:248:LYS:HB3	1.64	0.61
1:A:209:LEU:HD13	1:A:246:LEU:HD23	1.82	0.61
2:B:143:ALA:HB1	2:B:165:LEU:HD21	1.83	0.61
2:B:195:LYS:HD2	2:B:257:GLU:OE1	2.00	0.61
1:A:307:LYS:HD2	2:B:224:ALA:HB1	1.81	0.61
2:B:66:VAL:HA	2:B:85:VAL:HG21	1.83	0.61
1:A:248:LYS:NZ	1:A:248:LYS:HB3	2.16	0.61
1:A:327:TRP:CE2	1:A:385:PRO:HG3	2.36	0.61
2:B:214:LEU:HD23	2:B:214:LEU:C	2.21	0.61
2:B:215:LEU:O	2:B:216:ASN:HB2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:PRO:HB2	1:A:273:PHE:CE1	2.35	0.61
1:A:390:SER:O	1:A:415:ILE:HD11	2.01	0.60
1:A:281:PHE:CE1	1:A:295:VAL:HG13	2.36	0.60
1:A:16:GLY:H	1:A:132:HIS:CD2	2.19	0.60
1:A:5:LYS:H	1:A:5:LYS:CD	2.14	0.60
1:A:20:HIS:CE1	1:A:119:ALA:H	2.20	0.60
1:A:333:TYR:CE2	1:A:376:ASP:HA	2.37	0.60
1:A:138:ILE:HG23	1:A:410:TRP:CG	2.37	0.59
2:B:138:THR:O	2:B:141:GLU:HB3	2.02	0.59
1:A:151:VAL:O	1:A:153:VAL:N	2.35	0.59
1:A:307:LYS:O	1:A:308:ALA:C	2.40	0.59
2:B:14:ILE:O	2:B:15:LEU:HB3	2.02	0.59
2:B:143:ALA:HA	2:B:150:ILE:HD12	1.83	0.59
2:B:240:SER:O	2:B:241:GLU:C	2.40	0.59
2:B:89:GLU:O	2:B:93:LYS:HB2	2.03	0.59
2:B:71:VAL:HG22	2:B:78:VAL:HG22	1.84	0.59
1:A:68:TYR:CE1	1:A:196:GLU:HG3	2.37	0.59
2:B:170:LYS:CE	2:B:173:GLU:HG3	2.31	0.58
2:B:179:MET:SD	2:B:239:ALA:CB	2.92	0.58
1:A:13:GLY:HA3	1:A:111:MET:SD	2.43	0.58
2:B:156:VAL:O	2:B:158:GLU:OE1	2.22	0.58
1:A:104:MET:CE	1:A:108:ALA:HB2	2.32	0.58
1:A:207:ARG:NE	1:A:291:PRO:HB2	2.17	0.58
1:A:73:SER:HB3	1:A:75:LYS:HE2	1.84	0.57
1:A:342:ALA:HB2	1:A:406:ARG:NH1	2.19	0.57
1:A:406:ARG:HD3	6:A:538:HOH:O	2.04	0.57
2:B:5:ARG:N	2:B:127:TRP:CZ2	2.72	0.57
1:A:17:HIS:HA	1:A:128:GLN:HB3	1.86	0.57
1:A:306:THR:O	1:A:306:THR:OG1	2.22	0.57
1:A:339:VAL:HG11	1:A:401:ILE:CD1	2.32	0.57
2:B:1:MET:HE3	2:B:3:TYR:CZ	2.40	0.57
2:B:207:ILE:CD1	2:B:245:GLN:NE2	2.68	0.57
1:A:162:GLN:HA	1:A:165:GLN:NE2	2.18	0.57
1:A:183:VAL:HG23	1:A:184:SER:N	2.18	0.57
1:A:353:ALA:O	1:A:354:LYS:HB2	2.04	0.57
2:B:142:LYS:HB2	2:B:150:ILE:HD13	1.87	0.57
2:B:43:TRP:CZ3	2:B:58:LEU:HD11	2.40	0.57
2:B:162:LYS:HB2	2:B:162:LYS:NZ	2.20	0.57
1:A:229:GLN:O	1:A:231:ASN:N	2.38	0.56
2:B:211:TYR:CD1	2:B:245:GLN:NE2	2.59	0.56
2:B:212:GLU:HG2	2:B:213:SER:H	1.64	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:ILE:HG22	1:A:291:PRO:HG3	1.86	0.56
2:B:158:GLU:C	2:B:159:ILE:HD12	2.26	0.56
1:A:151:VAL:HG11	1:A:182:PRO:HB2	1.88	0.56
1:A:163:TYR:CE1	1:A:180:ILE:HB	2.41	0.56
1:A:209:LEU:HD13	1:A:246:LEU:CD2	2.36	0.56
1:A:231:ASN:HB2	1:A:232:GLU:OE2	2.06	0.56
1:A:355:GLU:OE2	1:A:357:LEU:HD21	2.06	0.56
1:A:65:PRO:O	1:A:67:ALA:N	2.39	0.56
1:A:110:LEU:HD12	1:A:110:LEU:N	2.21	0.55
1:A:145:ILE:HD12	1:A:198:ILE:HG22	1.88	0.55
1:A:155:SER:HB3	1:A:158:GLU:CG	2.36	0.55
1:A:74:CYS:C	1:A:76:SER:H	2.10	0.55
1:A:180:ILE:N	1:A:180:ILE:HD12	2.21	0.55
1:A:5:LYS:O	1:A:5:LYS:HG2	2.05	0.55
2:B:219:ILE:HD12	2:B:229:VAL:CG1	2.34	0.55
1:A:79:SER:OG	1:A:80:ASP:N	2.37	0.55
1:A:155:SER:HB3	1:A:158:GLU:HB2	1.88	0.55
1:A:249:VAL:HG23	1:A:287:LYS:O	2.07	0.55
2:B:170:LYS:HE3	2:B:170:LYS:HA	1.88	0.55
1:A:15:VAL:HB	1:A:132:HIS:HD2	1.72	0.55
2:B:162:LYS:HB2	2:B:163:PRO:HD3	1.89	0.55
2:B:175:ARG:O	2:B:234:THR:HA	2.05	0.55
1:A:18:VAL:HG22	1:A:19:ASP:N	2.22	0.55
1:A:17:HIS:HA	1:A:128:GLN:CB	2.37	0.54
1:A:229:GLN:HB3	1:A:231:ASN:ND2	2.16	0.54
2:B:22:VAL:HG22	2:B:58:LEU:HD22	1.89	0.54
2:B:15:LEU:HD11	2:B:31:LEU:HD22	1.87	0.54
2:B:203:ALA:HB1	2:B:249:ASN:HB3	1.89	0.54
1:A:104:MET:HE2	1:A:108:ALA:HB2	1.88	0.54
2:B:93:LYS:HG3	2:B:96:GLN:NE2	2.22	0.54
2:B:156:VAL:O	2:B:157:PRO:C	2.46	0.54
2:B:93:LYS:HA	2:B:96:GLN:NE2	2.23	0.54
1:A:148:GLN:O	1:A:182:PRO:HA	2.08	0.54
1:A:221:PHE:CD2	1:A:222:ASP:N	2.67	0.54
2:B:15:LEU:CD1	2:B:31:LEU:HD22	2.37	0.54
2:B:93:LYS:HG3	2:B:96:GLN:HE22	1.72	0.54
2:B:235:ASN:OD1	2:B:238:GLU:HG3	2.08	0.54
1:A:20:HIS:CD2	1:A:119:ALA:HB2	2.43	0.54
1:A:73:SER:CB	1:A:75:LYS:HE2	2.37	0.54
1:A:64:LYS:HG2	1:A:67:ALA:HB3	1.90	0.53
2:B:149:LYS:O	2:B:149:LYS:HD3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:159:ILE:N	2:B:159:ILE:CD1	2.71	0.53
2:B:190:PRO:HB2	2:B:191:LEU:HD12	1.89	0.53
2:B:159:ILE:O	2:B:163:PRO:HG2	2.08	0.53
2:B:212:GLU:HG2	2:B:213:SER:HB3	1.90	0.53
2:B:20:LYS:HG2	2:B:21:GLN:HG3	1.90	0.53
2:B:105:LYS:HZ2	2:B:234:THR:HG21	1.72	0.53
2:B:177:VAL:O	2:B:232:VAL:HA	2.08	0.53
1:A:87:ARG:NH2	1:A:204:THR:N	2.56	0.53
1:A:307:LYS:NZ	2:B:224:ALA:CB	2.72	0.53
2:B:187:THR:CG2	2:B:189:GLU:HG2	2.34	0.53
1:A:87:ARG:HH21	1:A:204:THR:H	1.56	0.53
2:B:4:SER:HA	2:B:127:TRP:HZ2	1.74	0.52
2:B:46:VAL:HG11	2:B:54:ILE:HD11	1.91	0.52
1:A:151:VAL:HG23	1:A:152:ASP:N	2.24	0.52
2:B:216:ASN:HB3	2:B:232:VAL:CG2	2.40	0.52
2:B:253:ILE:O	2:B:257:GLU:HB2	2.09	0.52
1:A:15:VAL:HB	1:A:132:HIS:CD2	2.45	0.52
1:A:261:VAL:HG21	1:A:270:GLU:OE1	2.09	0.52
2:B:24:ASP:O	2:B:43:TRP:NE1	2.38	0.52
2:B:216:ASN:HB3	2:B:232:VAL:HG23	1.91	0.52
1:A:233:LEU:HD11	2:B:227:TYR:CE2	2.38	0.52
2:B:127:TRP:O	2:B:130:GLU:HB3	2.10	0.52
1:A:194:LEU:O	1:A:198:ILE:HG23	2.10	0.52
1:A:389:TRP:CZ2	1:A:393:ILE:HD12	2.44	0.52
1:A:400:GLN:O	1:A:400:GLN:HG2	2.10	0.52
2:B:53:ASN:C	2:B:55:ARG:N	2.62	0.52
1:A:218:ILE:C	1:A:219:ARG:HG2	2.27	0.52
2:B:235:ASN:HB3	2:B:238:GLU:OE1	2.09	0.52
1:A:340:VAL:HG23	1:A:340:VAL:O	2.10	0.51
2:B:148:GLU:HB2	2:B:161:VAL:CG1	2.39	0.51
2:B:195:LYS:O	2:B:199:VAL:HG22	2.10	0.51
2:B:259:VAL:HG12	2:B:261:ILE:HG13	1.92	0.51
1:A:160:LEU:O	1:A:164:ARG:HG2	2.10	0.51
2:B:125:VAL:HA	2:B:156:VAL:HG13	1.92	0.51
1:A:3:TRP:CE3	1:A:72:PRO:HG3	2.45	0.51
1:A:230:PHE:HB2	2:B:200:ILE:HD12	1.92	0.51
2:B:136:PRO:O	2:B:140:ILE:HG13	2.10	0.51
2:B:193:VAL:O	2:B:197:LYS:HG3	2.10	0.51
2:B:222:ILE:HG22	2:B:226:ARG:O	2.10	0.51
2:B:15:LEU:O	2:B:15:LEU:HD12	2.10	0.51
1:A:140:GLY:O	1:A:142:LYS:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:14:ILE:O	2:B:15:LEU:CB	2.59	0.51
2:B:114:LEU:HD12	2:B:160:TRP:CZ3	2.46	0.51
2:B:142:LYS:CB	2:B:150:ILE:HD13	2.40	0.51
1:A:87:ARG:HH21	1:A:204:THR:N	2.09	0.51
1:A:103:THR:O	1:A:106:SER:HB3	2.10	0.51
1:A:116:LEU:H	1:A:144:LEU:HD11	1.75	0.51
2:B:240:SER:HB2	2:B:244:ASN:OD1	2.10	0.51
1:A:8:PRO:HB2	1:A:293:GLY:CA	2.40	0.51
2:B:65:ILE:HD13	2:B:90:ARG:HA	1.93	0.51
1:A:87:ARG:NH2	1:A:204:THR:H	2.09	0.51
1:A:207:ARG:HG2	1:A:291:PRO:CB	2.40	0.51
2:B:66:VAL:HG21	2:B:80:VAL:HG21	1.92	0.51
2:B:172:ALA:HB1	2:B:176:LYS:HZ3	1.72	0.51
1:A:63:LYS:O	1:A:66:GLU:HG3	2.11	0.50
1:A:333:TYR:CE1	1:A:351:ILE:HD12	2.46	0.50
1:A:259:LEU:HD12	1:A:260:ARG:N	2.24	0.50
2:B:13:GLU:O	2:B:68:VAL:HG23	2.10	0.50
2:B:83:LYS:HD3	2:B:83:LYS:C	2.31	0.50
2:B:102:ARG:HD2	2:B:137:ILE:CD1	2.39	0.50
1:A:20:HIS:CG	1:A:119:ALA:HB2	2.47	0.50
2:B:29:VAL:HG22	2:B:30:SER:H	1.77	0.50
2:B:41:LEU:HD21	2:B:82:LEU:HD21	1.92	0.50
1:A:392:ASN:O	1:A:393:ILE:C	2.50	0.50
2:B:222:ILE:HD13	2:B:222:ILE:C	2.31	0.50
2:B:247:ILE:O	2:B:251:ILE:HG13	2.11	0.50
1:A:203:LYS:HD2	1:A:204:THR:O	2.12	0.50
1:A:339:VAL:CG2	1:A:346:LEU:HG	2.41	0.50
2:B:147:GLY:C	2:B:149:LYS:H	2.14	0.50
2:B:254:GLY:C	2:B:256:GLU:N	2.65	0.50
1:A:155:SER:HB3	1:A:158:GLU:CB	2.41	0.50
1:A:162:GLN:HA	1:A:165:GLN:HE21	1.76	0.49
1:A:352:ARG:O	1:A:355:GLU:HB2	2.11	0.49
2:B:97:TRP:O	2:B:101:GLN:N	2.45	0.49
2:B:182:LEU:CD2	2:B:228:ARG:HE	2.25	0.49
1:A:101:MET:HG3	1:A:105:LEU:HD21	1.94	0.49
2:B:148:GLU:HB3	2:B:165:LEU:CD1	2.39	0.49
1:A:59:CYS:CB	1:A:74:CYS:SG	3.00	0.49
1:A:87:ARG:HD3	1:A:89:ILE:HG23	1.94	0.49
2:B:124:GLN:HB3	2:B:157:PRO:HD2	1.94	0.49
1:A:29:ILE:O	1:A:29:ILE:HG22	2.11	0.49
1:A:178:VAL:O	1:A:180:ILE:HD12	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:28:TYR:CE1	2:B:40:PHE:HD1	2.31	0.49
2:B:143:ALA:N	2:B:150:ILE:HD12	2.27	0.49
1:A:132:HIS:O	1:A:136:LEU:HG	2.12	0.49
1:A:207:ARG:HG2	1:A:291:PRO:HG2	1.94	0.49
1:A:248:LYS:N	1:A:251:GLN:OE1	2.42	0.49
1:A:307:LYS:NZ	2:B:224:ALA:HB2	2.28	0.49
2:B:45:GLU:HG3	2:B:69:ILE:HD11	1.95	0.49
1:A:169:PHE:C	1:A:171:LYS:H	2.16	0.49
1:A:100:LEU:O	1:A:101:MET:C	2.51	0.49
1:A:229:GLN:C	1:A:231:ASN:N	2.64	0.49
2:B:4:SER:CA	2:B:127:TRP:HZ2	2.25	0.49
2:B:254:GLY:O	2:B:256:GLU:N	2.43	0.49
2:B:14:ILE:CG2	2:B:15:LEU:N	2.75	0.48
1:A:10:VAL:HG22	1:A:11:ASN:N	2.29	0.48
2:B:167:GLU:O	2:B:171:HIS:HB2	2.12	0.48
2:B:20:LYS:O	2:B:21:GLN:HG3	2.14	0.48
2:B:43:TRP:O	2:B:45:GLU:N	2.46	0.48
1:A:84:LYS:HE3	1:A:86:LEU:HD21	1.96	0.48
2:B:143:ALA:CA	2:B:150:ILE:HD12	2.43	0.48
1:A:18:VAL:CG2	1:A:19:ASP:N	2.75	0.48
1:A:209:LEU:HD22	1:A:246:LEU:HB3	1.94	0.48
1:A:238:ILE:CG2	1:A:316:ILE:HD11	2.43	0.48
1:A:277:SER:N	1:A:298:GLY:O	2.46	0.48
1:A:171:LYS:C	1:A:171:LYS:HE3	2.34	0.48
1:A:361:VAL:HG23	1:A:361:VAL:O	2.13	0.48
2:B:32:ASP:C	2:B:34:TYR:H	2.16	0.48
1:A:7:GLN:HE22	1:A:290:LYS:N	2.09	0.48
2:B:1:MET:O	2:B:104:ASP:OD1	2.30	0.48
2:B:211:TYR:CE2	2:B:241:GLU:HB3	2.49	0.48
1:A:334:ASN:O	1:A:335:LEU:HD23	2.14	0.47
2:B:179:MET:HG3	2:B:239:ALA:CA	2.41	0.47
2:B:232:VAL:O	2:B:232:VAL:HG23	2.13	0.47
1:A:16:GLY:H	1:A:132:HIS:HD2	1.59	0.47
1:A:179:PRO:C	1:A:180:ILE:HD12	2.33	0.47
2:B:123:GLU:HG3	2:B:127:TRP:HD1	1.79	0.47
2:B:211:TYR:CD2	2:B:241:GLU:HB3	2.49	0.47
1:A:134:VAL:HG11	1:A:340:VAL:HG21	1.95	0.47
1:A:163:TYR:CZ	1:A:180:ILE:HB	2.50	0.47
2:B:72:ASP:O	2:B:76:GLY:N	2.47	0.47
2:B:4:SER:HA	2:B:127:TRP:CZ2	2.49	0.47
2:B:190:PRO:C	2:B:191:LEU:HD12	2.34	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:215:LEU:CB	2:B:233:GLY:HA2	2.41	0.47
1:A:29:ILE:HD11	1:A:194:LEU:HD23	1.96	0.47
1:A:339:VAL:HG12	1:A:348:VAL:CG2	2.43	0.47
2:B:154:ALA:HB3	2:B:156:VAL:HG23	1.95	0.47
1:A:48:LYS:HE3	6:A:521:HOH:O	2.15	0.47
2:B:160:TRP:O	2:B:161:VAL:C	2.52	0.47
1:A:7:GLN:NE2	1:A:290:LYS:HG3	2.28	0.47
1:A:57:GLY:O	1:A:69:VAL:HG22	2.15	0.47
1:A:144:LEU:HD12	1:A:145:ILE:N	2.29	0.47
1:A:274:THR:OG1	1:A:301:LEU:HD23	2.14	0.47
2:B:172:ALA:O	2:B:176:LYS:HG3	2.14	0.47
2:B:242:ALA:O	2:B:246:ILE:HG13	2.15	0.47
1:A:59:CYS:SG	1:A:74:CYS:SG	3.13	0.47
1:A:230:PHE:CD2	2:B:219:ILE:HB	2.49	0.47
1:A:207:ARG:HG2	1:A:291:PRO:CG	2.45	0.47
1:A:326:LEU:HD23	1:A:388:VAL:CG2	2.45	0.47
1:A:382:LEU:HD13	1:A:386:VAL:HG13	1.97	0.47
2:B:16:ILE:HG12	2:B:97:TRP:CE3	2.50	0.47
2:B:129:LEU:HB2	2:B:136:PRO:HB3	1.97	0.47
2:B:179:MET:HG3	2:B:239:ALA:CB	2.44	0.47
2:B:161:VAL:O	2:B:164:LEU:HB2	2.15	0.46
2:B:240:SER:HB2	2:B:244:ASN:CG	2.34	0.46
1:A:307:LYS:HZ1	2:B:224:ALA:HB2	1.80	0.46
2:B:13:GLU:HG2	2:B:14:ILE:O	2.14	0.46
1:A:151:VAL:C	1:A:153:VAL:H	2.19	0.46
1:A:151:VAL:CG2	1:A:152:ASP:N	2.78	0.46
1:A:251:GLN:O	1:A:275:LYS:HA	2.15	0.46
2:B:22:VAL:HG22	2:B:58:LEU:CD2	2.46	0.46
2:B:43:TRP:C	2:B:45:GLU:N	2.68	0.46
2:B:97:TRP:CA	2:B:100:ILE:HG22	2.44	0.46
2:B:2:ILE:O	2:B:2:ILE:HG22	2.14	0.46
2:B:127:TRP:CE3	2:B:127:TRP:CA	2.97	0.46
1:A:124:PHE:CD1	1:A:124:PHE:C	2.88	0.46
1:A:235:GLY:HA2	2:B:193:VAL:HG21	1.98	0.46
1:A:331:ILE:O	1:A:377:GLU:HA	2.15	0.46
1:A:80:ASP:O	1:A:81:ASP:C	2.53	0.46
2:B:4:SER:C	2:B:127:TRP:HZ2	2.19	0.46
1:A:8:PRO:HB2	1:A:293:GLY:HA3	1.98	0.46
1:A:358:MET:HB3	1:A:398:SER:HB2	1.97	0.46
2:B:90:ARG:O	2:B:94:ASN:HB2	2.14	0.46
2:B:94:ASN:O	2:B:97:TRP:HB3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:125:VAL:HG12	2:B:126:ALA:N	2.31	0.46
1:A:122:GLU:O	1:A:124:PHE:N	2.49	0.46
1:A:326:LEU:N	1:A:326:LEU:HD22	2.30	0.46
1:A:164:ARG:O	1:A:167:LYS:HB3	2.16	0.45
1:A:179:PRO:HG2	1:A:201:TYR:CZ	2.50	0.45
1:A:389:TRP:CE2	1:A:393:ILE:HD12	2.52	0.45
1:A:270:GLU:HA	1:A:271:PRO:HD3	1.79	0.45
2:B:170:LYS:HA	2:B:173:GLU:CG	2.47	0.45
1:A:215:MET:SD	1:A:316:ILE:HD12	2.56	0.45
2:B:66:VAL:HG12	2:B:82:LEU:HB3	1.98	0.45
1:A:57:GLY:C	1:A:69:VAL:HG22	2.37	0.45
1:A:73:SER:OG	1:A:75:LYS:HE2	2.16	0.45
1:A:218:ILE:HA	1:A:312:LEU:CD1	2.46	0.45
2:B:108:GLU:O	2:B:112:GLN:HB2	2.17	0.45
2:B:212:GLU:HG2	2:B:213:SER:CA	2.43	0.45
1:A:6:VAL:O	1:A:88:ARG:HD2	2.17	0.45
1:A:74:CYS:HB3	1:A:79:SER:O	2.17	0.45
1:A:77:CYS:SG	1:A:77:CYS:O	2.75	0.45
1:A:110:LEU:N	1:A:110:LEU:CD1	2.80	0.45
2:B:22:VAL:CG2	2:B:58:LEU:HD22	2.46	0.45
2:B:160:TRP:O	2:B:163:PRO:CD	2.63	0.45
1:A:326:LEU:HD23	1:A:388:VAL:HG21	1.98	0.45
2:B:86:THR:HG22	2:B:87:ASP:N	2.31	0.45
1:A:130:ARG:O	1:A:134:VAL:HG13	2.17	0.45
1:A:169:PHE:O	1:A:171:LYS:N	2.50	0.45
1:A:134:VAL:HG22	1:A:407:MET:CE	2.46	0.45
2:B:74:ARG:HG2	2:B:74:ARG:HH11	1.82	0.45
1:A:352:ARG:HG3	1:A:352:ARG:NH1	2.32	0.44
2:B:148:GLU:HB2	2:B:161:VAL:HG13	1.99	0.44
1:A:384:ARG:NH2	6:A:532:HOH:O	2.49	0.44
2:B:91:ARG:O	2:B:94:ASN:HB3	2.17	0.44
1:A:176:GLU:CG	1:A:177:ASN:N	2.75	0.44
2:B:1:MET:CE	2:B:3:TYR:CZ	3.01	0.44
2:B:43:TRP:C	2:B:45:GLU:H	2.20	0.44
2:B:132:LYS:O	2:B:133:TYR:C	2.55	0.44
2:B:218:LYS:O	2:B:219:ILE:HD13	2.17	0.44
2:B:176:LYS:NZ	2:B:215:LEU:HD21	2.33	0.44
1:A:11:ASN:ND2	1:A:90:SER:OG	2.50	0.44
1:A:228:THR:O	2:B:221:THR:HG22	2.18	0.44
2:B:148:GLU:CB	2:B:165:LEU:HD11	2.43	0.44
1:A:338:ARG:HD2	1:A:345:MET:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:143:ALA:HB1	2:B:165:LEU:CD2	2.47	0.44
1:A:17:HIS:HB2	1:A:129:THR:OG1	2.18	0.44
2:B:210:ASP:O	2:B:212:GLU:N	2.51	0.44
1:A:170:THR:O	1:A:175:ALA:O	2.36	0.43
1:A:208:ASP:CG	1:A:210:SER:HG	2.20	0.43
2:B:68:VAL:O	2:B:69:ILE:C	2.57	0.43
1:A:152:ASP:CG	5:A:912:GNP:HN1	2.21	0.43
2:B:53:ASN:C	2:B:55:ARG:H	2.21	0.43
2:B:203:ALA:HB1	2:B:249:ASN:CB	2.47	0.43
1:A:12:ILE:HG12	1:A:202:ILE:HG21	2.01	0.43
2:B:207:ILE:HD11	2:B:211:TYR:HB2	1.99	0.43
1:A:71:GLU:O	1:A:73:SER:N	2.49	0.43
2:B:217:ILE:HA	2:B:230:ASP:O	2.19	0.43
2:B:240:SER:O	2:B:243:LEU:N	2.51	0.43
1:A:215:MET:HG2	1:A:216:LEU:N	2.32	0.43
1:A:124:PHE:CB	1:A:125:PRO:CD	2.94	0.43
2:B:224:ALA:CB	2:B:225:PRO:HD3	2.37	0.43
1:A:25:LEU:HD13	1:A:183:VAL:HG21	2.00	0.43
2:B:171:HIS:CE1	2:B:175:ARG:HG3	2.54	0.43
1:A:13:GLY:HA2	1:A:92:ILE:HB	2.01	0.43
1:A:247:PHE:HA	1:A:251:GLN:OE1	2.19	0.43
1:A:69:VAL:HG11	1:A:83:PRO:HG2	2.00	0.43
1:A:74:CYS:O	1:A:76:SER:N	2.49	0.43
1:A:224:ASN:ND2	1:A:233:LEU:HD22	2.34	0.43
1:A:229:GLN:C	1:A:231:ASN:H	2.22	0.43
2:B:178:LYS:HB2	2:B:232:VAL:HG12	2.01	0.43
1:A:346:LEU:HD11	1:A:401:ILE:CD1	2.45	0.42
2:B:86:THR:HB	2:B:89:GLU:HG3	2.00	0.42
2:B:170:LYS:HA	2:B:173:GLU:HG2	2.00	0.42
1:A:11:ASN:HD21	1:A:293:GLY:CA	2.30	0.42
1:A:261:VAL:CG2	1:A:270:GLU:OE1	2.66	0.42
2:B:212:GLU:CG	2:B:213:SER:H	2.24	0.42
1:A:190:ASN:HD22	1:A:190:ASN:HA	1.58	0.42
2:B:5:ARG:N	2:B:127:TRP:HZ2	2.15	0.42
1:A:146:ILE:HG13	1:A:178:VAL:CG1	2.48	0.42
1:A:248:LYS:HZ1	1:A:288:GLU:HB3	1.82	0.42
1:A:388:VAL:HG12	1:A:390:SER:O	2.20	0.42
2:B:162:LYS:O	2:B:163:PRO:C	2.57	0.42
1:A:213:PRO:HG3	1:A:246:LEU:H	1.83	0.42
1:A:369:ILE:O	1:A:369:ILE:HG12	2.19	0.42
2:B:66:VAL:HA	2:B:85:VAL:CG2	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:101:GLN:HG2	2:B:101:GLN:O	2.19	0.42
1:A:142:LYS:O	1:A:144:LEU:N	2.52	0.42
2:B:185:VAL:HG13	2:B:261:ILE:HG12	2.02	0.42
2:B:211:TYR:HD1	2:B:245:GLN:CD	2.20	0.42
1:A:307:LYS:NZ	2:B:224:ALA:HB3	2.34	0.42
1:A:327:TRP:CD2	1:A:385:PRO:HG3	2.54	0.42
2:B:207:ILE:HD13	2:B:245:GLN:NE2	2.33	0.42
1:A:307:LYS:HZ2	2:B:224:ALA:HB3	1.84	0.42
2:B:81:SER:OG	2:B:84:LYS:HG2	2.20	0.42
2:B:92:LYS:C	2:B:94:ASN:H	2.22	0.42
2:B:124:GLN:O	2:B:128:LYS:HB2	2.20	0.42
2:B:183:ILE:O	2:B:226:ARG:HA	2.19	0.42
1:A:116:LEU:HD23	1:A:117:VAL:N	2.34	0.42
1:A:117:VAL:O	1:A:117:VAL:HG12	2.19	0.42
1:A:400:GLN:O	1:A:401:ILE:C	2.57	0.42
2:B:97:TRP:HA	2:B:100:ILE:CG2	2.46	0.41
1:A:22:LYS:HE2	1:A:22:LYS:HB2	1.86	0.41
1:A:45:MET:HB2	5:A:912:GNP:O1G	2.21	0.41
1:A:133:PHE:O	1:A:174:TRP:HH2	2.02	0.41
1:A:175:ALA:HB1	1:A:178:VAL:HG21	2.01	0.41
1:A:95:PRO:HG2	1:A:103:THR:OG1	2.20	0.41
1:A:59:CYS:SG	1:A:59:CYS:O	2.78	0.41
2:B:45:GLU:OE1	2:B:84:LYS:HE3	2.20	0.41
2:B:257:GLU:OE1	2:B:257:GLU:O	2.37	0.41
1:A:18:VAL:HG22	1:A:19:ASP:HB2	2.02	0.41
1:A:118:VAL:HG11	1:A:124:PHE:CD1	2.56	0.41
1:A:328:ASN:HA	1:A:380:VAL:O	2.21	0.41
2:B:210:ASP:HB2	2:B:211:TYR:H	1.77	0.41
1:A:134:VAL:HG23	1:A:138:ILE:HD12	2.02	0.41
2:B:199:VAL:HG23	2:B:200:ILE:N	2.35	0.41
1:A:63:LYS:H	1:A:63:LYS:HG2	1.43	0.41
1:A:391:ASN:OD1	1:A:415:ILE:N	2.51	0.41
1:A:339:VAL:HG21	1:A:346:LEU:HG	2.02	0.41
1:A:359:LEU:HD22	1:A:359:LEU:N	2.36	0.41
2:B:16:ILE:HG12	2:B:97:TRP:CD2	2.55	0.41
2:B:31:LEU:HG	2:B:37:LEU:O	2.21	0.41
2:B:40:PHE:HB3	2:B:79:ASP:OD1	2.20	0.41
2:B:182:LEU:HD21	2:B:228:ARG:CZ	2.50	0.41
2:B:243:LEU:CD2	2:B:247:ILE:HD12	2.51	0.41
1:A:179:PRO:HG2	1:A:201:TYR:CD2	2.56	0.41
1:A:352:ARG:HA	1:A:352:ARG:HD3	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:45:GLU:HG3	2:B:69:ILE:CD1	2.51	0.41
2:B:196:ILE:O	2:B:200:ILE:HG13	2.21	0.41
1:A:8:PRO:HA	1:A:88:ARG:HG2	2.02	0.40
1:A:372:SER:HB3	1:A:379:GLU:HB2	2.02	0.40
2:B:103:LEU:HD11	2:B:136:PRO:HB2	2.03	0.40
2:B:135:ASP:O	2:B:136:PRO:C	2.55	0.40
1:A:104:MET:O	1:A:108:ALA:N	2.49	0.40
1:A:27:GLN:O	1:A:27:GLN:HG2	2.21	0.40
1:A:404:ARG:HD3	1:A:406:ARG:HH22	1.77	0.40
2:B:147:GLY:O	2:B:149:LYS:N	2.51	0.40
2:B:240:SER:HA	2:B:243:LEU:HB3	2.04	0.40
1:A:304:SER:O	1:A:307:LYS:HG2	2.20	0.40
1:A:333:TYR:H	1:A:333:TYR:HD2	1.69	0.40
2:B:43:TRP:HA	2:B:43:TRP:HE3	1.85	0.40
2:B:98:LYS:NZ	2:B:208:GLU:OE1	2.41	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	395/414 (95%)	326 (82%)	51 (13%)	18 (5%)	2 14
2	B	255/266 (96%)	190 (74%)	47 (18%)	18 (7%)	1 5
All	All	650/680 (96%)	516 (79%)	98 (15%)	36 (6%)	2 10

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	66	GLU
1	A	80	ASP
1	A	124	PHE

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Mol	Chain	Res	Type
1	A	152	ASP
1	A	176	GLU
1	A	308	ALA
1	A	393	ILE
2	B	69	ILE
2	B	161	VAL
2	B	210	ASP
2	B	239	ALA
1	A	170	THR
1	A	173	THR
1	A	230	PHE
1	A	310	ASN
1	A	401	ILE
2	B	125	VAL
2	B	148	GLU
2	B	255	LYS
1	A	123	PRO
1	A	141	VAL
2	B	15	LEU
2	B	33	GLU
2	B	115	LYS
2	B	164	LEU
1	A	65	PRO
1	A	75	LYS
2	B	133	TYR
2	B	146	GLU
2	B	157	PRO
2	B	216	ASN
2	B	241	GLU
2	B	165	LEU
1	A	72	PRO
2	B	35	GLY
1	A	83	PRO

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	344/356 (97%)	306 (89%)	38 (11%)	6 25
2	B	231/239 (97%)	205 (89%)	26 (11%)	6 24
All	All	575/595 (97%)	511 (89%)	64 (11%)	6 25

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	PRO
1	A	5	LYS
1	A	7	GLN
1	A	19	ASP
1	A	33	TRP
1	A	59	CYS
1	A	61	SER
1	A	62	CYS
1	A	66	GLU
1	A	74	CYS
1	A	75	LYS
1	A	80	ASP
1	A	87	ARG
1	A	103	THR
1	A	104	MET
1	A	111	MET
1	A	134	VAL
1	A	149	ASN
1	A	160	LEU
1	A	168	GLN
1	A	171	LYS
1	A	190	ASN
1	A	192	ASP
1	A	219	ARG
1	A	221	PHE
1	A	246	LEU
1	A	248	LYS
1	A	290	LYS
1	A	295	VAL
1	A	309	ASP
1	A	333	TYR
1	A	343	LYS
1	A	344	GLU
1	A	366	THR
1	A	369	ILE

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Mol	Chain	Res	Type
1	A	376	ASP
1	A	404	ARG
1	A	415	ILE
2	B	18	THR
2	B	56	ASP
2	B	58	LEU
2	B	62	ARG
2	B	64	VAL
2	B	65	ILE
2	B	82	LEU
2	B	103	LEU
2	B	108	GLU
2	B	127	TRP
2	B	135	ASP
2	B	136	PRO
2	B	144	VAL
2	B	157	PRO
2	B	158	GLU
2	B	170	LYS
2	B	173	GLU
2	B	174	GLU
2	B	175	ARG
2	B	186	ARG
2	B	187	THR
2	B	204	LEU
2	B	210	ASP
2	B	214	LEU
2	B	221	THR
2	B	222	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	11	ASN
1	A	132	HIS
1	A	149	ASN
1	A	162	GLN
1	A	187	HIS
1	A	190	ASN
1	A	229	GLN
1	A	231	ASN

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Mol	Chain	Res	Type
1	A	400	GLN
2	B	21	GLN
2	B	53	ASN
2	B	61	ASN
2	B	94	ASN
2	B	96	GLN
2	B	101	GLN
2	B	124	GLN
2	B	206	ASN
2	B	209	GLN
2	B	216	ASN
2	B	245	GLN
2	B	249	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	GNP	A	912	3	29,34,34	2.24	12 (41%)	33,54,54	2.81	9 (27%)

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
5	GNP	A	912	3	-	3/14/38/38	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	912	GNP	C2-N2	5.35	1.44	1.33
5	A	912	GNP	C6-N1	4.22	1.40	1.33
5	A	912	GNP	PB-O3A	3.45	1.63	1.59
5	A	912	GNP	PG-N3B	3.43	1.72	1.63
5	A	912	GNP	PG-O3G	-2.89	1.49	1.56
5	A	912	GNP	PG-O1G	2.81	1.50	1.46
5	A	912	GNP	PB-O2B	-2.63	1.49	1.56
5	A	912	GNP	O6-C6	-2.54	1.18	1.24
5	A	912	GNP	C5-C6	2.50	1.45	1.41
5	A	912	GNP	C2-N1	2.37	1.39	1.35
5	A	912	GNP	C2'-C1'	-2.09	1.50	1.53
5	A	912	GNP	O4'-C4'	-2.01	1.40	1.45

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	912	GNP	C5-C6-N1	-9.10	110.98	123.43
5	A	912	GNP	C2-N3-C4	-7.22	107.11	115.36
5	A	912	GNP	O1G-PG-N3B	-6.20	102.63	111.77
5	A	912	GNP	N2-C2-N1	-4.79	109.80	117.25
5	A	912	GNP	N3-C2-N1	4.61	133.37	127.22
5	A	912	GNP	O2B-PB-O1B	3.42	117.09	109.92
5	A	912	GNP	O3A-PB-N3B	-2.42	99.88	106.59
5	A	912	GNP	O4'-C4'-C5'	2.06	116.15	109.37
5	A	912	GNP	C2-N1-C6	2.02	119.14	115.93

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	912	GNP	PG-N3B-PB-O1B
5	A	912	GNP	PG-N3B-PB-O3A
5	A	912	GNP	PA-O3A-PB-O2B

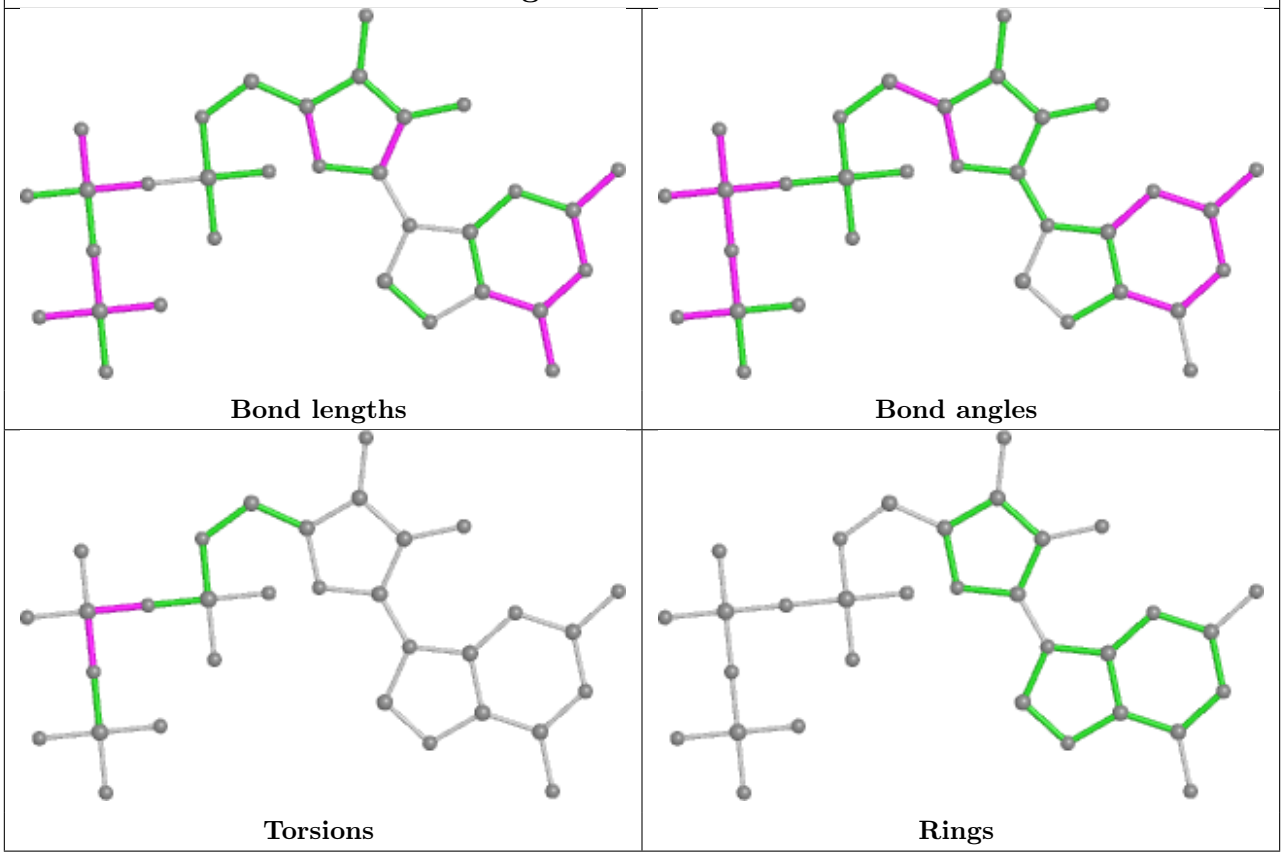
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	912	GNP	2	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 then 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.

Ligand GNP A 912



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	401/414 (96%)	-0.45	1 (0%)	95	87	12, 36, 68, 87	0
2	B	259/266 (97%)	-0.08	5 (1%)	66	37	27, 57, 85, 105	0
All	All	660/680 (97%)	-0.30	6 (0%)	84	63	12, 47, 80, 105	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	211	TYR	3.3
2	B	212	GLU	2.6
2	B	170	LYS	2.3
1	A	2	ALA	2.3
2	B	133	TYR	2.2
2	B	171	HIS	2.2

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

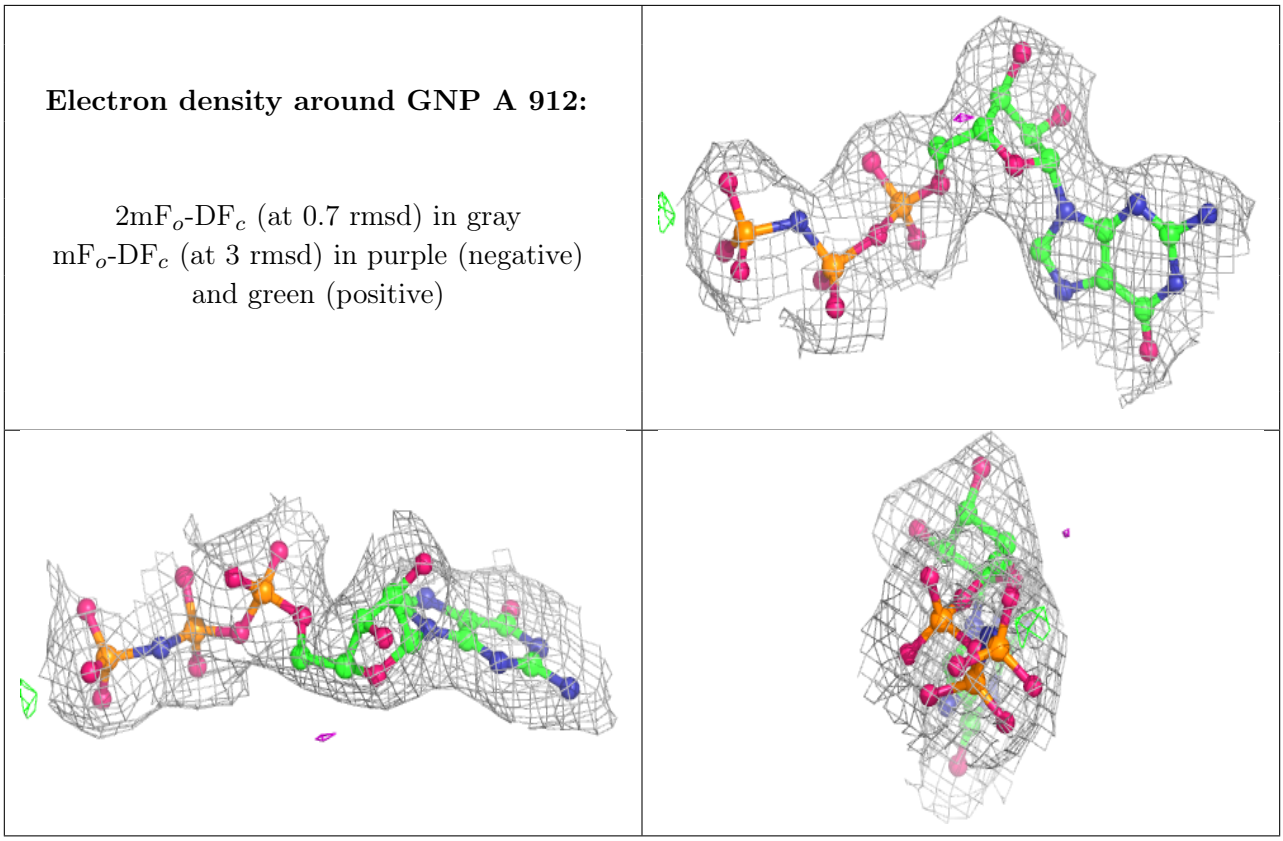
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	ZN	A	914	1/1	0.73	0.14	200,200,200,200	0
3	MG	A	913	1/1	0.96	0.16	19,19,19,19	0
5	GNP	A	912	32/32	0.98	0.16	26,43,44,45	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 GNP A 912:

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 (i)

There are no such residues in this entry.