Full wwPDB X-ray Structure Validation Report (i)

Jun 23, 2024 – 12:39 PM EDT

PDB ID	:	5IZM
Title	:	The crystal structure of human eEFSec in complex with GDPNP
Authors	:	Dobosz-Bartoszek, M.; Otwinowski, Z.; Simonovic, M.
Deposited on	:	2016-03-25
Resolution	:	3.40 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:

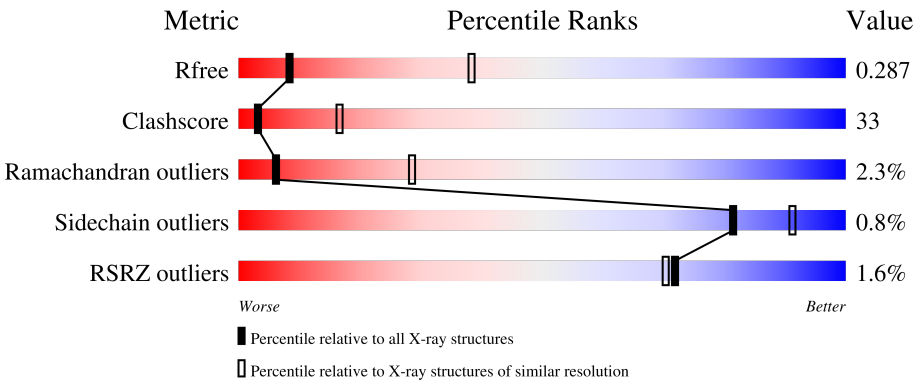
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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	616	2% 43% 30% • 25%
1	B	616	48% 31% • 20%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6632 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 Selenocysteine-specific elongation factor.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	460	3147	2026	544	554	9	14	0	1	0
1	B	495	3419	2212	579	604	9	15	0	0	0

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MSE	-	initiating methionine	UNP P57772
A	-18	GLY	-	expression tag	UNP P57772
A	-17	SER	-	expression tag	UNP P57772
A	-16	SER	-	expression tag	UNP P57772
A	-15	HIS	-	expression tag	UNP P57772
A	-14	HIS	-	expression tag	UNP P57772
A	-13	HIS	-	expression tag	UNP P57772
A	-12	HIS	-	expression tag	UNP P57772
A	-11	HIS	-	expression tag	UNP P57772
A	-10	HIS	-	expression tag	UNP P57772
A	-9	SER	-	expression tag	UNP P57772
A	-8	SER	-	expression tag	UNP P57772
A	-7	GLY	-	expression tag	UNP P57772
A	-6	LEU	-	expression tag	UNP P57772
A	-5	VAL	-	expression tag	UNP P57772
A	-4	PRO	-	expression tag	UNP P57772
A	-3	ARG	-	expression tag	UNP P57772
A	-2	GLY	-	expression tag	UNP P57772
A	-1	SER	-	expression tag	UNP P57772
A	0	HIS	-	expression tag	UNP P57772
A	1	MSE	-	expression tag	UNP P57772
B	-19	MSE	-	initiating methionine	UNP P57772
B	-18	GLY	-	expression tag	UNP P57772
B	-17	SER	-	expression tag	UNP P57772
B	-16	SER	-	expression tag	UNP P57772

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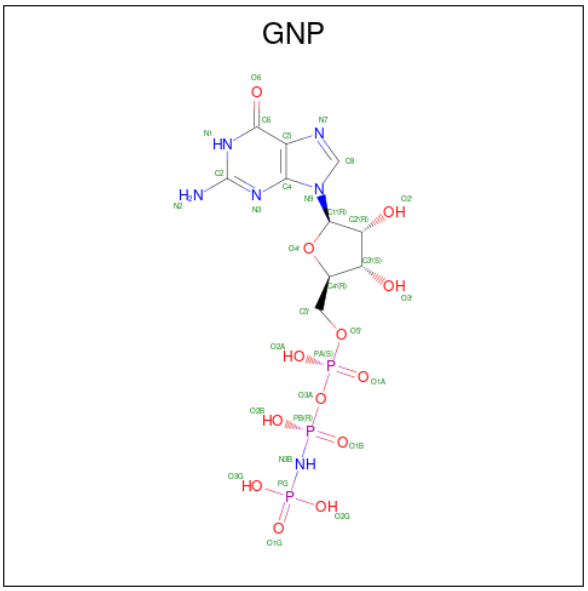
Chain	Residue	Modelled	Actual	Comment	Reference
B	-15	HIS	-	expression tag	UNP P57772
B	-14	HIS	-	expression tag	UNP P57772
B	-13	HIS	-	expression tag	UNP P57772
B	-12	HIS	-	expression tag	UNP P57772
B	-11	HIS	-	expression tag	UNP P57772
B	-10	HIS	-	expression tag	UNP P57772
B	-9	SER	-	expression tag	UNP P57772
B	-8	SER	-	expression tag	UNP P57772
B	-7	GLY	-	expression tag	UNP P57772
B	-6	LEU	-	expression tag	UNP P57772
B	-5	VAL	-	expression tag	UNP P57772
B	-4	PRO	-	expression tag	UNP P57772
B	-3	ARG	-	expression tag	UNP P57772
B	-2	GLY	-	expression tag	UNP P57772
B	-1	SER	-	expression tag	UNP P57772
B	0	HIS	-	expression tag	UNP P57772
B	1	MSE	-	expression tag	UNP P57772

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mn		
2	A	1	1	1	0	0
			Total	Mn		
2	B	1	1	1	0	0

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$).



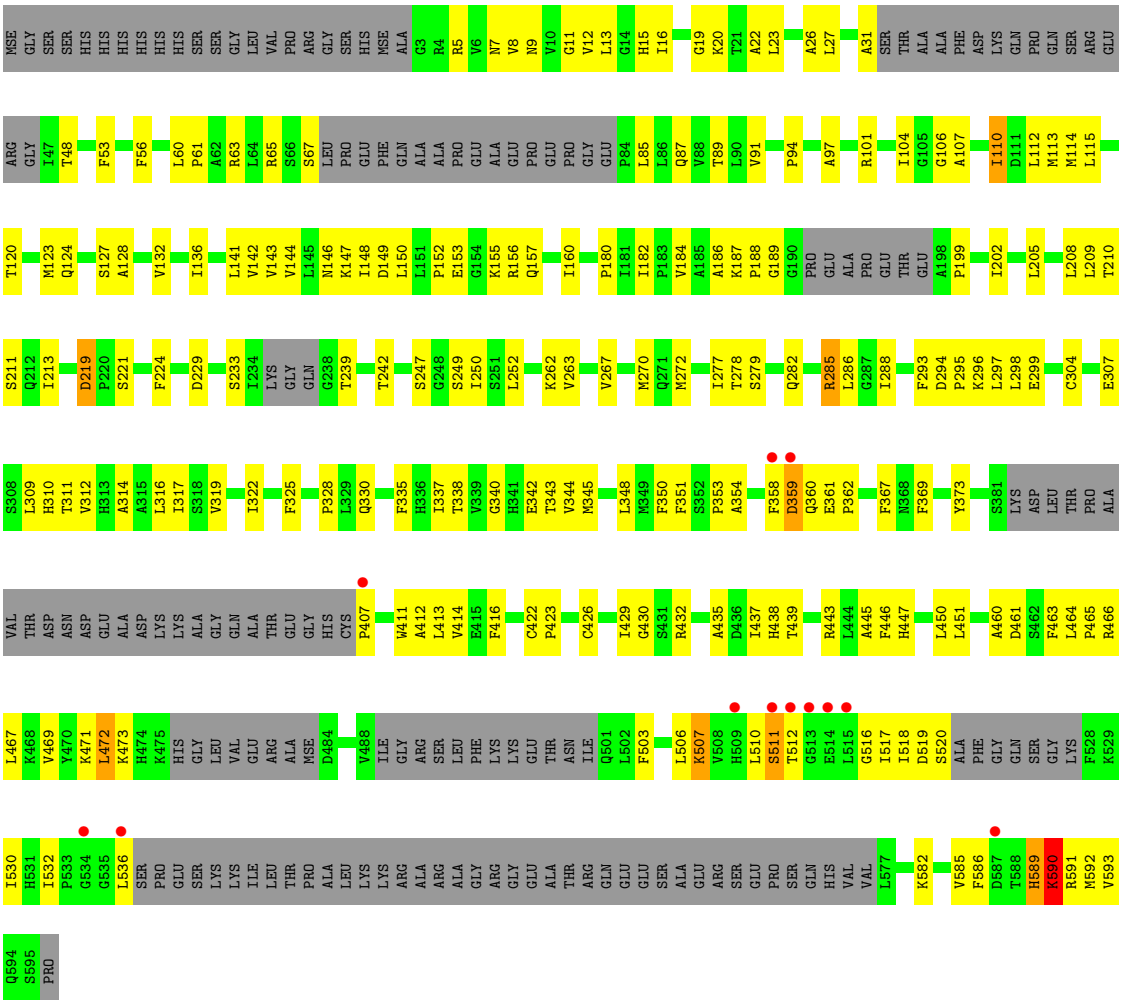
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	32	10	6	13	3	0	0
			Total	C	N	O	P		
3	B	1	32	10	6	13	3	0	0

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.

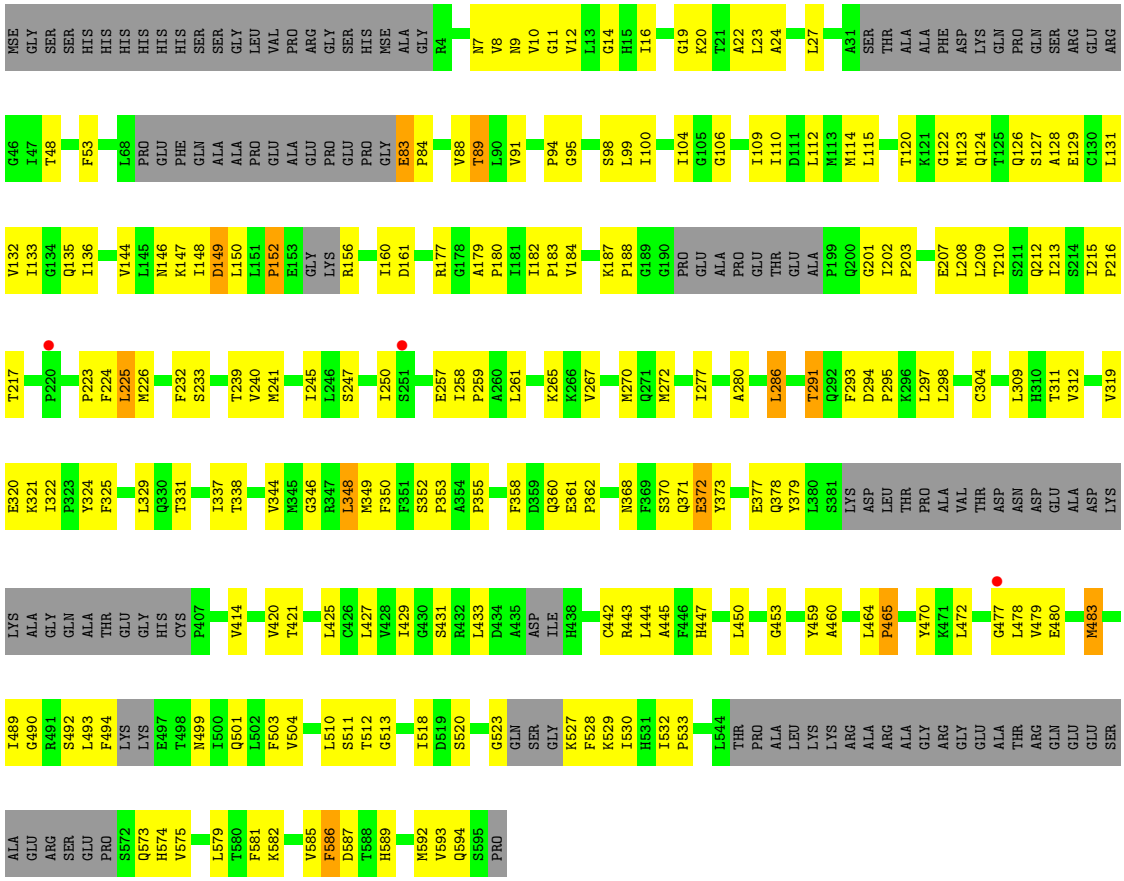
• Molecule 1: Selenocysteine-specific elongation factor

Chain A: 2% 43% 30% • 25%



• Molecule 1: Selenocysteine-specific elongation factor

Chain B: 48% 31% • 20%


MSE GLY SER SER HIS HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS MSE ALA GLY R4 N7 V8 N9 V10 G11 V12 L13 G14 H15 I16 G19 K20 T21 A22 L23 A24 L27 A31 SER THR ALA ALA PHE ASP LYS GLN PRO GLN SER ARG GLU ARG
G46 I47 T48 F53 L68 PRO GLU PHE GLN ALA ALA PRO GLU ALA GLU PRO GLU PRO GLY E83 P84 V88 T89 L90 V91 P94 G95 S98 L99 I100 I104 G105 G106 I109 I110 D111 L112 M113 M114 L115 T120 K121 G122 M123 Q124 T125 Q126 S127 A128 E129 C130 L131
V132 I133 G134 Q135 I136 V144 L145 N146 K147 I148 D149 L150 L151 P152 E153 GLY LYS R156 I160 D161 R177 G178 A179 P180 I181 I182 P183 V184 K187 P188 G189 G190 PRO GLU ALA PRO GLU THR GLU ALA P199 Q200 G201 I202 P203 E207 L208 L209 T210 S211 Q212 I213 S214 I215 P216
T217 P220 P223 F224 L225 M226 F232 S233 T239 V240 M241 I245 L246 S247 I250 S251 E257 I258 P259 A260 L261 K265 K266 V267 M270 Q271 M272 I277 A280 L286 T291 Q292 F293 D294 P295 K296 L297 L298 C304 L309 H310 T311 V312 V319
E320 K321 I322 P323 Y324 F325 L329 Q330 T331 I337 T338 V344 M345 G346 R347 L348 M349 F350 F351 S352 P353 A354 P355 F358 D359 Q360 E361 P362 N368 F369 S370 Q371 E372 Y373 E377 Q378 Y379 L380 S381 LYS ASP LEU THR PRO ALA VAL THR ASP ASN ASP GLU ALA ASP LYS
LYS ALA GLY GLN ALA THR GLU GLY HIS CYS P407 V414 V420 T421 L425 C426 L427 V428 I429 G430 S431 R432 L433 D434 A435 ASP ILE H438 C442 R443 L444 A445 F446 H447 L450 G453 Y459 A460 L464 P465 Y470 K471 L472 G477 L478 V479 E480 M483
I489 G490 R491 S492 L493 F494 LYS LYS E497 T498 N499 I500 Q501 L502 F503 V504 L510 S511 T512 G513 I518 D519 S520 G523 GLN SER GLY K527 F528 K529 I530 H531 I532 P533 L544 THR PRO ALA LEU LYS LYS ARG ALA ARG ALA GLY ARG GLY GLU ALA THR ARG GLN GLU GLU SER
ALA GLU ARG SER GLU PRO S572 Q573 H574 V575 L579 T580 F581 K582 V585 F586 D587 T588 H589 M592 V593 Q594 S595 PRO

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	92.32Å 112.40Å 327.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.16 – 3.40 46.16 – 3.38	Depositor EDS
% Data completeness (in resolution range)	78.4 (46.16-3.40) 84.9 (46.16-3.38)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.98 (at 3.40Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.235 , 0.285 0.236 , 0.287	Depositor DCC
R_{free} test set	1114 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å^2)	41.9	Xtriage
Anisotropy	0.030	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 33.3	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	0.79	EDS
Total number of atoms	6632	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

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

[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: GNP, MN

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	0.40	0/3193	0.77	12/4335 (0.3%)
1	B	0.37	0/3467	0.72	9/4708 (0.2%)
All	All	0.39	0/6660	0.75	21/9043 (0.2%)

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	262	LYS	CB-CA-C	-7.40	95.59	110.40
1	B	225	LEU	N-CA-CB	-6.58	97.25	110.40
1	A	592	MSE	CB-CA-C	-6.37	97.66	110.40
1	B	445	ALA	CB-CA-C	-6.24	100.75	110.10
1	A	511	SER	N-CA-C	6.23	127.83	111.00
1	B	177	ARG	CB-CA-C	-6.09	98.22	110.40
1	A	590	LYS	N-CA-CB	6.03	121.45	110.60
1	B	348	LEU	CB-CA-C	-5.81	99.17	110.20
1	A	307	GLU	N-CA-CB	-5.74	100.26	110.60
1	B	291	THR	N-CA-C	5.73	126.47	111.00
1	B	149	ASP	CB-CG-OD1	5.61	123.35	118.30
1	B	445	ALA	N-CA-C	5.56	126.01	111.00
1	A	285	ARG	N-CA-C	-5.44	96.32	111.00
1	A	299	GLU	CB-CA-C	5.42	121.25	110.40
1	B	89	THR	N-CA-C	-5.28	96.76	111.00
1	A	219	ASP	CB-CG-OD2	5.20	122.97	118.30
1	A	263	VAL	N-CA-CB	5.19	122.92	111.50
1	A	589	HIS	N-CA-CB	-5.12	101.37	110.60
1	A	359	ASP	N-CA-C	-5.10	97.22	111.00
1	A	361	GLU	C-N-CD	5.07	139.05	128.40
1	B	83	GLU	C-N-CD	5.07	139.04	128.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3147	0	2871	206	0
1	B	3419	0	3163	219	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	32	0	13	7	0
3	B	32	0	13	2	0
All	All	6632	0	6060	424	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 33.

All (424) 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:B:272:MSE:CB	1:B:286:LEU:HD23	1.20	1.64
1:B:272:MSE:CE	1:B:286:LEU:HD21	1.17	1.58
1:B:272:MSE:CG	1:B:286:LEU:HD23	1.45	1.43
1:B:272:MSE:HB2	1:B:286:LEU:CD2	1.55	1.37
1:B:272:MSE:CB	1:B:286:LEU:CD2	2.05	1.34
1:B:272:MSE:CE	1:B:286:LEU:CD2	2.10	1.30
1:B:272:MSE:CG	1:B:286:LEU:CD2	2.08	1.29
1:B:280:ALA:CB	1:B:286:LEU:HD13	1.59	1.29
1:B:182:ILE:HD11	1:B:208:LEU:CD2	1.68	1.22
1:A:219:ASP:OD2	1:A:221:SER:CB	1.92	1.18
1:B:182:ILE:HD11	1:B:208:LEU:HD23	1.17	1.15
1:B:490:GLY:O	1:B:528:PHE:CB	1.96	1.13
1:B:272:MSE:HE2	1:B:286:LEU:CD2	1.72	1.12
1:B:280:ALA:CB	1:B:286:LEU:CD1	2.25	1.12
1:B:280:ALA:HB1	1:B:286:LEU:CD1	1.79	1.12
1:B:490:GLY:O	1:B:528:PHE:HB3	1.45	1.12
1:A:585:VAL:HG12	1:A:589:HIS:HB3	1.19	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:272:MSE:HE3	1:B:286:LEU:HD21	1.19	1.08
1:A:582:LYS:HB2	1:A:585:VAL:CG2	1.84	1.07
1:B:272:MSE:HE2	1:B:286:LEU:HD21	1.13	1.06
1:A:9:ASN:O	1:A:110:ILE:HG23	1.54	1.05
1:B:272:MSE:HG3	1:B:286:LEU:CD2	1.86	1.05
1:B:371:GLN:O	1:B:373:TYR:CE1	2.10	1.05
1:A:328:PRO:HB2	1:A:330:GLN:HE21	1.18	1.04
1:B:272:MSE:HG3	1:B:286:LEU:CG	1.87	1.04
1:A:304:CYS:CB	1:A:309:LEU:HD13	1.88	1.03
1:A:348:LEU:HD11	1:A:414:VAL:HG22	1.42	1.00
1:B:272:MSE:HG3	1:B:286:LEU:HD23	1.41	1.00
1:A:348:LEU:CD1	1:A:414:VAL:HG22	1.93	0.99
1:A:582:LYS:CB	1:A:585:VAL:CG2	2.41	0.99
1:B:272:MSE:SE	1:B:286:LEU:HD21	2.12	0.98
1:B:272:MSE:HE2	1:B:286:LEU:HD11	1.45	0.98
1:A:582:LYS:CB	1:A:585:VAL:HG21	1.95	0.97
1:A:460:ALA:HA	1:A:464:LEU:HD12	1.46	0.97
1:B:272:MSE:HE2	1:B:286:LEU:CD1	1.95	0.95
1:B:146:ASN:OD1	1:B:147:LYS:N	2.00	0.94
1:B:280:ALA:HB1	1:B:286:LEU:HD11	1.48	0.94
1:A:304:CYS:HB3	1:A:309:LEU:HD13	1.47	0.93
1:A:219:ASP:CG	1:A:221:SER:CB	2.36	0.93
1:A:358:PHE:O	1:A:360:GLN:N	2.02	0.92
1:A:585:VAL:HG12	1:A:589:HIS:CB	2.00	0.92
1:A:316:LEU:HD21	1:A:467:LEU:HD13	1.54	0.90
1:B:280:ALA:HB3	1:B:286:LEU:HD13	1.51	0.89
1:B:19:GLY:O	1:B:23:LEU:N	2.06	0.89
1:B:7:ASN:HD21	1:B:89:THR:HG23	1.38	0.88
1:A:586:PHE:HA	1:A:590:LYS:H	1.38	0.87
1:A:582:LYS:HB2	1:A:585:VAL:HG21	1.55	0.87
1:B:272:MSE:HE2	1:B:286:LEU:CG	2.04	0.87
1:B:272:MSE:SE	1:B:286:LEU:CD2	2.71	0.86
1:B:321:LYS:N	1:B:379:TYR:OH	2.06	0.86
1:B:272:MSE:HB2	1:B:286:LEU:HD23	0.88	0.86
1:A:335:PHE:CE1	1:A:432:ARG:NE	2.44	0.85
1:B:272:MSE:HG3	1:B:286:LEU:HG	1.55	0.85
1:A:582:LYS:HB2	1:A:585:VAL:HG23	1.56	0.84
1:A:582:LYS:CB	1:A:585:VAL:HG23	2.08	0.83
1:B:528:PHE:HD1	1:B:529:LYS:H	1.21	0.82
1:B:182:ILE:CD1	1:B:208:LEU:HD23	2.06	0.82
1:B:207:GLU:HA	1:B:210:THR:HG22	1.60	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:182:ILE:HD11	1:B:208:LEU:HD22	1.59	0.81
1:A:150:LEU:HD13	3:A:1002:GNP:HN21	1.44	0.81
1:A:9:ASN:O	1:A:110:ILE:CG2	2.28	0.81
1:B:7:ASN:HD21	1:B:89:THR:CG2	1.94	0.79
1:B:280:ALA:HB2	1:B:286:LEU:HD13	1.61	0.78
1:A:304:CYS:HB3	1:A:309:LEU:CD1	2.15	0.77
1:B:371:GLN:O	1:B:373:TYR:HE1	1.67	0.77
1:A:65:ARG:C	1:A:67:SER:H	1.86	0.76
1:A:423:PRO:HG2	1:A:426:CYS:HB3	1.68	0.76
1:A:414:VAL:HG11	1:A:416:PHE:CE1	2.21	0.76
1:B:9:ASN:ND2	1:B:89:THR:OG1	2.14	0.76
1:A:585:VAL:CG1	1:A:589:HIS:HB3	2.11	0.75
1:A:15:HIS:CD2	1:A:16:ILE:H	2.04	0.75
1:B:523:GLY:HA3	1:B:527:LYS:HA	1.67	0.75
1:A:312:VAL:CG1	1:A:314:ALA:O	2.34	0.75
1:B:331:THR:HG22	1:B:350:PHE:H	1.51	0.75
1:B:490:GLY:O	1:B:528:PHE:HB2	1.86	0.75
1:A:187:LYS:O	3:A:1002:GNP:C6	2.35	0.74
1:A:328:PRO:HB2	1:A:330:GLN:NE2	1.98	0.74
1:B:360:GLN:HG3	1:B:361:GLU:H	1.51	0.74
1:A:27:LEU:HD21	1:A:205:LEU:HD23	1.68	0.74
1:A:340:GLY:C	1:A:342:GLU:H	1.91	0.73
1:A:19:GLY:O	1:A:23:LEU:N	2.23	0.72
1:A:312:VAL:HG13	1:A:314:ALA:O	1.90	0.72
1:B:372:GLU:O	1:B:373:TYR:CD1	2.43	0.71
1:A:335:PHE:HE1	1:A:432:ARG:NE	1.87	0.71
1:A:414:VAL:CG1	1:A:416:PHE:CE1	2.74	0.71
1:B:272:MSE:HB2	1:B:286:LEU:HD22	1.69	0.70
1:A:182:ILE:HD11	1:A:208:LEU:HD22	1.72	0.70
1:B:493:LEU:HD12	1:B:575:VAL:CG2	2.21	0.70
1:B:321:LYS:HB3	1:B:379:TYR:CE2	2.25	0.70
1:B:149:ASP:OD1	1:B:150:LEU:N	2.25	0.70
1:B:149:ASP:OD2	1:B:188:PRO:HA	1.92	0.69
1:A:219:ASP:OD1	1:A:221:SER:CB	2.40	0.69
1:B:493:LEU:HD12	1:B:575:VAL:HG21	1.75	0.69
1:B:272:MSE:CG	1:B:286:LEU:CG	2.60	0.68
1:A:250:ILE:HD11	1:A:267:VAL:HG21	1.76	0.67
1:B:277:ILE:HD13	1:B:286:LEU:HD22	1.76	0.67
1:A:586:PHE:HA	1:A:590:LYS:N	2.08	0.67
1:B:371:GLN:O	1:B:373:TYR:CD1	2.48	0.67
1:B:232:PHE:CE1	1:B:240:VAL:HB	2.29	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:582:LYS:CG	1:A:585:VAL:HG21	2.25	0.67
1:A:239:THR:OG1	1:A:293:PHE:CE2	2.47	0.66
1:A:358:PHE:CE2	1:A:407:PRO:HD3	2.30	0.66
1:A:340:GLY:O	1:A:342:GLU:N	2.23	0.66
1:A:582:LYS:HB3	1:A:585:VAL:CG2	2.25	0.66
1:A:316:LEU:CD1	1:A:413:LEU:HD12	2.26	0.65
1:A:353:PRO:HD3	1:A:411:TRP:CZ3	2.32	0.65
1:B:523:GLY:HA3	1:B:527:LYS:CA	2.27	0.65
1:B:7:ASN:ND2	1:B:89:THR:HG23	2.08	0.65
1:A:12:VAL:HG12	1:A:20:LYS:HG2	1.77	0.65
1:B:325:PHE:HA	1:B:442:CYS:HB3	1.77	0.64
1:B:232:PHE:CZ	1:B:240:VAL:HB	2.31	0.64
1:A:328:PRO:CB	1:A:330:GLN:HE21	2.04	0.64
1:A:517:ILE:O	1:A:530:ILE:HG23	1.97	0.64
1:B:372:GLU:C	1:B:373:TYR:CD1	2.71	0.64
1:B:11:GLY:HA3	1:B:110:ILE:HD13	1.80	0.64
1:A:11:GLY:N	1:A:110:ILE:HG21	2.13	0.64
1:B:19:GLY:N	3:B:1002:GNP:O2B	2.30	0.64
1:B:207:GLU:HA	1:B:210:THR:CG2	2.28	0.63
1:B:122:GLY:O	1:B:124:GLN:HG3	1.97	0.63
1:B:182:ILE:CD1	1:B:208:LEU:CD2	2.63	0.63
1:A:120:THR:HG21	1:A:150:LEU:HB3	1.81	0.63
1:A:187:LYS:O	3:A:1002:GNP:N1	2.32	0.63
1:A:471:LYS:O	1:A:473:LYS:N	2.32	0.63
1:B:272:MSE:CG	1:B:286:LEU:HG	2.27	0.63
1:A:353:PRO:HG2	1:A:358:PHE:HA	1.80	0.62
1:A:304:CYS:SG	1:A:309:LEU:HD13	2.39	0.62
1:A:348:LEU:HD11	1:A:414:VAL:CG2	2.24	0.62
1:A:15:HIS:ND1	1:A:124:GLN:OE1	2.33	0.62
1:A:13:LEU:HD22	1:A:113:MSE:SE	2.50	0.62
1:A:340:GLY:C	1:A:342:GLU:N	2.52	0.62
1:A:582:LYS:HB3	1:A:585:VAL:HG23	1.82	0.62
1:A:582:LYS:HG3	1:A:585:VAL:HG21	1.83	0.61
1:B:270:MSE:HB2	1:B:277:ILE:HG23	1.82	0.61
1:B:470:TYR:HB3	1:B:582:LYS:HG2	1.83	0.61
1:B:477:GLY:HA2	1:B:492:SER:O	2.01	0.61
1:A:5:ARG:HG2	1:A:85:LEU:HB2	1.82	0.60
1:A:15:HIS:HD1	1:A:124:GLN:CB	2.13	0.60
1:A:358:PHE:HE2	1:A:407:PRO:HD3	1.66	0.60
1:A:316:LEU:HD12	1:A:413:LEU:HD12	1.82	0.60
1:B:511:SER:HB3	1:B:573:GLN:HB2	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:414:VAL:HG11	1:A:416:PHE:HE1	1.65	0.59
1:A:186:ALA:O	1:A:199:PRO:HB3	2.03	0.59
1:A:464:LEU:C	1:A:466:ARG:H	2.07	0.58
1:B:129:GLU:OE1	1:B:443:ARG:NH2	2.35	0.58
1:A:15:HIS:O	1:A:20:LYS:NZ	2.34	0.58
1:B:250:ILE:HD11	1:B:267:VAL:HG21	1.84	0.58
1:B:321:LYS:CB	1:B:379:TYR:CE2	2.86	0.58
1:A:219:ASP:OD1	1:A:221:SER:N	2.36	0.58
1:A:354:ALA:O	1:A:358:PHE:HD1	1.86	0.58
1:A:319:VAL:HG11	1:A:350:PHE:HE1	1.69	0.58
1:A:120:THR:CG2	1:A:150:LEU:O	2.51	0.58
1:A:358:PHE:CD2	1:A:407:PRO:N	2.72	0.58
1:A:507:LYS:O	1:A:507:LYS:HG3	2.02	0.58
1:B:232:PHE:CZ	1:B:240:VAL:HG11	2.38	0.58
1:B:320:GLU:HA	1:B:379:TYR:OH	2.04	0.57
1:A:338:THR:HG23	1:A:343:THR:HB	1.86	0.57
1:B:88:VAL:C	1:B:89:THR:O	2.38	0.57
1:B:311:THR:HA	1:B:421:THR:HA	1.86	0.57
1:A:150:LEU:HD13	3:A:1002:GNP:N2	2.18	0.57
1:B:480:GLU:H	1:B:490:GLY:HA2	1.70	0.57
1:A:113:MSE:HE3	1:A:115:LEU:HB2	1.86	0.57
1:A:65:ARG:C	1:A:67:SER:N	2.56	0.56
1:A:460:ALA:HA	1:A:464:LEU:CD1	2.29	0.56
1:A:348:LEU:CG	1:A:414:VAL:HG22	2.36	0.56
1:B:585:VAL:O	1:B:586:PHE:CB	2.53	0.56
1:B:465:PRO:HB3	1:B:585:VAL:HA	1.87	0.56
1:A:15:HIS:CD2	1:A:16:ILE:HG13	2.40	0.56
1:A:15:HIS:CG	1:A:16:ILE:H	2.24	0.56
1:B:126:GLN:HA	1:B:129:GLU:HB3	1.88	0.55
1:B:377:GLU:O	1:B:378:GLN:HG3	2.07	0.55
1:A:180:PRO:HB3	1:A:208:LEU:HD11	1.88	0.55
1:B:161:ASP:OD1	1:B:161:ASP:O	2.24	0.55
1:B:511:SER:C	1:B:513:GLY:H	2.08	0.55
1:A:31:ALA:HB1	1:A:56:PHE:HB2	1.89	0.55
1:A:437:ILE:HG13	1:A:438:HIS:ND1	2.21	0.55
1:A:152:PRO:O	1:A:156:ARG:N	2.40	0.55
1:B:324:TYR:HB3	1:B:442:CYS:SG	2.47	0.55
1:A:112:LEU:HD11	1:A:142:VAL:HG23	1.89	0.55
1:B:123:MSE:HE3	1:B:128:ALA:HB2	1.88	0.55
1:B:110:ILE:CG2	1:B:112:LEU:O	2.55	0.54
1:B:265:LYS:HE3	1:B:293:PHE:HB3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:GLY:O	1:A:110:ILE:CD1	2.55	0.54
1:B:272:MSE:CE	1:B:286:LEU:HD11	2.30	0.54
1:B:180:PRO:HB2	1:B:208:LEU:HD21	1.88	0.54
1:B:209:LEU:O	1:B:213:ILE:HG12	2.06	0.54
1:A:104:ILE:HG23	1:A:429:ILE:HD12	1.90	0.53
1:B:312:VAL:HG11	1:B:453:GLY:HA3	1.90	0.53
1:B:207:GLU:CA	1:B:210:THR:HG22	2.33	0.53
1:B:224:PHE:CE1	1:B:245:ILE:HG23	2.44	0.53
1:B:272:MSE:HE3	1:B:286:LEU:CD2	2.07	0.53
1:A:233:SER:HB3	1:A:239:THR:HG22	1.89	0.53
1:B:104:ILE:HG21	1:B:338:THR:HG21	1.90	0.53
1:B:483:MSE:HG2	1:B:489:ILE:HG22	1.89	0.53
1:A:463:PHE:C	1:A:465:PRO:HD2	2.29	0.53
1:B:425:LEU:HA	1:B:450:LEU:O	2.08	0.53
1:B:215:ILE:HD12	1:B:216:PRO:O	2.09	0.53
1:A:272:MSE:HE3	1:A:277:ILE:HG13	1.91	0.52
1:B:100:ILE:HG21	1:B:433:LEU:HD22	1.92	0.52
1:B:579:LEU:HD22	1:B:592:MSE:HG3	1.91	0.52
1:A:65:ARG:O	1:A:67:SER:N	2.43	0.52
1:B:182:ILE:CD1	1:B:208:LEU:HD22	2.37	0.52
1:B:329:LEU:HD12	1:B:379:TYR:CD1	2.44	0.52
1:A:471:LYS:O	1:A:472:LEU:C	2.48	0.52
1:B:280:ALA:HB2	1:B:286:LEU:CD1	2.28	0.52
1:B:272:MSE:SE	1:B:286:LEU:HG	2.60	0.52
1:A:146:ASN:OD1	1:A:147:LYS:N	2.35	0.52
1:A:337:ILE:HD12	1:A:414:VAL:HG11	1.91	0.52
1:B:523:GLY:HA3	1:B:527:LYS:CB	2.40	0.52
1:B:581:PHE:CD1	1:B:592:MSE:SE	3.13	0.52
1:A:519:ASP:O	1:A:520:SER:C	2.46	0.52
1:B:344:VAL:HG11	1:B:420:VAL:HG21	1.92	0.52
1:B:353:PRO:HG2	1:B:358:PHE:HA	1.92	0.52
1:B:232:PHE:CZ	1:B:240:VAL:CB	2.93	0.52
1:B:232:PHE:CZ	1:B:240:VAL:CG1	2.93	0.52
1:B:477:GLY:CA	1:B:492:SER:O	2.57	0.52
1:B:489:ILE:HG23	1:B:489:ILE:O	2.10	0.52
1:B:493:LEU:HD12	1:B:575:VAL:HG23	1.92	0.52
1:A:182:ILE:HD12	1:A:205:LEU:HD12	1.91	0.51
1:B:88:VAL:O	1:B:89:THR:C	2.48	0.51
1:A:106:GLY:O	1:A:110:ILE:HD11	2.10	0.51
1:A:219:ASP:O	1:A:282:GLN:NE2	2.25	0.51
1:A:464:LEU:N	1:A:465:PRO:HD2	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:516:GLY:C	1:A:517:ILE:HG13	2.31	0.51
1:B:518:ILE:HG23	1:B:528:PHE:CE1	2.45	0.51
1:B:12:VAL:HG12	1:B:20:LYS:HB3	1.92	0.51
1:B:9:ASN:HA	1:B:89:THR:OG1	2.10	0.51
1:B:8:VAL:HG11	1:B:213:ILE:HD12	1.93	0.50
1:B:83:GLU:CB	1:B:84:PRO:CD	2.89	0.50
1:B:272:MSE:SE	1:B:286:LEU:CG	3.09	0.50
1:B:110:ILE:HG21	1:B:112:LEU:O	2.11	0.50
1:A:304:CYS:CB	1:A:309:LEU:CD1	2.75	0.50
1:B:106:GLY:O	1:B:110:ILE:HD11	2.12	0.50
1:A:15:HIS:HD1	1:A:124:GLN:HB2	1.76	0.50
1:B:187:LYS:O	3:B:1002:GNP:C6	2.60	0.50
1:B:261:LEU:HD21	1:B:297:LEU:HB3	1.94	0.50
1:B:352:SER:HB2	1:B:353:PRO:HD2	1.94	0.50
1:A:414:VAL:HG12	1:A:416:PHE:CE1	2.47	0.50
1:A:589:HIS:O	1:A:591:ARG:N	2.45	0.50
1:B:11:GLY:N	1:B:110:ILE:HG21	2.27	0.50
1:B:184:VAL:HG12	1:B:201:GLY:O	2.11	0.50
1:B:224:PHE:CZ	1:B:226:MSE:HB2	2.46	0.49
1:A:350:PHE:CD1	1:A:412:ALA:HB2	2.46	0.49
1:B:321:LYS:CB	1:B:379:TYR:CZ	2.95	0.49
1:B:241:MSE:HE3	1:B:293:PHE:CZ	2.48	0.49
1:A:101:ARG:HD2	1:A:343:THR:HG21	1.95	0.49
1:A:152:PRO:HG2	1:A:155:LYS:HB2	1.94	0.49
1:B:431:SER:HB3	1:B:444:LEU:HD23	1.94	0.49
1:B:144:VAL:CG1	1:B:184:VAL:HG22	2.43	0.49
1:B:152:PRO:O	1:B:156:ARG:HA	2.12	0.49
1:A:123:MSE:HE2	1:A:128:ALA:HA	1.95	0.49
1:A:267:VAL:HG13	1:A:288:ILE:HG23	1.94	0.48
1:A:149:ASP:OD2	1:A:188:PRO:HA	2.13	0.48
1:A:353:PRO:HA	1:A:373:TYR:HD1	1.79	0.48
1:B:321:LYS:HB2	1:B:379:TYR:CZ	2.49	0.48
1:B:208:LEU:O	1:B:212:GLN:HG2	2.12	0.48
1:B:270:MSE:HB2	1:B:277:ILE:CG2	2.43	0.48
1:B:280:ALA:CB	1:B:286:LEU:HD11	2.19	0.48
1:A:295:PRO:O	1:A:298:LEU:O	2.31	0.48
1:A:187:LYS:C	1:A:189:GLY:H	2.17	0.48
1:A:8:VAL:HB	1:A:213:ILE:HD11	1.96	0.48
1:A:219:ASP:OD1	1:A:221:SER:CA	2.61	0.48
1:A:312:VAL:HG12	1:A:314:ALA:H	1.78	0.48
1:B:511:SER:HB2	1:B:574:HIS:H	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:LEU:C	1:A:211:SER:H	2.18	0.47
1:A:141:LEU:HD21	1:A:143:VAL:HG23	1.95	0.47
1:A:335:PHE:CD2	1:A:446:PHE:HE2	2.32	0.47
1:B:355:PRO:HA	1:B:358:PHE:HB2	1.95	0.47
1:A:15:HIS:CD2	1:A:16:ILE:N	2.79	0.47
1:A:22:ALA:O	1:A:186:ALA:HB1	2.15	0.47
1:A:224:PHE:HA	1:A:247:SER:O	2.15	0.47
1:A:229:ASP:OD2	1:A:285:ARG:NH1	2.48	0.47
1:A:373:TYR:O	1:A:469:VAL:HA	2.14	0.47
1:A:585:VAL:O	1:A:589:HIS:N	2.48	0.47
1:B:215:ILE:HG13	1:B:215:ILE:O	2.15	0.47
1:A:242:THR:O	1:A:242:THR:OG1	2.32	0.47
1:A:310:HIS:O	1:A:311:THR:CG2	2.62	0.47
1:A:510:LEU:HD12	1:A:512:THR:H	1.78	0.47
1:B:272:MSE:HE3	1:B:277:ILE:CD1	2.45	0.47
1:A:148:ILE:HD13	1:A:148:ILE:HA	1.76	0.47
1:A:107:ALA:HA	1:A:110:ILE:HD12	1.96	0.47
1:B:272:MSE:HG3	1:B:286:LEU:CB	2.44	0.47
1:B:361:GLU:HA	1:B:362:PRO:HD2	1.82	0.46
1:A:150:LEU:CD1	3:A:1002:GNP:HN21	2.19	0.46
1:B:329:LEU:HB3	1:B:350:PHE:CZ	2.49	0.46
1:A:270:MSE:HE1	1:A:279:SER:HA	1.97	0.46
1:B:16:ILE:HA	1:B:95:GLY:HA3	1.97	0.46
1:A:153:GLU:HA	1:A:156:ARG:HB2	1.96	0.46
1:A:310:HIS:O	1:A:311:THR:HG23	2.16	0.46
1:A:322:ILE:HG13	1:A:446:PHE:HA	1.98	0.46
1:A:353:PRO:O	1:A:354:ALA:C	2.54	0.46
1:B:483:MSE:HG2	1:B:489:ILE:CG2	2.45	0.46
1:B:14:GLY:HA2	1:B:115:LEU:HD12	1.96	0.46
1:B:131:LEU:O	1:B:135:GLN:HG3	2.16	0.46
1:B:490:GLY:O	1:B:528:PHE:CG	2.65	0.46
1:A:422:CYS:HB2	1:A:426:CYS:SG	2.55	0.46
1:A:48:THR:O	1:A:94:PRO:HB3	2.16	0.45
1:A:115:LEU:HD21	1:A:123:MSE:HE3	1.98	0.45
1:A:464:LEU:N	1:A:465:PRO:CD	2.79	0.45
1:A:150:LEU:CD1	3:A:1002:GNP:N2	2.77	0.45
1:B:337:ILE:HD12	1:B:346:GLY:HA3	1.98	0.45
1:A:414:VAL:HG12	1:A:416:PHE:CD1	2.51	0.45
1:B:8:VAL:HG11	1:B:213:ILE:HG23	1.98	0.45
1:A:312:VAL:HG12	1:A:314:ALA:N	2.31	0.45
1:A:510:LEU:HD12	1:A:510:LEU:C	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20:LYS:O	1:B:24:ALA:N	2.42	0.45
1:B:224:PHE:HE1	1:B:245:ILE:HG12	1.81	0.45
1:B:523:GLY:CA	1:B:527:LYS:CB	2.94	0.45
1:A:16:ILE:HG23	3:A:1002:GNP:O2G	2.16	0.45
1:B:304:CYS:SG	1:B:309:LEU:HG	2.56	0.45
1:B:493:LEU:HD22	1:B:494:PHE:CE1	2.51	0.45
1:A:464:LEU:C	1:A:466:ARG:N	2.70	0.45
1:B:348:LEU:HD23	1:B:414:VAL:HG12	1.99	0.44
1:B:372:GLU:O	1:B:373:TYR:CG	2.70	0.44
1:A:15:HIS:CG	1:A:16:ILE:N	2.86	0.44
1:A:503:PHE:HA	1:A:506:LEU:HD12	1.98	0.44
1:B:180:PRO:CB	1:B:208:LEU:HD21	2.48	0.44
1:B:10:VAL:HG11	1:B:114:MSE:HE2	1.98	0.44
1:A:15:HIS:HD2	1:A:16:ILE:HG13	1.82	0.44
1:A:461:ASP:O	1:A:465:PRO:HG3	2.18	0.44
1:B:148:ILE:HG23	1:B:160:ILE:HD11	1.99	0.44
1:B:258:ILE:HG23	1:B:298:LEU:CD1	2.48	0.44
1:B:291:THR:O	1:B:291:THR:HG22	2.16	0.44
1:B:324:TYR:CB	1:B:442:CYS:SG	3.06	0.44
1:B:478:LEU:HA	1:B:574:HIS:HA	1.99	0.44
1:B:586:PHE:O	1:B:589:HIS:C	2.56	0.44
1:A:63:ARG:HH21	1:A:211:SER:HA	1.82	0.44
1:A:353:PRO:HD3	1:A:411:TRP:HZ3	1.78	0.44
1:A:148:ILE:HG12	1:A:184:VAL:O	2.18	0.44
1:A:124:GLN:O	1:A:127:SER:OG	2.33	0.44
1:A:325:PHE:CD2	1:A:445:ALA:HA	2.52	0.44
1:B:529:LYS:O	1:B:530:ILE:HG13	2.17	0.44
1:A:7:ASN:ND2	1:A:87:GLN:OE1	2.51	0.43
1:B:132:VAL:HG11	1:B:322:ILE:HD13	2.00	0.43
1:B:133:ILE:HA	1:B:136:ILE:HD12	2.00	0.43
1:A:11:GLY:HA3	1:A:110:ILE:HD13	1.99	0.43
1:A:27:LEU:HD23	1:A:202:ILE:HG23	1.99	0.43
1:B:53:PHE:CE2	1:B:91:VAL:HG22	2.54	0.43
1:B:499:ASN:C	1:B:501:GLN:N	2.71	0.43
1:B:19:GLY:CA	1:B:22:ALA:HB3	2.48	0.43
1:B:368:ASN:ND2	1:B:370:SER:OG	2.52	0.43
1:B:110:ILE:HG22	1:B:112:LEU:O	2.19	0.43
1:A:348:LEU:HG	1:A:414:VAL:HG22	2.01	0.42
1:B:144:VAL:CG1	1:B:184:VAL:CG2	2.97	0.42
1:B:321:LYS:N	1:B:379:TYR:CZ	2.81	0.42
1:A:97:ALA:O	1:A:443:ARG:NH2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:PHE:C	1:A:360:GLN:N	2.69	0.42
1:B:460:ALA:HA	1:B:464:LEU:HD12	2.01	0.42
1:B:586:PHE:O	1:B:587:ASP:C	2.58	0.42
1:A:286:LEU:HD23	1:A:288:ILE:HD11	2.02	0.42
1:B:510:LEU:O	1:B:513:GLY:N	2.51	0.42
1:A:7:ASN:ND2	1:A:89:THR:OG1	2.46	0.42
1:A:589:HIS:O	1:A:590:LYS:C	2.58	0.42
1:A:26:ALA:HB1	1:A:202:ILE:HG13	2.02	0.42
1:B:298:LEU:O	1:B:298:LEU:HD23	2.19	0.42
1:B:319:VAL:HG11	1:B:350:PHE:HE2	1.85	0.42
1:A:132:VAL:HG11	1:A:322:ILE:HD13	2.02	0.42
1:A:510:LEU:HD12	1:A:510:LEU:O	2.20	0.42
1:B:110:ILE:HG22	1:B:112:LEU:H	1.84	0.42
1:B:124:GLN:H	1:B:127:SER:HB2	1.84	0.42
1:B:294:ASP:HA	1:B:295:PRO:HD3	1.70	0.42
1:B:470:TYR:HE2	1:B:472:LEU:HB2	1.85	0.42
1:A:295:PRO:O	1:A:297:LEU:N	2.52	0.42
1:B:202:ILE:N	1:B:203:PRO:HD2	2.34	0.42
1:B:258:ILE:HG23	1:B:298:LEU:HD13	2.01	0.42
1:B:23:LEU:O	1:B:27:LEU:HD12	2.20	0.41
1:B:225:LEU:HD13	1:B:309:LEU:HD21	2.02	0.41
1:B:232:PHE:O	1:B:239:THR:HG23	2.19	0.41
1:B:532:ILE:HA	1:B:533:PRO:HD3	1.77	0.41
1:A:317:ILE:HG22	1:A:450:LEU:HA	2.02	0.41
1:A:337:ILE:CD1	1:A:414:VAL:HG11	2.50	0.41
1:A:586:PHE:HA	1:A:590:LYS:HA	2.03	0.41
1:A:430:GLY:HA3	1:A:446:PHE:CZ	2.55	0.41
1:B:98:SER:HB2	1:B:99:LEU:HD12	2.02	0.41
1:B:120:THR:HG21	1:B:150:LEU:HD22	2.03	0.41
1:B:179:ALA:HA	1:B:180:PRO:HD3	1.95	0.41
1:B:331:THR:HG22	1:B:349:MSE:HA	2.01	0.41
1:B:503:PHE:O	1:B:504:VAL:C	2.58	0.41
1:B:511:SER:C	1:B:513:GLY:N	2.74	0.41
1:A:11:GLY:H	1:A:110:ILE:HG21	1.85	0.41
1:A:187:LYS:C	1:A:189:GLY:N	2.72	0.41
1:A:353:PRO:O	1:A:354:ALA:O	2.39	0.41
1:B:459:TYR:CG	1:B:460:ALA:N	2.88	0.41
1:A:60:LEU:HD23	1:A:61:PRO:O	2.19	0.41
1:A:224:PHE:HB2	1:A:249:SER:O	2.20	0.41
1:A:312:VAL:CG1	1:A:314:ALA:H	2.34	0.41
1:A:53:PHE:CE2	1:A:91:VAL:HG22	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:ILE:HG22	1:A:279:SER:H	1.86	0.41
1:A:293:PHE:HD1	1:A:294:ASP:O	2.04	0.41
1:B:429:ILE:HD13	1:B:447:HIS:HB2	2.02	0.41
1:B:528:PHE:CD1	1:B:529:LYS:N	2.73	0.41
1:A:209:LEU:HD12	1:A:209:LEU:HA	1.93	0.41
1:A:141:LEU:HD23	1:A:142:VAL:N	2.35	0.41
1:A:252:LEU:HG	1:A:278:THR:HA	2.03	0.41
1:A:316:LEU:CD2	1:A:467:LEU:HD13	2.39	0.41
1:A:337:ILE:HD11	1:A:348:LEU:HD11	2.01	0.41
1:B:100:ILE:O	1:B:104:ILE:HD12	2.21	0.41
1:B:128:ALA:O	1:B:132:VAL:HG23	2.21	0.41
1:B:224:PHE:HA	1:B:247:SER:O	2.20	0.41
1:B:331:THR:HG22	1:B:350:PHE:N	2.28	0.41
1:B:470:TYR:HA	1:B:582:LYS:HA	2.02	0.41
1:A:149:ASP:OD1	1:A:149:ASP:N	2.53	0.41
1:A:367:PHE:HB3	1:A:369:PHE:CE1	2.56	0.41
1:A:319:VAL:HG21	1:A:412:ALA:HB3	2.03	0.40
1:A:451:LEU:HD23	1:A:451:LEU:HA	1.79	0.40
1:B:499:ASN:C	1:B:501:GLN:H	2.23	0.40
1:B:511:SER:O	1:B:513:GLY:N	2.54	0.40
1:A:278:THR:O	1:A:278:THR:HG22	2.21	0.40
1:A:344:VAL:HG22	1:A:345:MSE:H	1.86	0.40
1:A:516:GLY:C	1:A:517:ILE:CG1	2.89	0.40
1:B:257:GLU:HG2	1:B:259:PRO:HD3	2.03	0.40
1:A:136:ILE:HD13	1:A:447:HIS:HB3	2.03	0.40
1:A:351:PHE:CZ	1:A:411:TRP:HB2	2.55	0.40
1:A:435:ALA:O	1:B:98:SER:HA	2.21	0.40
1:B:126:GLN:HA	1:B:129:GLU:CB	2.52	0.40
1:B:126:GLN:NE2	1:B:129:GLU:OE1	2.54	0.40
1:A:532:ILE:HD13	1:A:536:LEU:CB	2.52	0.40
1:B:48:THR:HB	1:B:94:PRO:HA	2.02	0.40
1:B:109:ILE:O	1:B:109:ILE:HG22	2.22	0.40
1:A:27:LEU:HD23	1:A:27:LEU:HA	1.87	0.40
1:A:114:MSE:HE2	1:A:144:VAL:HG21	2.04	0.40
1:A:157:GLN:O	1:A:160:ILE:N	2.55	0.40
1:B:12:VAL:CG1	1:B:20:LYS:HB3	2.52	0.40
1:B:136:ILE:HG22	1:B:427:LEU:HD11	2.03	0.40
1:B:479:VAL:HA	1:B:490:GLY:HA3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	441/616 (72%)	350 (79%)	81 (18%)	10 (2%)	6 28
1	B	475/616 (77%)	377 (79%)	87 (18%)	11 (2%)	6 28
All	All	916/1232 (74%)	727 (79%)	168 (18%)	21 (2%)	6 28

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	590	LYS
1	A	296	LYS
1	A	359	ASP
1	A	439	THR
1	A	511	SER
1	A	593	VAL
1	B	372	GLU
1	B	512	THR
1	A	472	LEU
1	B	217	THR
1	B	586	PHE
1	B	593	VAL
1	A	210	THR
1	B	152	PRO
1	B	520	SER
1	A	518	ILE
1	B	223	PRO
1	B	483	MSE
1	A	362	PRO
1	B	465	PRO
1	B	183	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	278/507 (55%)	276 (99%)	2 (1%)	84 92
1	B	312/507 (62%)	309 (99%)	3 (1%)	76 88
All	All	590/1014 (58%)	585 (99%)	5 (1%)	81 91

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	110	ILE
1	A	507	LYS
1	B	233	SER
1	B	286	LEU
1	B	594	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	330	GLN
1	B	7	ASN
1	B	9	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 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	$\#\|Z\| > 2$
3	GNP	B	1002	2	29,34,34	3.18	10 (34%)	33,54,54	2.18	9 (27%)
3	GNP	A	1002	2	29,34,34	3.18	10 (34%)	33,54,54	2.18	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
3	GNP	B	1002	2	-	2/14/38/38	0/3/3/3
3	GNP	A	1002	2	-	5/14/38/38	0/3/3/3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1002	GNP	PG-O1G	10.21	1.62	1.46
3	A	1002	GNP	PG-O1G	10.19	1.62	1.46
3	A	1002	GNP	PB-O1B	10.17	1.62	1.46
3	B	1002	GNP	PB-O1B	10.14	1.62	1.46
3	B	1002	GNP	C5-C6	-4.57	1.33	1.41
3	A	1002	GNP	C5-C6	-4.51	1.33	1.41
3	A	1002	GNP	C6-N1	4.08	1.40	1.33
3	B	1002	GNP	C6-N1	4.04	1.40	1.33
3	A	1002	GNP	PG-O3G	-2.94	1.48	1.56
3	A	1002	GNP	PB-O2B	-2.94	1.48	1.56
3	B	1002	GNP	PG-O3G	-2.92	1.48	1.56
3	B	1002	GNP	PB-O2B	-2.92	1.48	1.56
3	A	1002	GNP	C5-C4	-2.68	1.33	1.40
3	B	1002	GNP	C5-C4	-2.65	1.33	1.40
3	A	1002	GNP	C2-N1	2.54	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1002	GNP	C2-N1	2.52	1.39	1.35
3	A	1002	GNP	PG-O2G	2.09	1.62	1.56
3	B	1002	GNP	PG-O2G	2.06	1.62	1.56
3	B	1002	GNP	O4'-C1'	2.04	1.43	1.41
3	A	1002	GNP	O4'-C1'	2.01	1.43	1.41

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1002	GNP	N3-C2-N1	-5.89	119.36	127.22
3	A	1002	GNP	N3-C2-N1	-5.89	119.36	127.22
3	A	1002	GNP	C2-N3-C4	4.67	120.69	115.36
3	B	1002	GNP	C2-N3-C4	4.64	120.66	115.36
3	A	1002	GNP	O1B-PB-N3B	-4.54	105.09	111.77
3	B	1002	GNP	O1B-PB-N3B	-4.50	105.15	111.77
3	B	1002	GNP	PB-O3A-PA	-3.59	119.96	132.62
3	A	1002	GNP	PB-O3A-PA	-3.58	119.99	132.62
3	B	1002	GNP	O1G-PG-N3B	-3.39	106.78	111.77
3	A	1002	GNP	O1G-PG-N3B	-3.39	106.78	111.77
3	B	1002	GNP	O2G-PG-O1G	-3.33	105.07	113.45
3	A	1002	GNP	O2G-PG-O1G	-3.33	105.09	113.45
3	A	1002	GNP	C5-C6-N1	-2.77	119.64	123.43
3	B	1002	GNP	C5-C6-N1	-2.74	119.68	123.43
3	A	1002	GNP	O2B-PB-O3A	2.74	113.77	104.64
3	B	1002	GNP	O2B-PB-O3A	2.72	113.73	104.64
3	B	1002	GNP	C3'-C2'-C1'	2.06	104.08	100.98
3	A	1002	GNP	C3'-C2'-C1'	2.05	104.07	100.98

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1002	GNP	PB-N3B-PG-O1G
3	A	1002	GNP	PG-N3B-PB-O1B
3	B	1002	GNP	PB-N3B-PG-O1G
3	B	1002	GNP	PG-N3B-PB-O1B
3	A	1002	GNP	O4'-C4'-C5'-O5'
3	A	1002	GNP	C3'-C4'-C5'-O5'
3	A	1002	GNP	PB-O3A-PA-O2A

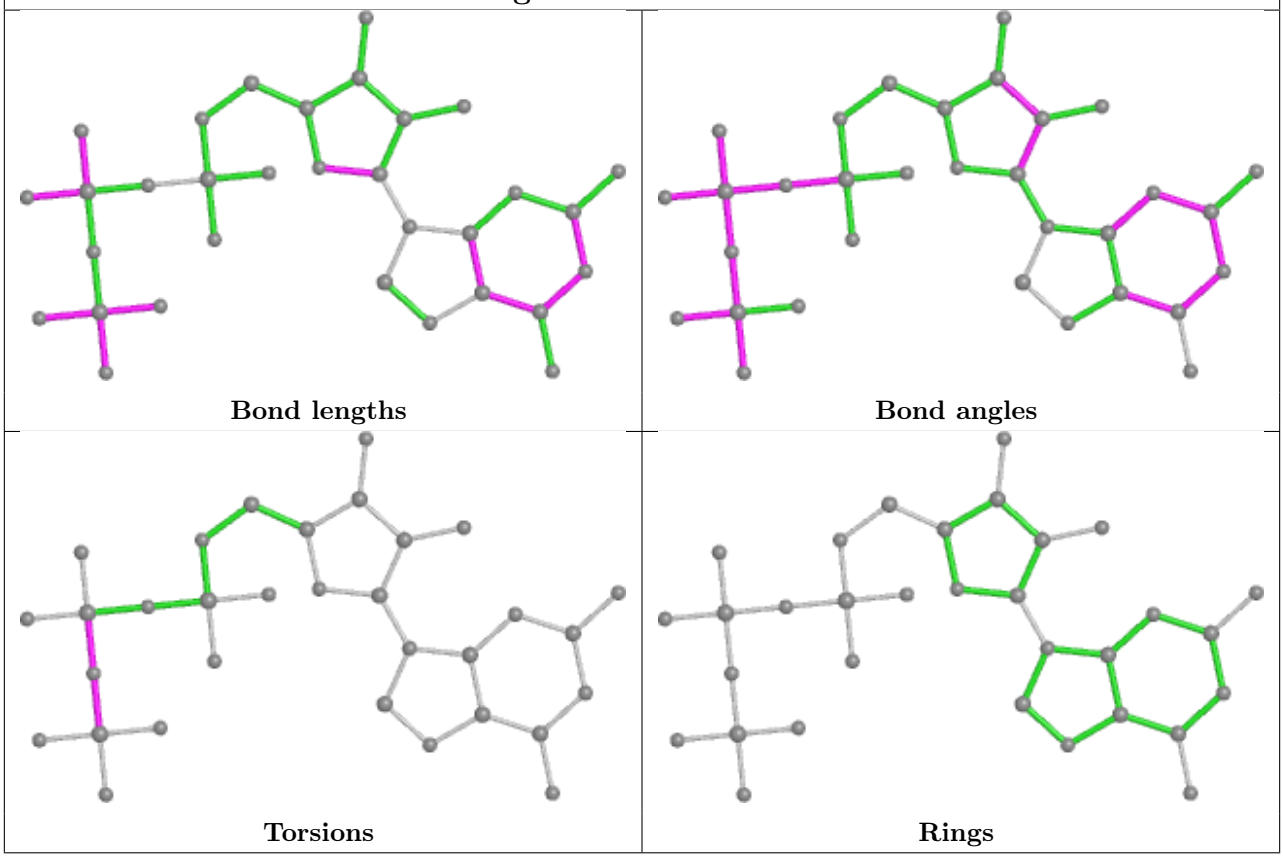
There are no ring outliers.

2 monomers are involved in 9 short contacts:

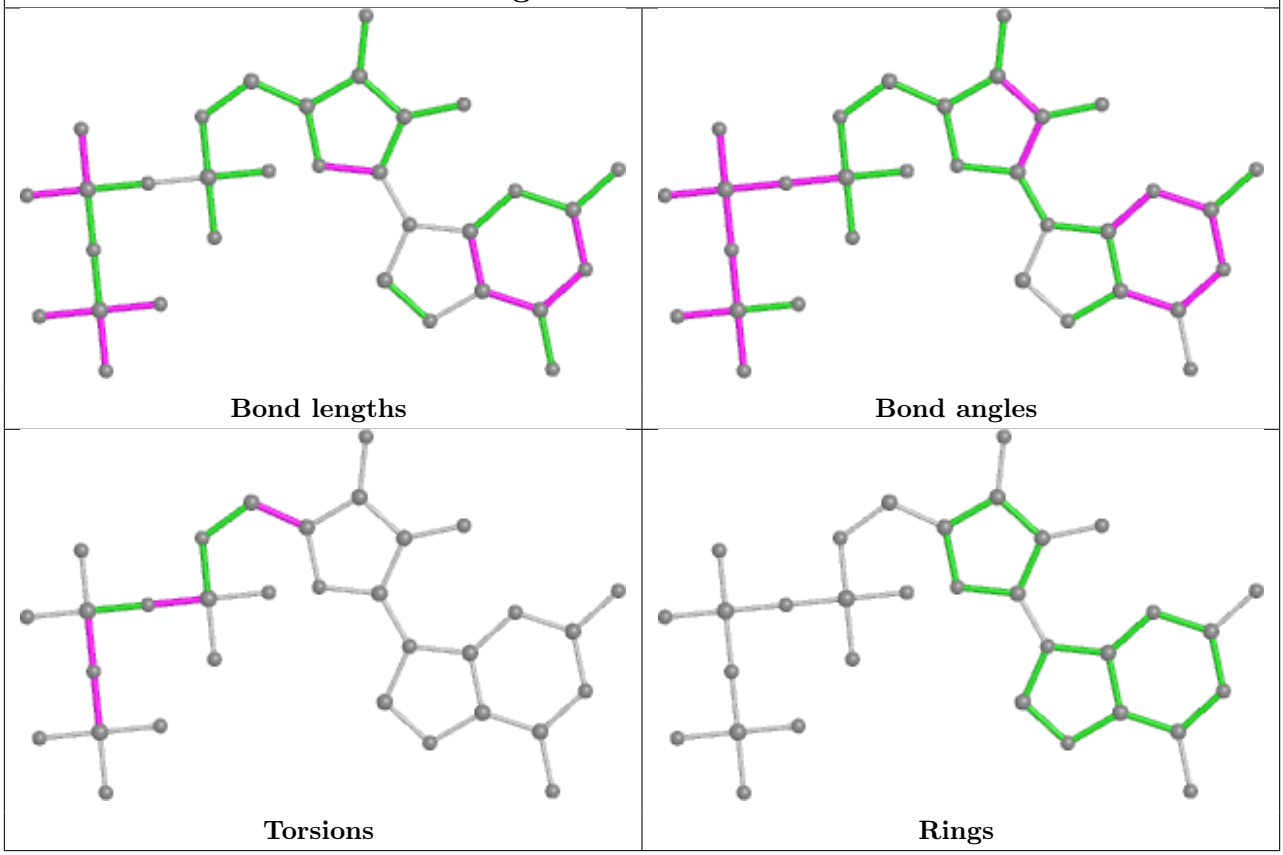
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1002	GNP	2	0
3	A	1002	GNP	7	0

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 B 1002



Ligand GNP A 1002



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	446/616 (72%)	-0.03	12 (2%)	54	53	6, 31, 70, 104	0
1	B	480/616 (77%)	-0.19	3 (0%)	89	89	8, 28, 55, 76	0
All	All	926/1232 (75%)	-0.11	15 (1%)	72	70	6, 30, 64, 104	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	359	ASP	3.2
1	A	514	GLU	2.8
1	A	536	LEU	2.8
1	A	515	LEU	2.6
1	A	534	GLY	2.6
1	A	512	THR	2.5
1	B	251	SER	2.5
1	A	587	ASP	2.4
1	A	509	HIS	2.3
1	A	513	GLY	2.3
1	A	407	PRO	2.3
1	B	477	GLY	2.2
1	B	220	PRO	2.1
1	A	358	PHE	2.1
1	A	511	SER	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

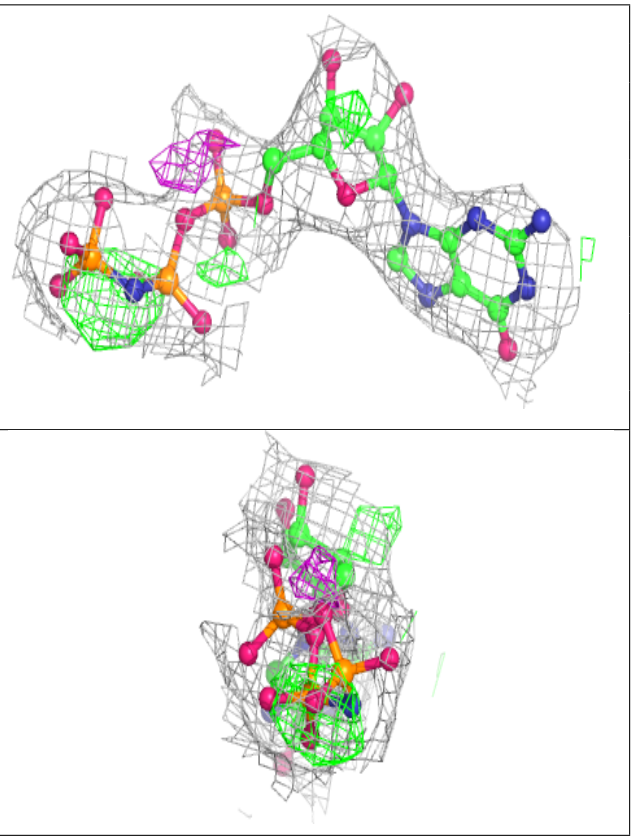
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GNP	B	1002	32/32	0.89	0.26	24,54,66,96	0
3	GNP	A	1002	32/32	0.90	0.27	17,47,78,96	0
2	MN	A	1001	1/1	0.97	0.07	16,16,16,16	0
2	MN	B	1001	1/1	0.97	0.13	15,15,15,15	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.

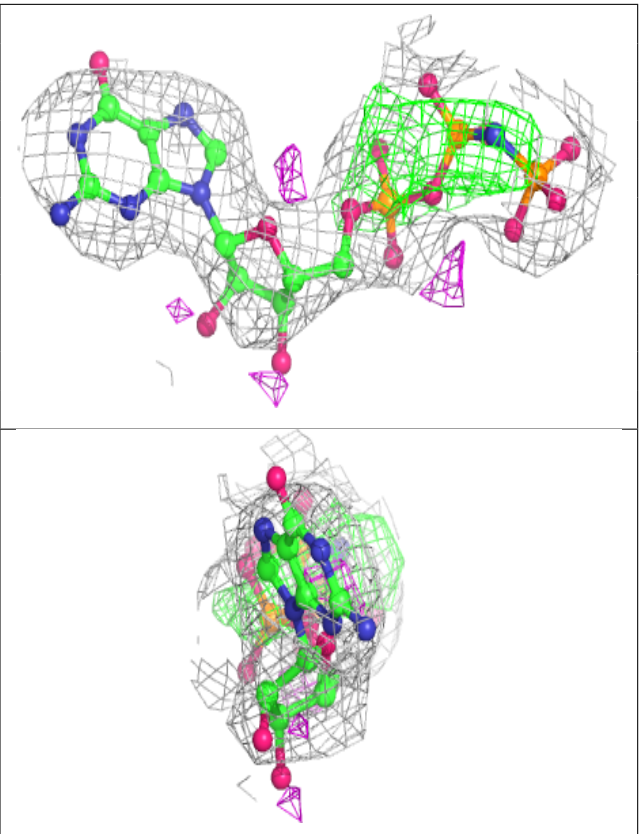
Electron density around GNP B 1002:

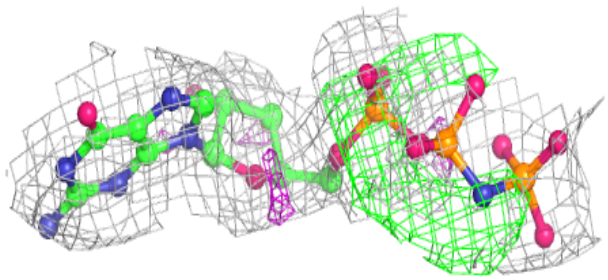
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around GNP A 1002:

$2mF_o$-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.