



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:34 AM UTC

PDB ID : 5IZM / pdb_00005izm
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 ⓘ symbol.

The types of validation reports are described at

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

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

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

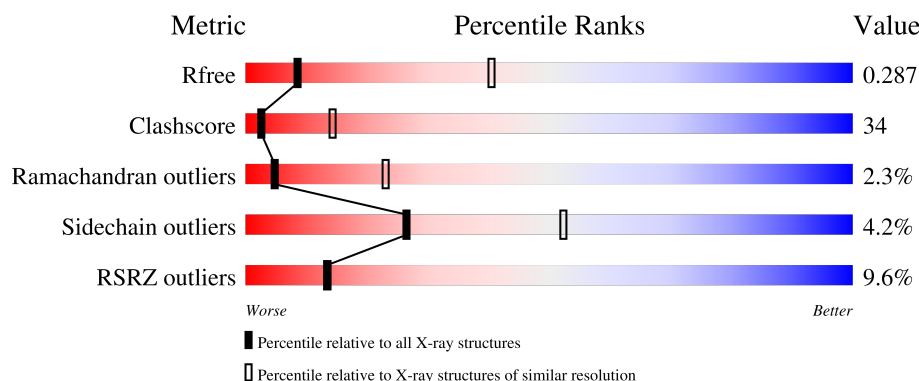
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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}	180053	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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

Mol	Chain	Length	Quality of chain
1	A	616	
1	B	616	

2 Entry composition

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
1	A	460	Total	C	N	O	S	Se	0	1	0
			3147	2026	544	554	9	14			
1	B	495	Total	C	N	O	S	Se	0	0	0
			3419	2212	579	604	9	15			

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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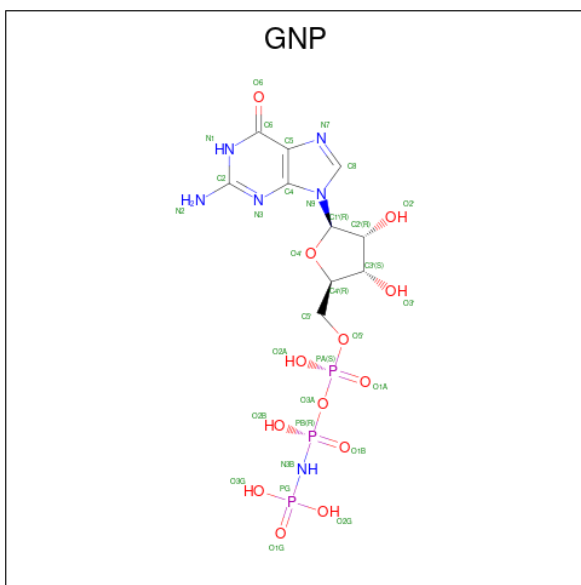
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-15	HIS	-	expression tag	UNP P57772
B	-14	HIS	-	expression tag	UNP P57772
B	-13	HIS	-	expression tag	UNP P57772
B	-12	HIS	-	expression tag	UNP P57772
B	-11	HIS	-	expression tag	UNP P57772
B	-10	HIS	-	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 (CCD ID: MN) (formula: Mn).

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

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (CCD ID: GNP) (formula: C₁₀H₁₇N₆O₁₃P₃).

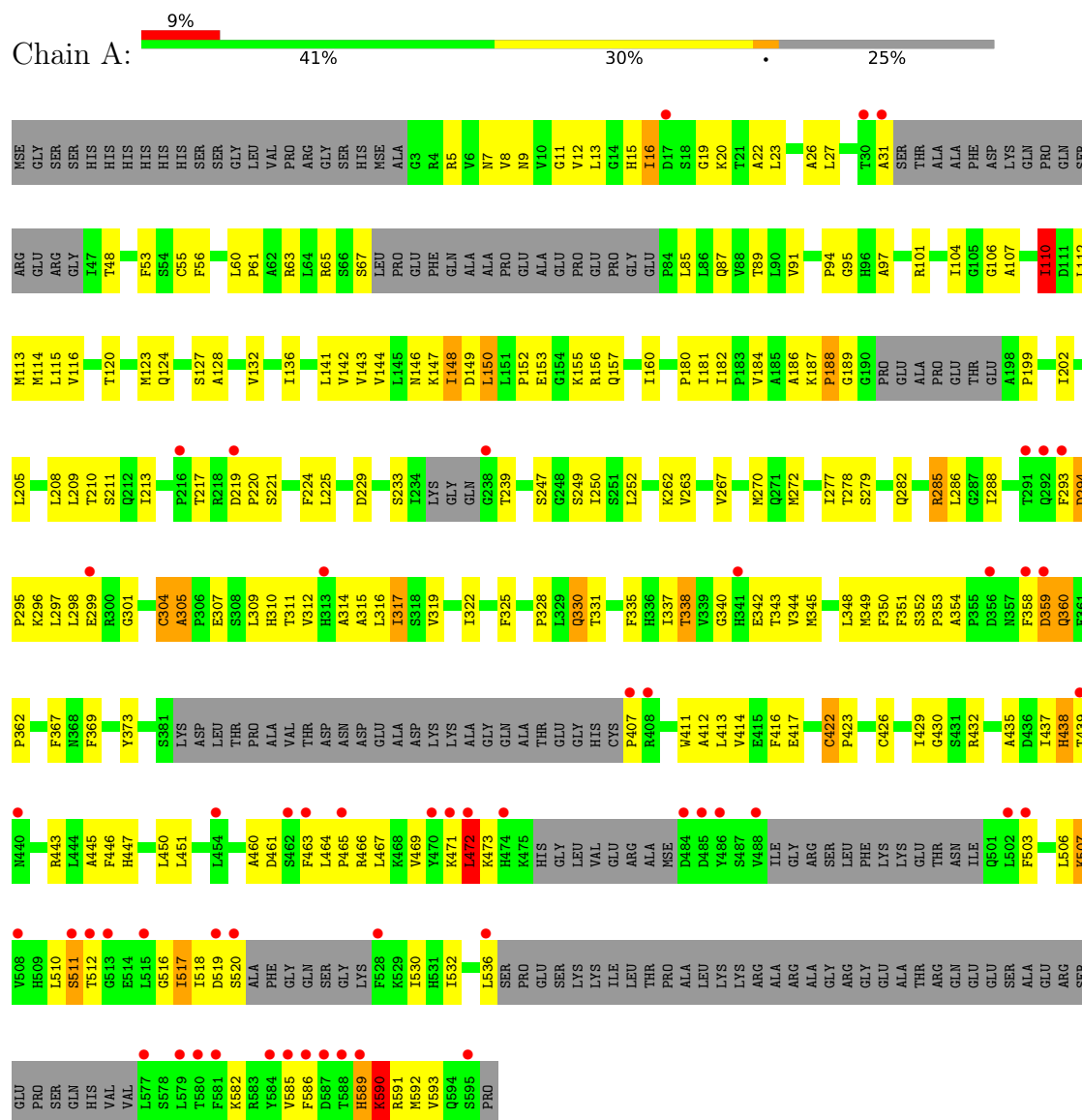


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 32	C 10	N 6	O 13	P 3	0	0
3	B	1	Total 32	C 10	N 6	O 13	P 3	0	0

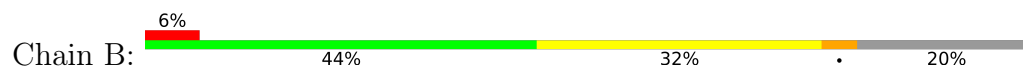
3 Residue-property plots

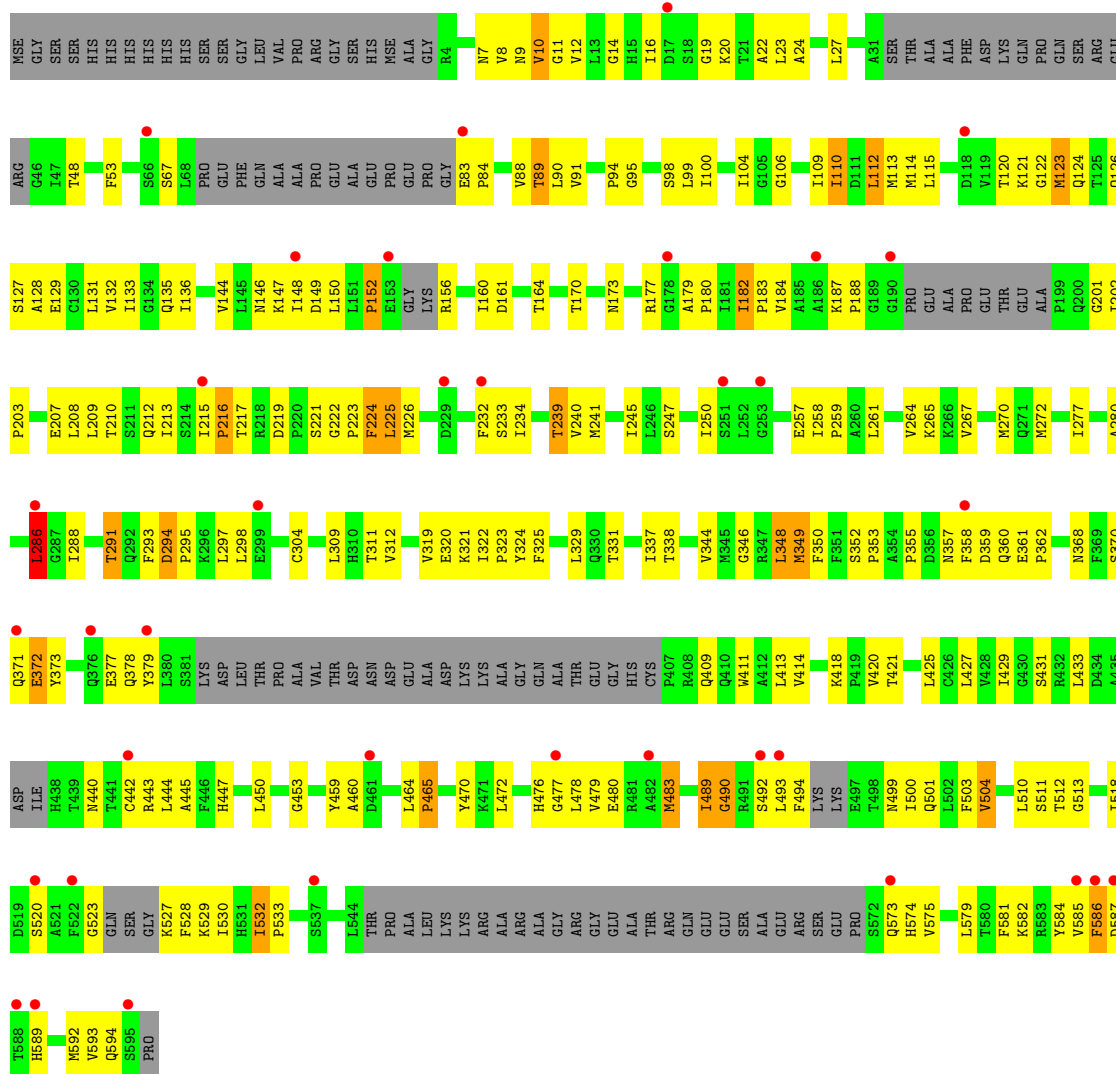
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



• Molecule 1: Selenocysteine-specific elongation factor





4 Data and refinement statistics

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 – 3.40	Depositor EDS
% Data completeness (in resolution range)	78.4 (46.16-3.40) 86.1 (46.16-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 3.40Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.235 , 0.285 0.237 , 0.287	Depositor DCC
R_{free} test set	1114 reflections (4.57%)	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)	0.30 , 47.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.81	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MN, 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	0.56	2/3193 (0.1%)	1.14	34/4335 (0.8%)
1	B	0.49	2/3467 (0.1%)	1.10	30/4708 (0.6%)
All	All	0.52	4/6660 (0.1%)	1.12	64/9043 (0.7%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	584	TYR	CA-C	-5.89	1.48	1.52
1	A	294	ASP	CA-C	-5.88	1.45	1.52
1	A	517	ILE	C-O	-5.42	1.18	1.23
1	B	490	GLY	C-O	-5.41	1.17	1.24

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	445	ALA	N-CA-C	13.49	126.01	111.03
1	B	291	THR	N-CA-C	10.18	126.47	110.70
1	A	299	GLU	CB-CA-C	9.37	121.25	109.16
1	A	110	ILE	N-CA-C	8.88	121.40	108.53
1	B	294	ASP	CA-C-N	8.45	127.76	118.97
1	B	294	ASP	C-N-CA	8.45	127.76	118.97
1	A	511	SER	N-CA-C	8.00	127.83	110.80
1	A	285	ARG	N-CA-C	-7.93	96.32	109.24
1	A	220	PRO	CB-CA-C	-7.89	101.35	112.64
1	A	262	LYS	CB-CA-C	-7.72	95.59	110.65
1	B	225	LEU	N-CA-CB	-7.67	97.25	111.13
1	A	299	GLU	N-CA-C	-7.58	105.20	114.75
1	A	592	MSE	CB-CA-C	-7.54	97.66	109.80
1	A	263	VAL	N-CA-CB	7.09	122.92	111.23
1	B	121	LYS	N-CA-C	-7.08	97.70	108.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	220	PRO	N-CA-C	-7.04	102.12	112.26
1	B	288	ILE	N-CA-C	7.00	117.91	108.11
1	B	224	PHE	N-CA-C	6.82	120.38	110.42
1	A	330	GLN	N-CA-C	6.72	119.65	108.96
1	A	589	HIS	N-CA-CB	-6.70	101.37	111.15
1	B	216	PRO	CB-CA-C	-6.66	100.56	111.56
1	A	307	GLU	N-CA-CB	-6.63	100.26	111.27
1	B	89	THR	N-CA-C	-6.59	96.76	110.80
1	A	360	GLN	N-CA-C	-6.58	98.25	109.24
1	B	445	ALA	CB-CA-C	-6.58	100.75	110.95
1	A	590	LYS	N-CA-CB	6.49	121.45	110.49
1	A	331	THR	N-CA-C	-6.46	100.75	110.24
1	A	359	ASP	N-CA-C	-6.38	97.22	110.80
1	B	291	THR	CB-CA-C	-6.27	102.38	111.91
1	A	188	PRO	N-CA-C	-6.24	104.06	112.48
1	A	422	CYS	N-CA-C	6.07	118.07	108.23
1	A	589	HIS	N-CA-C	5.92	122.20	114.75
1	B	177	ARG	CB-CA-C	-5.86	98.22	110.17
1	B	532	ILE	CA-C-N	5.85	125.39	119.19
1	B	532	ILE	C-N-CA	5.85	125.39	119.19
1	A	301	GLY	N-CA-C	5.74	117.64	110.29
1	A	422	CYS	CA-C-N	-5.65	113.97	119.90
1	A	422	CYS	C-N-CA	-5.65	113.97	119.90
1	A	315	ALA	N-CA-C	5.62	117.65	108.55
1	A	217	THR	N-CA-C	-5.59	99.69	108.63
1	B	286	LEU	N-CA-C	5.43	117.27	108.41
1	A	352	SER	CA-C-N	-5.42	114.04	120.11
1	A	352	SER	C-N-CA	-5.42	114.04	120.11
1	B	348	LEU	CB-CA-C	-5.41	99.17	109.66
1	B	504	VAL	CB-CA-C	5.40	120.14	111.29
1	B	476	HIS	N-CA-C	5.39	118.40	110.59
1	A	305	ALA	N-CA-C	-5.34	98.00	109.81
1	A	472	LEU	N-CA-C	-5.32	99.46	110.80
1	A	438	HIS	N-CA-C	-5.31	106.57	112.57
1	A	55	CYS	N-CA-C	5.19	116.84	108.32
1	B	418	LYS	CA-C-N	5.19	126.33	119.84
1	B	418	LYS	C-N-CA	5.19	126.33	119.84
1	B	500	ILE	CB-CA-C	-5.19	102.79	111.29
1	B	112	LEU	CB-CA-C	5.17	118.32	109.99
1	B	222	GLY	CA-C-N	5.13	126.25	119.84
1	B	222	GLY	C-N-CA	5.13	126.25	119.84
1	B	234	ILE	CB-CA-C	-5.12	102.90	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	323	PRO	CB-CA-C	-5.10	104.95	113.06
1	B	440	ASN	N-CA-C	5.09	116.41	110.41
1	A	304	CYS	N-CA-C	5.08	117.98	109.96
1	A	417	GLU	N-CA-C	-5.08	99.98	110.80
1	B	173	ASN	N-CA-C	-5.05	106.89	113.16
1	B	67	SER	N-CA-C	5.03	121.51	110.80
1	A	317	ILE	N-CA-C	5.00	115.69	108.48

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3147	0	2871	211	0
1	B	3419	0	3163	224	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	434	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 34.

All (434) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:219:ASP:CG	1:A:221:SER:CB	2.36	0.97
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:65:ARG:C	1:A:67:SER:H	1.86	0.80
1:B:7:ASN:HD21	1:B:89:THR:CG2	1.94	0.79
1:A:340:GLY:C	1:A:342:GLU:H	1.91	0.78
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:372:GLU:C	1:B:373:TYR:CD1	2.71	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
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:C	1:A:342:GLU:N	2.52	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: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:A:65:ARG:C	1:A:67:SER:N	2.56	0.63
1:B:207:GLU:HA	1:B:210:THR:CG2	2.28	0.63
1:A:464:LEU:C	1:A:466:ARG:H	2.07	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:B:88:VAL:C	1:B:89:THR:O	2.38	0.62
1:A:304:CYS:SG	1:A:309:LEU:HD13	2.39	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C	1:B:513:GLY:H	2.08	0.60
1:B:511:SER:HB3	1:B:573:GLN:HB2	1.84	0.60
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: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:A:463:PHE:C	1:A:465:PRO:HD2	2.29	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:471:LYS:O	1:A:472:LEU:C	2.48	0.57
1:A:113:MSE:HE3	1:A:115:LEU:HB2	1.86	0.57
1:A:519:ASP:O	1:A:520:SER:C	2.46	0.56
1:B:88:VAL:O	1:B:89:THR:C	2.48	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:A:516:GLY:C	1:A:517:ILE:HG13	2.31	0.56
1:B:585:VAL:O	1:B:586:PHE:CB	2.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:187:LYS:C	1:A:189:GLY:H	2.17	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:209:LEU:C	1:A:211:SER:H	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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:A:353:PRO:O	1:A:354:ALA:C	2.54	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:A:510:LEU:HD12	1:A:510:LEU:C	2.37	0.49
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:MSE:HE2	1:A:128:ALA:HA	1.95	0.49
1:B:586:PHE:O	1:B:589:HIS:C	2.56	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:499:ASN:C	1:B:501:GLN:N	2.71	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: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
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:A:358:PHE:C	1:A:360:GLN:N	2.69	0.47
1:B:586:PHE:O	1:B:587:ASP:C	2.58	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: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:A:464:LEU:C	1:A:466:ARG:N	2.70	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:B:499:ASN:C	1:B:501:GLN:H	2.23	0.46
1:B:503:PHE:O	1:B:504:VAL:C	2.58	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:GLU:HA	1:A:156:ARG:HB2	1.96	0.46
1:A:187:LYS:C	1:A:189:GLY:N	2.72	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: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:511:SER:C	1:B:513:GLY:N	2.74	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:A:516:GLY:C	1:A:517:ILE:CG1	2.89	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: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:A:589:HIS:O	1:A:590:LYS:C	2.58	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: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:324:TYR:C	1:B:442:CYS:CB	2.91	0.44
1:B:478:LEU:HA	1:B:574:HIS:HA	1.99	0.44
1:B:409:GLN:HE21	1:B:411:TRP:NE1	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:15:HIS:HD1	1:A:124:GLN:CD	2.25	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:304:CYS:C	1:A:305:ALA:O	2.59	0.42
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
1:B:460:ALA:HA	1:B:464:LEU:HD12	2.01	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: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:B:219:ASP:C	1:B:221:SER:H	2.28	0.42
1:A:16:ILE:HG12	1:A:95:GLY:C	2.44	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:357:ASN:C	1:B:359:ASP:H	2.28	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:A:11:GLY:H	1:A:110:ILE:HG21	1.85	0.41
1:A:310:HIS:C	1:A:311:THR:HG23	2.45	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:B:510:LEU:O	1:B:511:SER:C	2.63	0.41
1:A:295:PRO:C	1:A:297:LEU:H	2.28	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:VAL:HG22	1:A:345:MSE:H	1.86	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:180:PRO:C	1:A:181:ILE:HG13	2.46	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 ⓘ

5.3.1 Protein backbone ⓘ

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%)	5	23
1	B	475/616 (77%)	377 (79%)	87 (18%)	11 (2%)	5	23
All	All	916/1232 (74%)	727 (79%)	168 (18%)	21 (2%)	5	23

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	590	LYS

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Mol	Chain	Res	Type
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 ⓘ

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%)	269 (97%)	9 (3%)	34	58
1	B	312/507 (62%)	296 (95%)	16 (5%)	21	48
All	All	590/1014 (58%)	565 (96%)	25 (4%)	26	52

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	ILE
1	A	110	ILE
1	A	116	VAL

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Mol	Chain	Res	Type
1	A	148	ILE
1	A	150	LEU
1	A	225	LEU
1	A	338	THR
1	A	349	MSE
1	A	507	LYS
1	B	10	VAL
1	B	90	LEU
1	B	110	ILE
1	B	113	MSE
1	B	123	MSE
1	B	164	THR
1	B	170	THR
1	B	182	ILE
1	B	233	SER
1	B	239	THR
1	B	264	VAL
1	B	286	LEU
1	B	349	MSE
1	B	413	LEU
1	B	489	ILE
1	B	594	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	ASN
1	A	330	GLN
1	B	7	ASN
1	B	9	ASN
1	B	15	HIS
1	B	139	GLN
1	B	212	GLN
1	B	474	HIS
1	B	509	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	A	1002	2	34,34,34	2.92	7 (20%)	47,54,54	1.96	14 (29%)
3	GNP	B	1002	2	34,34,34	2.92	7 (20%)	47,54,54	1.95	14 (29%)

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	A	1002	2	-	6/18/38/38	0/3/3/3
3	GNP	B	1002	2	-	2/18/38/38	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1002	GNP	PG-O1G	10.70	1.62	1.46
3	A	1002	GNP	PG-O1G	10.68	1.62	1.46
3	A	1002	GNP	PB-O1B	10.66	1.62	1.46
3	B	1002	GNP	PB-O1B	10.63	1.62	1.46
3	B	1002	GNP	C5-C6	-3.01	1.33	1.44
3	A	1002	GNP	PG-O3G	-3.00	1.48	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1002	GNP	PB-O2B	-3.00	1.48	1.56
3	B	1002	GNP	PG-O3G	-2.98	1.48	1.56
3	A	1002	GNP	C5-C6	-2.98	1.33	1.44
3	B	1002	GNP	PB-O2B	-2.98	1.48	1.56
3	B	1002	GNP	C5-N7	-2.76	1.33	1.39
3	A	1002	GNP	C5-N7	-2.76	1.33	1.39
3	A	1002	GNP	PG-O2G	2.10	1.62	1.56
3	B	1002	GNP	PG-O2G	2.07	1.62	1.56

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1002	GNP	C2-N3-C4	4.87	120.69	112.30
3	B	1002	GNP	C2-N3-C4	4.85	120.66	112.30
3	B	1002	GNP	C5-C4-N3	-4.56	121.13	128.39
3	A	1002	GNP	C5-C4-N3	-4.54	121.16	128.39
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	A	1002	GNP	C2-N1-C6	-3.80	118.22	125.11
3	B	1002	GNP	C2-N1-C6	-3.78	118.26	125.11
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	-3.34	105.07	113.45
3	A	1002	GNP	O2G-PG-O1G	-3.34	105.09	113.45
3	A	1002	GNP	N9-C8-N7	-3.03	107.79	113.40
3	B	1002	GNP	N9-C8-N7	-3.00	107.83	113.40
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	N9-C4-N3	2.60	131.14	125.95
3	A	1002	GNP	N9-C4-N3	2.58	131.12	125.95
3	B	1002	GNP	C5-C6-N1	2.52	119.68	113.25
3	A	1002	GNP	C5-C6-N1	2.51	119.64	113.25
3	B	1002	GNP	C4'-O4'-C1'	-2.49	103.96	109.47
3	A	1002	GNP	C4'-O4'-C1'	-2.49	103.96	109.47
3	A	1002	GNP	C8-N7-C5	2.22	108.21	104.26
3	B	1002	GNP	C8-N7-C5	2.22	108.21	104.26
3	B	1002	GNP	O6-C6-C5	-2.20	120.72	126.53
3	A	1002	GNP	O6-C6-C5	-2.19	120.75	126.53
3	B	1002	GNP	N1-C2-N3	-2.16	119.36	123.32
3	A	1002	GNP	N1-C2-N3	-2.16	119.36	123.32

There are no chirality outliers.

All (8) 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	PB-O3A-PA-O2A
3	A	1002	GNP	C3'-C4'-C5'-O5'
3	A	1002	GNP	PB-O3A-PA-O1A

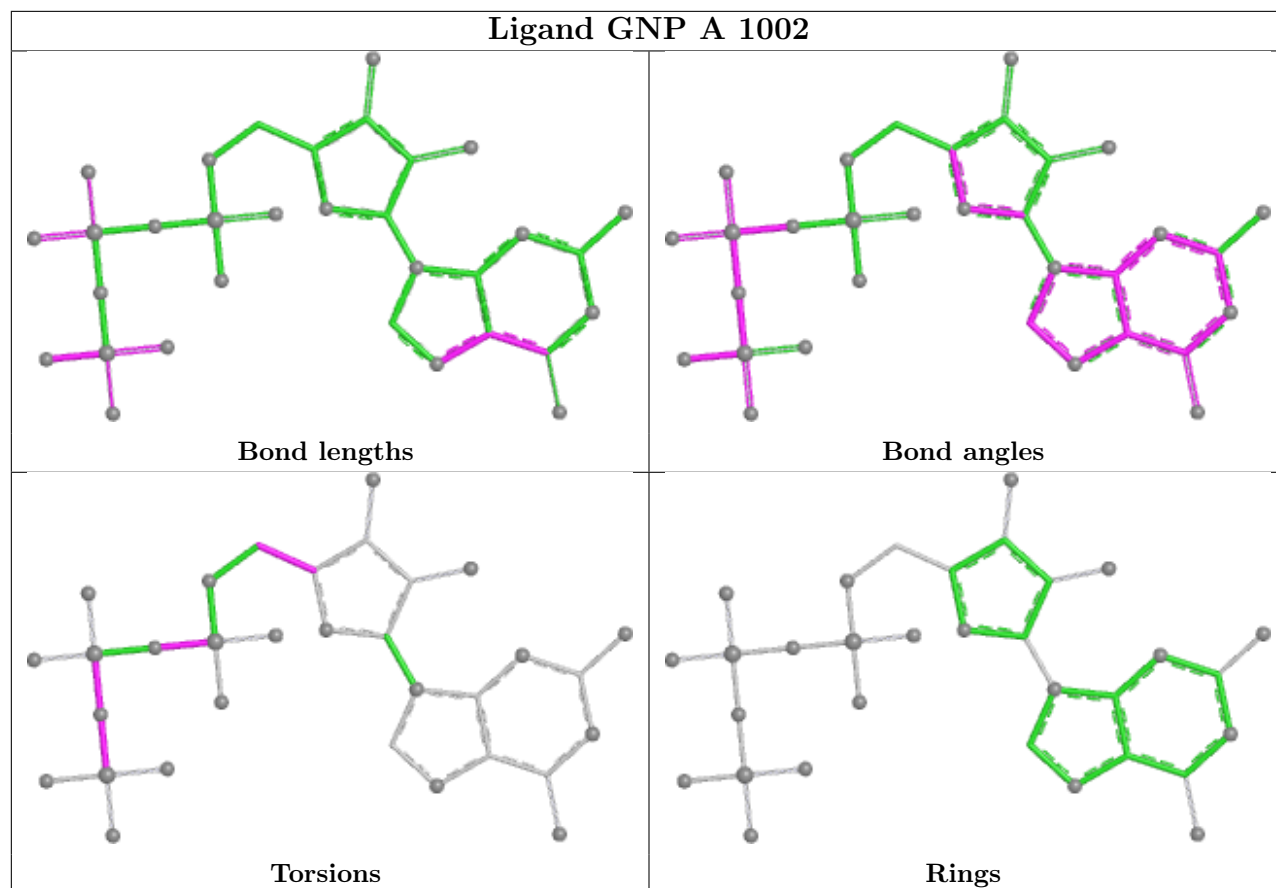
There are no ring outliers.

2 monomers are involved in 9 short contacts:

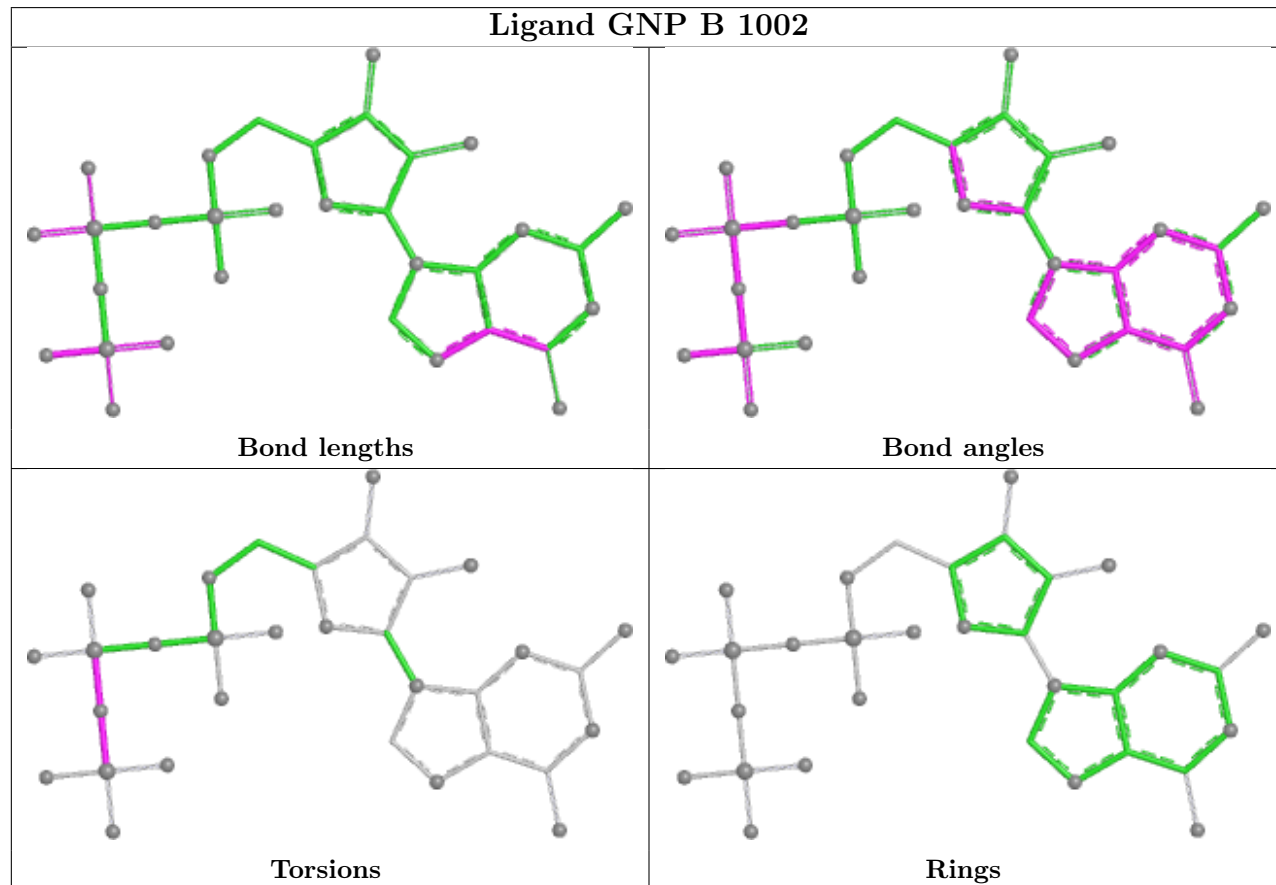
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1002	GNP	7	0
3	B	1002	GNP	2	0

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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand GNP A 1002



Ligand GNP B 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

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	446/616 (72%)	0.78	53 (11%)	9 10	6, 31, 70, 104	1 (0%)
1	B	480/616 (77%)	0.59	36 (7%)	20 17	8, 28, 55, 76	0
All	All	926/1232 (75%)	0.68	89 (9%)	13 13	6, 30, 64, 104	1 (0%)

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	587	ASP	5.1
1	A	520	SER	4.5
1	A	440	ASN	4.2
1	A	484	ASP	3.8
1	A	595	SER	3.8
1	A	341	HIS	3.7
1	A	508	VAL	3.7
1	A	589	HIS	3.6
1	B	286	LEU	3.6
1	B	153	GLU	3.5
1	A	528	PHE	3.5
1	A	536	LEU	3.5
1	A	486	TYR	3.5
1	A	515	LEU	3.5
1	A	472	LEU	3.4
1	B	376	GLN	3.2
1	B	588	THR	3.2
1	B	379	TYR	3.2
1	B	589	HIS	3.2
1	B	299	GLU	3.1
1	A	512	THR	3.1
1	A	470	TYR	3.1
1	A	586	PHE	3.1
1	B	493	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	584	TYR	3.0
1	A	488	VAL	3.0
1	B	17	ASP	2.9
1	A	465	PRO	2.9
1	A	313[A]	HIS	2.9
1	A	407	PRO	2.9
1	B	251	SER	2.9
1	B	586	PHE	2.8
1	A	588	THR	2.8
1	B	461	ASP	2.7
1	A	471	LYS	2.7
1	A	581	PHE	2.7
1	A	17	ASP	2.7
1	A	580	THR	2.6
1	B	371	GLN	2.6
1	B	442	CYS	2.6
1	A	585	VAL	2.6
1	B	595	SER	2.6
1	A	474	HIS	2.6
1	A	359	ASP	2.6
1	B	118	ASP	2.6
1	A	30	THR	2.6
1	A	293	PHE	2.6
1	A	291	THR	2.5
1	A	503	PHE	2.5
1	A	454	LEU	2.4
1	A	579	LEU	2.4
1	A	408	ARG	2.4
1	B	482	ALA	2.3
1	A	511	SER	2.3
1	B	83	GLU	2.3
1	B	477	GLY	2.3
1	B	232	PHE	2.3
1	A	356	ASP	2.3
1	A	485	ASP	2.3
1	A	299	GLU	2.2
1	B	186	ALA	2.2
1	B	148	ILE	2.2
1	A	519	ASP	2.2
1	A	31	ALA	2.2
1	A	462	SER	2.2
1	B	587	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	573	GLN	2.2
1	A	577	LEU	2.2
1	A	513	GLY	2.2
1	B	358	PHE	2.2
1	B	215	ILE	2.1
1	B	492	SER	2.1
1	B	537	SER	2.1
1	B	522	PHE	2.1
1	B	229	ASP	2.1
1	B	178	GLY	2.1
1	A	463	PHE	2.1
1	B	253	GLY	2.1
1	A	439	THR	2.1
1	A	238	GLY	2.1
1	B	585	VAL	2.0
1	B	520	SER	2.0
1	A	292	GLN	2.0
1	A	358	PHE	2.0
1	B	190	GLY	2.0
1	B	66	SER	2.0
1	A	219	ASP	2.0
1	A	216	PRO	2.0
1	A	502	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

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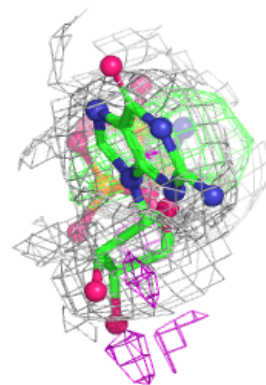
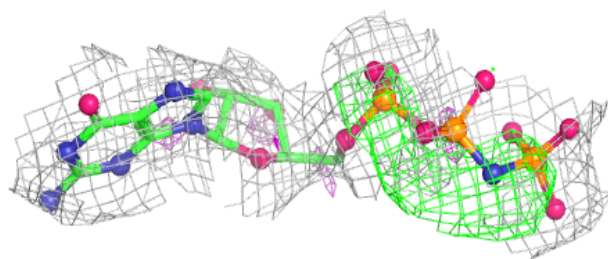
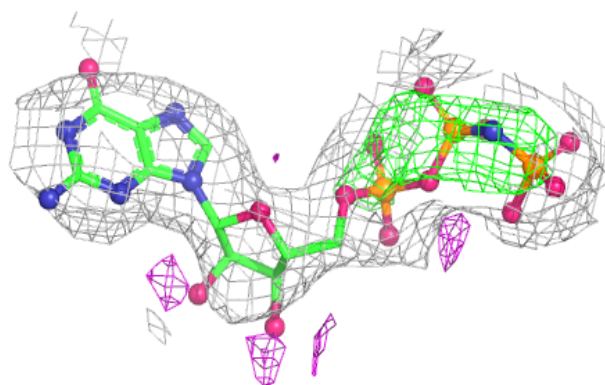
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GNP	A	1002	32/32	0.91	0.17	17,47,78,96	0
3	GNP	B	1002	32/32	0.91	0.15	24,54,66,96	0
2	MN	A	1001	1/1	0.99	0.03	16,16,16,16	0
2	MN	B	1001	1/1	0.99	0.05	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.

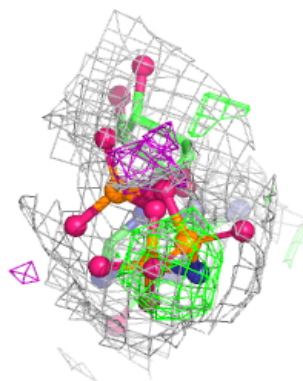
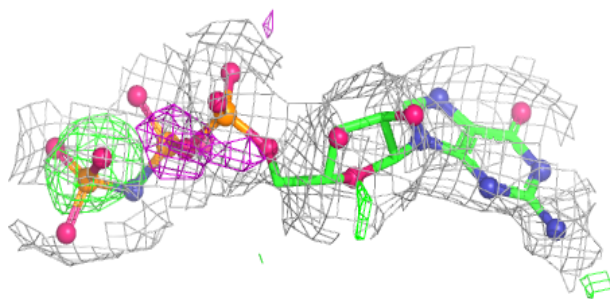
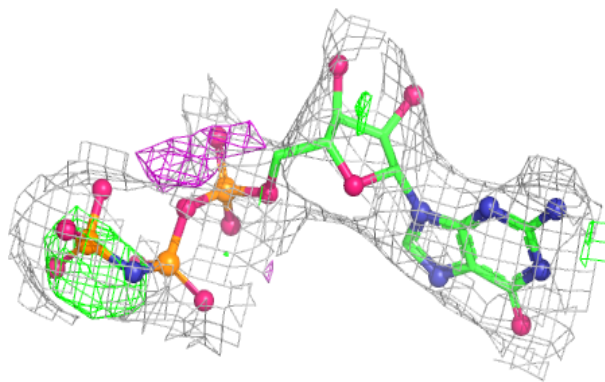
Electron density around GNP A 1002:

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



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)



6.5 Other polymers [i](#)

There are no such residues in this entry.