



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:54 AM UTC

PDB ID : 1FNM / pdb_00001fnn
Title : STRUCTURE OF THERMUS THERMOPHILUS EF-G H573A
Authors : Laurberg, M.; Kristensen, O.; Martemyanov, K.; Gudkov, A.T.; Nagaev, I.;
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Deposited on : 2000-08-22
Resolution : 2.80 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

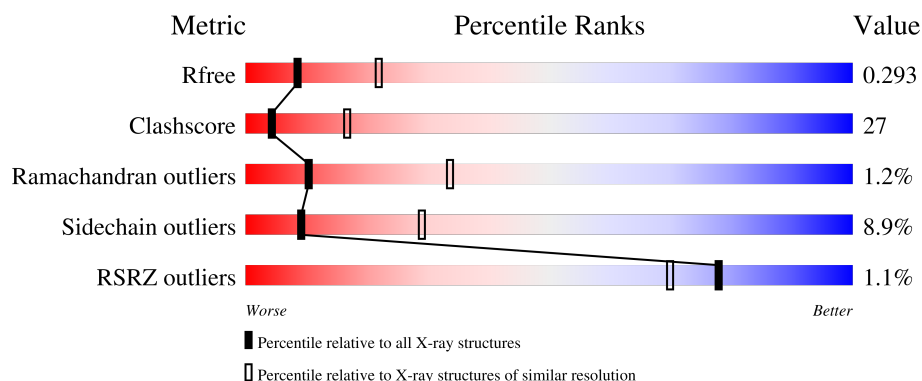
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	691	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5173 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 ELONGATION FACTOR G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	655	Total	C	N	O	S	0	0	0
			5126	3259	874	975	18			

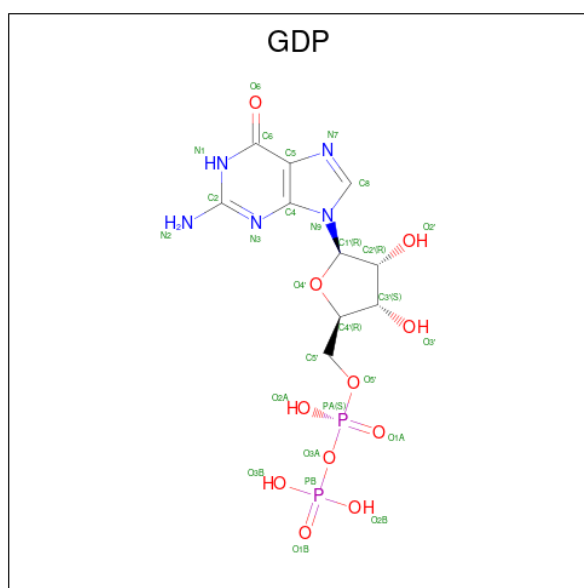
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	573	ALA	HIS	engineered mutation	UNP P13551

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 3 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

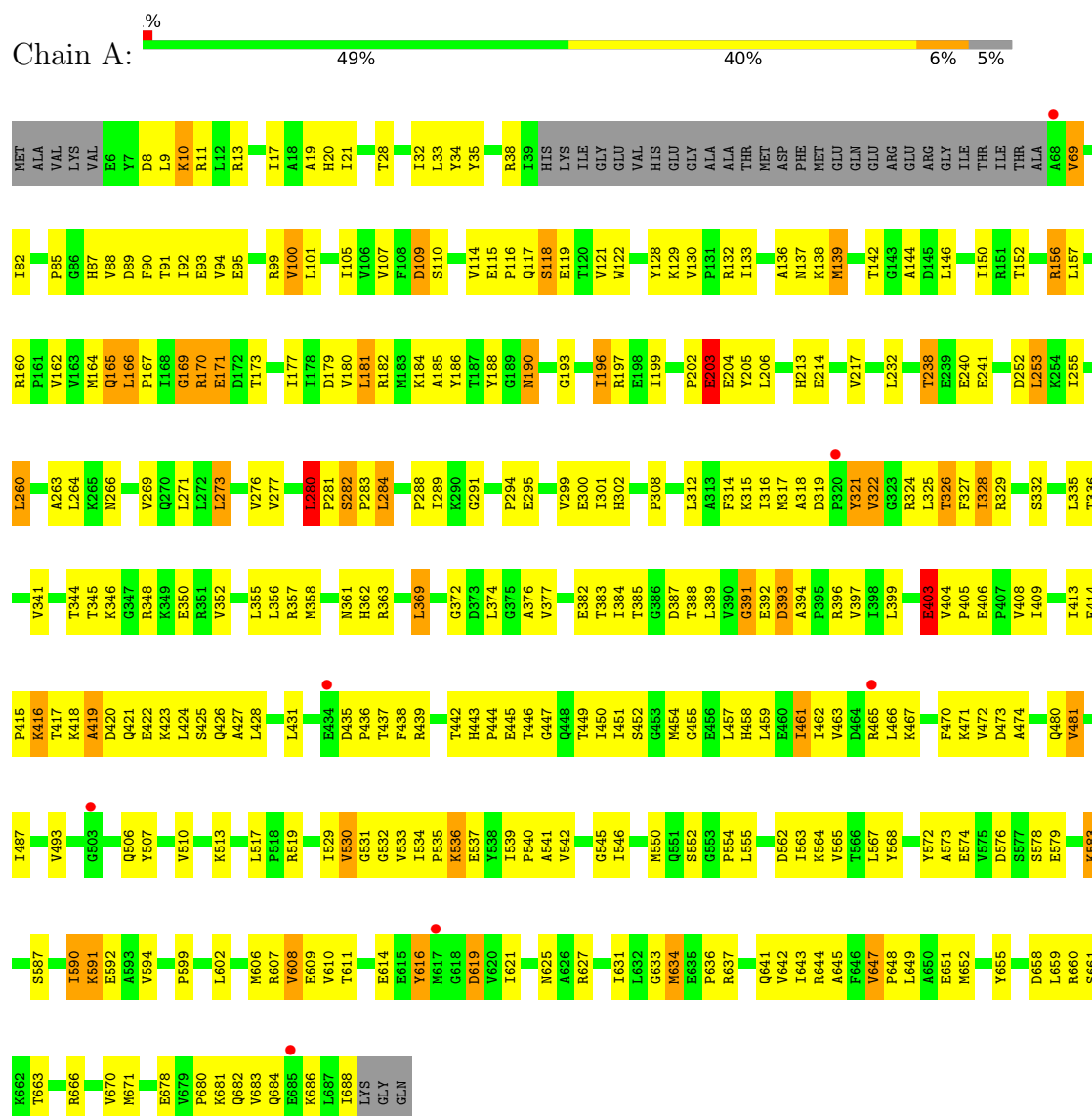
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	18	Total	O	0	0
			18	18		

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: ELONGATION FACTOR G



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	76.70Å 85.97Å 113.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.80 25.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	94.8 (25.00-2.80) 94.7 (25.00-2.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.64 (at 2.81Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.212 , 0.295 0.211 , 0.293	Depositor DCC
R_{free} test set	654 reflections (3.62%)	wwPDB-VP
Wilson B-factor (Å ²)	48.5	Xtriage
Anisotropy	0.363	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 58.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5173	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 4.56% 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: MG, GDP

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	0.50	1/5222 (0.0%)	1.04	28/7073 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	139	MET	SD-CE	-6.22	1.64	1.79

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	530	VAL	N-CA-C	16.83	126.26	112.12
1	A	532	GLY	N-CA-C	-9.79	99.83	114.90
1	A	280	LEU	CA-C-N	7.97	127.99	119.78
1	A	280	LEU	C-N-CA	7.97	127.99	119.78
1	A	169	GLY	N-CA-C	-7.71	103.66	112.29
1	A	529	ILE	CA-C-N	-7.35	115.06	122.77
1	A	529	ILE	C-N-CA	-7.35	115.06	122.77
1	A	419	ALA	N-CA-C	-6.73	104.03	111.36
1	A	591	LYS	N-CA-C	-6.70	103.98	111.28
1	A	530	VAL	CB-CA-C	-6.64	104.40	110.91
1	A	109	ASP	N-CA-C	-6.29	98.92	108.67
1	A	289	ILE	N-CA-C	-6.13	103.28	110.21
1	A	608	VAL	N-CA-C	6.10	116.66	107.75
1	A	645	ALA	N-CA-C	5.80	117.07	108.60
1	A	281	PRO	N-CA-C	5.52	119.99	111.21
1	A	156	ARG	N-CA-C	5.48	117.06	111.14
1	A	205	TYR	N-CA-C	-5.47	105.25	113.89
1	A	282	SER	N-CA-C	-5.39	102.18	110.58
1	A	357	ARG	N-CA-C	-5.36	100.44	109.07
1	A	663	THR	N-CA-C	-5.34	106.07	112.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	576	ASP	N-CA-C	5.25	119.40	112.89
1	A	179	ASP	N-CA-C	-5.23	101.25	109.25
1	A	552	SER	N-CA-C	5.22	116.08	107.20
1	A	416	LYS	N-CA-C	5.22	119.65	113.28
1	A	169	GLY	CA-C-O	-5.14	118.69	122.23
1	A	214	GLU	N-CA-C	-5.12	105.61	111.14
1	A	118	SER	N-CA-C	-5.05	105.05	111.11
1	A	393	ASP	N-CA-C	-5.01	104.64	111.56

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	5126	0	5186	278	0
2	A	1	0	0	0	0
3	A	28	0	12	1	0
4	A	18	0	0	1	0
All	All	5173	0	5198	278	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 27.

All (278) 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:142:THR:HA	1:A:171:GLU:HG2	1.50	0.91
1:A:137:ASN:HD21	1:A:263:ALA:H	1.20	0.88
1:A:165:GLN:HE21	1:A:260:LEU:H	1.24	0.84
1:A:415:PRO:HG3	1:A:421:GLN:HG2	1.60	0.84
1:A:238:THR:HG22	1:A:241:GLU:H	1.44	0.83
1:A:633:GLY:HA2	1:A:634:MET:HE2	1.61	0.81
1:A:316:ILE:HD12	1:A:324:ARG:HH21	1.46	0.81
1:A:413:ILE:HD13	1:A:451:ILE:HD11	1.63	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:GLN:HE21	1:A:260:LEU:HD13	1.47	0.79
1:A:531:GLY:H	1:A:533:VAL:HG23	1.48	0.78
1:A:321:TYR:O	1:A:322:VAL:HG13	1.86	0.75
1:A:13:ARG:HH11	1:A:277:VAL:HA	1.51	0.75
1:A:165:GLN:NE2	1:A:260:LEU:H	1.84	0.74
1:A:166:LEU:HD22	1:A:180:VAL:HG11	1.69	0.74
1:A:545:GLY:HA2	1:A:583:LYS:HE3	1.70	0.73
1:A:110:SER:HB3	1:A:139:MET:HE3	1.71	0.73
1:A:621:ILE:HD11	1:A:643:ILE:HD13	1.69	0.72
1:A:169:GLY:HA3	1:A:173:THR:O	1.89	0.72
1:A:536:LYS:HD2	1:A:537:GLU:N	2.05	0.71
1:A:321:TYR:O	1:A:322:VAL:HG22	1.91	0.70
1:A:405:PRO:HB2	1:A:454:MET:HG2	1.72	0.70
1:A:424:LEU:HD13	1:A:472:VAL:HG11	1.74	0.70
1:A:536:LYS:HD2	1:A:537:GLU:H	1.57	0.69
1:A:627:ARG:HD2	1:A:651:GLU:O	1.91	0.69
1:A:467:LYS:O	1:A:471:LYS:HA	1.91	0.69
1:A:238:THR:HG23	1:A:240:GLU:OE2	1.93	0.69
1:A:114:VAL:HG12	1:A:152:THR:OG1	1.92	0.68
1:A:539:ILE:O	1:A:542:VAL:HG12	1.94	0.68
1:A:423:LYS:HG3	1:A:472:VAL:HG22	1.76	0.68
1:A:607:ARG:HH22	1:A:644:ARG:HE	1.41	0.67
1:A:627:ARG:HH21	1:A:655:TYR:HD1	1.43	0.67
1:A:142:THR:HA	1:A:171:GLU:CG	2.23	0.66
1:A:517:LEU:HD13	1:A:564:LYS:HB2	1.77	0.66
1:A:13:ARG:NH1	1:A:277:VAL:O	2.29	0.66
1:A:608:VAL:HG21	1:A:652:MET:HE2	1.78	0.66
1:A:546:ILE:O	1:A:550:MET:HG3	1.96	0.65
1:A:110:SER:HB3	1:A:139:MET:CE	2.27	0.65
1:A:422:GLU:O	1:A:426:GLN:HG2	1.98	0.64
1:A:637:ARG:HG3	1:A:637:ARG:HH11	1.61	0.64
1:A:114:VAL:HG12	1:A:152:THR:CB	2.28	0.64
1:A:345:THR:O	1:A:346:LYS:HG3	1.97	0.64
1:A:139:MET:HE2	1:A:144:ALA:HB1	1.80	0.63
1:A:513:LYS:HG3	1:A:568:TYR:CE1	2.33	0.63
1:A:92:ILE:HG23	1:A:93:GLU:N	2.14	0.63
1:A:20:HIS:HD2	1:A:117:GLN:H	1.46	0.63
1:A:607:ARG:NH2	1:A:644:ARG:HE	1.97	0.63
1:A:9:LEU:HD13	1:A:284:LEU:HD13	1.80	0.62
1:A:166:LEU:HD22	1:A:180:VAL:CG1	2.28	0.62
1:A:316:ILE:HD13	1:A:326:THR:HB	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:GLU:HB3	1:A:128:TYR:OH	1.99	0.62
1:A:19:ALA:HB2	1:A:107:VAL:HB	1.82	0.62
1:A:129:LYS:HB3	1:A:253:LEU:HD21	1.82	0.62
1:A:413:ILE:HD13	1:A:451:ILE:CD1	2.29	0.61
1:A:105:ILE:HG12	1:A:133:ILE:HD11	1.83	0.61
1:A:139:MET:HE2	1:A:139:MET:HA	1.81	0.61
1:A:288:PRO:HG2	1:A:300:GLU:HG2	1.81	0.61
1:A:462:ILE:O	1:A:466:LEU:HD13	2.00	0.61
1:A:445:GLU:HG3	1:A:446:THR:H	1.66	0.61
1:A:405:PRO:HG3	1:A:437:THR:HB	1.83	0.61
1:A:190:ASN:C	1:A:190:ASN:HD22	2.10	0.60
1:A:427:ALA:HB1	1:A:470:PHE:CD2	2.37	0.60
1:A:110:SER:CB	1:A:139:MET:HE3	2.31	0.60
1:A:294:PRO:HD3	1:A:396:ARG:O	2.01	0.59
1:A:35:TYR:OH	1:A:193:GLY:HA3	2.03	0.59
1:A:181:LEU:HD12	1:A:181:LEU:O	2.02	0.59
1:A:619:ASP:N	1:A:619:ASP:OD2	2.36	0.59
1:A:409:ILE:HG13	1:A:455:GLY:HA2	1.85	0.59
1:A:621:ILE:CD1	1:A:643:ILE:HD13	2.31	0.59
1:A:684:GLN:O	1:A:688:ILE:HG13	2.03	0.58
1:A:417:THR:C	1:A:419:ALA:H	2.11	0.58
1:A:20:HIS:CD2	1:A:117:GLN:HB2	2.38	0.58
1:A:404:VAL:HG13	1:A:405:PRO:HD2	1.86	0.58
1:A:445:GLU:HG3	1:A:446:THR:N	2.18	0.58
1:A:137:ASN:ND2	1:A:263:ALA:H	1.95	0.58
1:A:682:GLN:HG3	1:A:686:LYS:HE3	1.86	0.58
1:A:213:HIS:O	1:A:217:VAL:HG23	2.03	0.58
1:A:238:THR:HG22	1:A:241:GLU:N	2.16	0.58
1:A:391:GLY:O	1:A:392:GLU:HB3	2.04	0.57
1:A:101:LEU:C	1:A:101:LEU:HD12	2.29	0.57
1:A:391:GLY:C	1:A:393:ASP:H	2.11	0.57
1:A:633:GLY:CA	1:A:634:MET:HE2	2.31	0.57
1:A:647:VAL:HG21	1:A:652:MET:SD	2.45	0.57
1:A:188:TYR:CE1	1:A:196:ILE:HG12	2.40	0.57
1:A:17:ILE:N	1:A:17:ILE:HD12	2.20	0.56
1:A:414:GLU:C	1:A:474:ALA:HB1	2.31	0.56
1:A:542:VAL:O	1:A:546:ILE:HG13	2.04	0.56
1:A:506:GLN:NE2	1:A:578:SER:OG	2.38	0.56
1:A:32:ILE:HG23	1:A:273:LEU:HD11	1.88	0.56
1:A:114:VAL:HG12	1:A:152:THR:HB	1.87	0.55
1:A:625:ASN:HD21	1:A:631:ILE:HD13	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:ARG:HH21	1:A:372:GLY:HA2	1.71	0.55
1:A:449:THR:O	1:A:450:ILE:HD13	2.07	0.55
1:A:363:ARG:HG3	1:A:363:ARG:HH11	1.71	0.55
1:A:170:ARG:HH11	1:A:170:ARG:HG2	1.73	0.54
1:A:238:THR:HB	1:A:241:GLU:OE1	2.07	0.54
1:A:417:THR:O	1:A:419:ALA:N	2.39	0.54
1:A:449:THR:C	1:A:450:ILE:HD13	2.33	0.54
1:A:648:PRO:HG2	1:A:651:GLU:CG	2.37	0.54
1:A:602:LEU:HD23	1:A:678:GLU:HA	1.89	0.54
1:A:137:ASN:ND2	1:A:138:LYS:H	2.06	0.53
1:A:165:GLN:NE2	1:A:260:LEU:HD13	2.21	0.53
1:A:316:ILE:CD1	1:A:326:THR:HB	2.38	0.53
1:A:85:PRO:HG2	1:A:94:VAL:CG2	2.39	0.53
1:A:160:ARG:HD3	1:A:255:ILE:HG22	1.91	0.53
1:A:425:SER:HA	1:A:428:LEU:HD12	1.90	0.53
1:A:115:GLU:HB3	1:A:116:PRO:HD2	1.90	0.52
1:A:181:LEU:HD12	1:A:181:LEU:C	2.34	0.52
1:A:115:GLU:HB3	1:A:116:PRO:CD	2.40	0.52
1:A:118:SER:O	1:A:121:VAL:HG22	2.10	0.52
1:A:546:ILE:HG23	1:A:590:ILE:HG12	1.92	0.52
1:A:606:MET:HE3	1:A:671:MET:HG2	1.91	0.52
1:A:114:VAL:CG1	1:A:152:THR:HB	2.40	0.51
1:A:431:LEU:HD11	1:A:465:ARG:HD3	1.93	0.51
1:A:550:MET:SD	1:A:563:ILE:HD11	2.49	0.51
1:A:344:THR:C	1:A:346:LYS:H	2.17	0.51
1:A:534:ILE:HD12	1:A:567:LEU:HD11	1.93	0.51
1:A:636:PRO:HD3	1:A:641:GLN:HE22	1.76	0.51
1:A:415:PRO:CG	1:A:421:GLN:HG2	2.35	0.51
1:A:454:MET:H	1:A:458:HIS:HD2	1.59	0.51
1:A:90:PHE:O	1:A:94:VAL:HG23	2.11	0.51
1:A:8:ASP:OD1	1:A:10:LYS:HE2	2.11	0.50
1:A:308:PRO:HB2	1:A:394:ALA:HB1	1.92	0.50
1:A:519:ARG:HA	1:A:519:ARG:HH11	1.76	0.50
1:A:519:ARG:HD3	1:A:562:ASP:OD1	2.12	0.50
1:A:182:ARG:HB2	1:A:184:LYS:HD2	1.93	0.50
1:A:335:LEU:HD11	1:A:341:VAL:HG11	1.94	0.49
1:A:85:PRO:HG2	1:A:94:VAL:N	2.27	0.49
1:A:384:ILE:HD13	1:A:436:PRO:HG3	1.94	0.49
1:A:85:PRO:HG2	1:A:94:VAL:CA	2.43	0.49
1:A:34:TYR:CZ	1:A:38:ARG:HD3	2.48	0.49
1:A:607:ARG:NH2	1:A:644:ARG:HH21	2.10	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:607:ARG:HH21	1:A:644:ARG:HH21	1.60	0.49
1:A:658:ASP:O	1:A:661:SER:HB3	2.13	0.49
1:A:166:LEU:CD2	1:A:180:VAL:HG11	2.41	0.49
1:A:85:PRO:HG3	1:A:93:GLU:HB3	1.95	0.49
1:A:536:LYS:HD2	1:A:537:GLU:HG3	1.95	0.49
1:A:87:HIS:HB3	1:A:90:PHE:CE1	2.48	0.48
1:A:328:ILE:HD13	1:A:328:ILE:O	2.13	0.48
1:A:507:TYR:CD1	1:A:507:TYR:C	2.91	0.48
1:A:291:GLY:O	1:A:299:VAL:N	2.45	0.48
1:A:312:LEU:HD23	1:A:399:LEU:HB2	1.96	0.48
1:A:417:THR:O	1:A:418:LYS:HB2	2.13	0.48
1:A:510:VAL:HG11	1:A:542:VAL:HG21	1.95	0.48
1:A:13:ARG:HH11	1:A:277:VAL:CA	2.23	0.48
1:A:122:TRP:CE3	1:A:157:LEU:HD13	2.49	0.47
1:A:361:ASN:O	1:A:362:HIS:HB3	2.14	0.47
1:A:122:TRP:CD2	1:A:157:LEU:HD13	2.49	0.47
1:A:89:ASP:O	1:A:91:THR:N	2.44	0.47
1:A:443:HIS:HB3	1:A:446:THR:OG1	2.13	0.47
1:A:114:VAL:HG13	1:A:114:VAL:O	2.15	0.47
1:A:8:ASP:O	1:A:9:LEU:C	2.58	0.47
1:A:417:THR:C	1:A:419:ALA:N	2.72	0.47
1:A:587:SER:O	1:A:591:LYS:HG2	2.15	0.47
1:A:99:ARG:HD3	4:A:1014:HOH:O	2.15	0.47
1:A:146:LEU:O	1:A:150:ILE:HG12	2.14	0.47
1:A:318:ALA:HA	1:A:324:ARG:HA	1.97	0.47
1:A:92:ILE:CG2	1:A:93:GLU:N	2.78	0.47
1:A:264:LEU:HD23	1:A:264:LEU:O	2.15	0.47
1:A:384:ILE:CD1	1:A:436:PRO:HG3	2.45	0.47
1:A:345:THR:C	1:A:346:LYS:HG3	2.39	0.46
1:A:9:LEU:O	1:A:11:ARG:N	2.48	0.46
1:A:555:LEU:HD21	1:A:599:PRO:HG2	1.98	0.46
1:A:196:ILE:HD13	1:A:197:ARG:N	2.31	0.46
1:A:363:ARG:HG3	1:A:363:ARG:NH1	2.31	0.46
1:A:316:ILE:HD12	1:A:324:ARG:NH2	2.23	0.46
1:A:606:MET:HE2	1:A:671:MET:HE3	1.98	0.46
1:A:138:LYS:HG2	3:A:900:GDP:C6	2.50	0.46
1:A:631:ILE:HD12	1:A:631:ILE:N	2.31	0.46
1:A:415:PRO:HA	1:A:474:ALA:HB2	1.97	0.46
1:A:583:LYS:C	1:A:583:LYS:HE2	2.41	0.45
1:A:637:ARG:HG3	1:A:637:ARG:NH1	2.29	0.45
1:A:110:SER:OG	1:A:136:ALA:HB1	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:ASP:HB2	1:A:325:LEU:HD12	1.98	0.45
1:A:458:HIS:CE1	1:A:462:ILE:HD11	2.51	0.45
1:A:609:GLU:HB2	1:A:670:VAL:CG2	2.46	0.45
1:A:636:PRO:HD3	1:A:641:GLN:NE2	2.31	0.45
1:A:282:SER:C	1:A:284:LEU:H	2.25	0.45
1:A:238:THR:HG22	1:A:241:GLU:HG3	1.99	0.45
1:A:345:THR:O	1:A:345:THR:HG22	2.17	0.45
1:A:461:ILE:O	1:A:465:ARG:HB2	2.17	0.45
1:A:608:VAL:HG12	1:A:610:VAL:HG23	1.99	0.45
1:A:260:LEU:HD22	1:A:260:LEU:C	2.42	0.45
1:A:493:VAL:HG11	1:A:592:GLU:HG3	1.99	0.45
1:A:519:ARG:HA	1:A:519:ARG:NH1	2.32	0.45
1:A:633:GLY:C	1:A:634:MET:HE2	2.42	0.45
1:A:413:ILE:CD1	1:A:451:ILE:HD11	2.40	0.44
1:A:418:LYS:HA	1:A:421:GLN:CB	2.47	0.44
1:A:403:GLU:HG2	1:A:404:VAL:N	2.31	0.44
1:A:438:PHE:HB2	1:A:452:SER:O	2.17	0.44
1:A:606:MET:HB3	1:A:671:MET:HG3	1.98	0.44
1:A:82:ILE:HG12	1:A:100:VAL:HG12	1.99	0.44
1:A:348:ARG:HH21	1:A:350:GLU:HA	1.83	0.44
1:A:406:GLU:O	1:A:408:VAL:HG13	2.17	0.44
1:A:680:PRO:HD2	1:A:683:VAL:HG21	2.00	0.44
1:A:409:ILE:O	1:A:452:SER:HA	2.18	0.44
1:A:20:HIS:CD2	1:A:117:GLN:H	2.31	0.44
1:A:28:THR:O	1:A:32:ILE:HG13	2.17	0.44
1:A:269:VAL:O	1:A:273:LEU:HD22	2.18	0.44
1:A:85:PRO:HG2	1:A:94:VAL:HA	1.99	0.44
1:A:146:LEU:HD13	1:A:146:LEU:C	2.42	0.44
1:A:616:TYR:HA	1:A:619:ASP:OD1	2.18	0.44
1:A:487:ILE:HA	1:A:599:PRO:HA	1.99	0.44
1:A:348:ARG:HH11	1:A:382:GLU:HG3	1.82	0.44
1:A:627:ARG:NH2	1:A:655:TYR:HD1	2.13	0.44
1:A:109:ASP:CG	1:A:138:LYS:HD2	2.42	0.44
1:A:276:VAL:O	1:A:280:LEU:HB2	2.18	0.44
1:A:288:PRO:HB2	1:A:301:ILE:O	2.18	0.43
1:A:20:HIS:O	1:A:21:ILE:C	2.61	0.43
1:A:114:VAL:O	1:A:114:VAL:HG22	2.17	0.43
1:A:252:ASP:O	1:A:253:LEU:HB2	2.18	0.43
1:A:324:ARG:NH2	1:A:383:THR:O	2.52	0.43
1:A:280:LEU:HD12	1:A:280:LEU:HA	1.75	0.43
1:A:321:TYR:O	1:A:322:VAL:CG1	2.62	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:LEU:HD13	1:A:369:LEU:HD22	2.00	0.43
1:A:481:VAL:HB	1:A:649:LEU:HD23	1.99	0.43
1:A:487:ILE:CG2	1:A:594:VAL:HA	2.47	0.43
1:A:88:VAL:HG12	1:A:121:VAL:HG12	2.00	0.43
1:A:627:ARG:O	1:A:651:GLU:HG3	2.18	0.43
1:A:92:ILE:HG23	1:A:93:GLU:H	1.81	0.43
1:A:85:PRO:HG2	1:A:94:VAL:HG22	2.01	0.43
1:A:414:GLU:O	1:A:474:ALA:HB1	2.19	0.43
1:A:20:HIS:CE1	1:A:21:ILE:HG22	2.54	0.43
1:A:185:ALA:HB3	1:A:199:ILE:O	2.19	0.43
1:A:435:ASP:OD1	1:A:435:ASP:C	2.62	0.43
1:A:164:MET:C	1:A:180:VAL:HG22	2.44	0.42
1:A:317:MET:O	1:A:325:LEU:N	2.51	0.42
1:A:573:ALA:O	1:A:574:GLU:C	2.62	0.42
1:A:546:ILE:HD13	1:A:565:VAL:HG11	2.01	0.42
1:A:324:ARG:O	1:A:324:ARG:HG3	2.20	0.42
1:A:203:GLU:HA	1:A:206:LEU:HB2	2.01	0.42
1:A:186:TYR:HB3	1:A:196:ILE:HD11	2.01	0.42
1:A:240:GLU:H	1:A:240:GLU:CD	2.27	0.42
1:A:344:THR:HG21	1:A:396:ARG:HA	2.02	0.42
1:A:682:GLN:HG3	1:A:686:LYS:CE	2.49	0.42
1:A:459:LEU:O	1:A:463:VAL:HG23	2.20	0.42
1:A:442:THR:HG23	1:A:447:GLY:O	2.20	0.42
1:A:9:LEU:HD22	1:A:283:PRO:HB2	2.02	0.42
1:A:391:GLY:C	1:A:393:ASP:N	2.77	0.42
1:A:416:LYS:HG2	1:A:474:ALA:HA	2.02	0.42
1:A:308:PRO:HB2	1:A:394:ALA:CB	2.50	0.42
1:A:409:ILE:HA	1:A:480:GLN:O	2.20	0.42
1:A:427:ALA:HB1	1:A:470:PHE:CG	2.55	0.42
1:A:454:MET:H	1:A:458:HIS:CD2	2.38	0.42
1:A:530:VAL:O	1:A:530:VAL:CG1	2.63	0.42
1:A:634:MET:HE2	1:A:634:MET:N	2.35	0.42
1:A:110:SER:CB	1:A:139:MET:CE	2.95	0.41
1:A:202:PRO:O	1:A:203:GLU:C	2.63	0.41
1:A:9:LEU:O	1:A:10:LYS:C	2.63	0.41
1:A:321:TYR:O	1:A:322:VAL:CG2	2.65	0.41
1:A:345:THR:HG21	1:A:387:ASP:OD1	2.20	0.41
1:A:302:HIS:O	1:A:332:SER:HB3	2.20	0.41
1:A:611:THR:OG1	1:A:642:VAL:HG22	2.20	0.41
1:A:100:VAL:HG21	1:A:314:PHE:CD2	2.55	0.41
1:A:301:ILE:HD12	1:A:399:LEU:HD11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:680:PRO:O	1:A:681:LYS:C	2.63	0.41
1:A:13:ARG:HD3	1:A:276:VAL:O	2.21	0.41
1:A:156:ARG:NH2	1:A:666:ARG:HG2	2.36	0.41
1:A:537:GLU:H	1:A:537:GLU:HG3	1.58	0.41
1:A:535:PRO:HD3	1:A:572:TYR:CD1	2.55	0.41
1:A:648:PRO:HG2	1:A:651:GLU:HG3	2.02	0.41
1:A:327:PHE:CE1	1:A:376:ALA:HB2	2.56	0.41
1:A:9:LEU:C	1:A:11:ARG:N	2.79	0.41
1:A:88:VAL:CG1	1:A:121:VAL:HG12	2.50	0.41
1:A:329:ARG:HD2	1:A:374:LEU:HG	2.03	0.41
1:A:350:GLU:OE2	1:A:383:THR:OG1	2.32	0.41
1:A:388:THR:HG21	1:A:397:VAL:O	2.21	0.41
1:A:438:PHE:O	1:A:439:ARG:HD2	2.21	0.41
1:A:539:ILE:N	1:A:540:PRO:HD2	2.36	0.41
1:A:609:GLU:HB2	1:A:670:VAL:HG22	2.04	0.40
1:A:116:PRO:O	1:A:119:GLU:HB3	2.21	0.40
1:A:356:LEU:HB2	1:A:358:MET:CE	2.52	0.40
1:A:546:ILE:HG23	1:A:590:ILE:CG1	2.51	0.40
1:A:177:ILE:HD12	1:A:271:LEU:HD12	2.03	0.40
1:A:579:GLU:O	1:A:583:LYS:HB2	2.21	0.40
1:A:457:LEU:O	1:A:458:HIS:C	2.64	0.40
1:A:193:GLY:CA	1:A:266:ASN:HB3	2.52	0.40
1:A:541:ALA:O	1:A:583:LYS:HA	2.21	0.40
1:A:648:PRO:HG2	1:A:651:GLU:HG2	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	651/691 (94%)	592 (91%)	51 (8%)	8 (1%)	10 34

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	322	VAL
1	A	10	LYS
1	A	403	GLU
1	A	444	PRO
1	A	69	VAL
1	A	203	GLU
1	A	554	PRO
1	A	391	GLY

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	553/581 (95%)	504 (91%)	49 (9%)	9 29

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	LEU
1	A	69	VAL
1	A	100	VAL
1	A	130	VAL
1	A	132	ARG
1	A	162	VAL
1	A	165	GLN
1	A	166	LEU
1	A	167	PRO
1	A	170	ARG
1	A	171	GLU
1	A	181	LEU
1	A	190	ASN
1	A	196	ILE
1	A	203	GLU
1	A	204	GLU
1	A	232	LEU

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Mol	Chain	Res	Type
1	A	238	THR
1	A	253	LEU
1	A	260	LEU
1	A	273	LEU
1	A	280	LEU
1	A	284	LEU
1	A	295	GLU
1	A	315	LYS
1	A	321	TYR
1	A	326	THR
1	A	328	ILE
1	A	336	THR
1	A	352	VAL
1	A	369	LEU
1	A	377	VAL
1	A	385	THR
1	A	389	LEU
1	A	403	GLU
1	A	420	ASP
1	A	461	ILE
1	A	473	ASP
1	A	481	VAL
1	A	536	LYS
1	A	583	LYS
1	A	590	ILE
1	A	614	GLU
1	A	616	TYR
1	A	619	ASP
1	A	634	MET
1	A	647	VAL
1	A	659	LEU
1	A	660	ARG

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	20	HIS
1	A	80	ASN
1	A	124	GLN
1	A	137	ASN
1	A	154	GLN
1	A	165	GLN

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Mol	Chain	Res	Type
1	A	208	GLN
1	A	226	ASN
1	A	426	GLN
1	A	443	HIS
1	A	448	GLN
1	A	458	HIS
1	A	475	ASN
1	A	480	GLN
1	A	500	GLN
1	A	506	GLN
1	A	543	GLN
1	A	551	GLN
1	A	625	ASN
1	A	641	GLN
1	A	664	GLN
1	A	677	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is 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
3	GDP	A	900	2	29,30,30	1.24	2 (6%)	45,47,47	0.76	1 (2%)

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	GDP	A	900	2	-	3/16/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	900	GDP	PA-O3A	4.68	1.64	1.59
3	A	900	GDP	PB-O2B	-2.27	1.46	1.54

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	900	GDP	O3'-C3'-C4'	-2.24	104.64	111.08

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	900	GDP	PA-O3A-PB-O3B
3	A	900	GDP	PA-O3A-PB-O2B
3	A	900	GDP	PA-O3A-PB-O1B

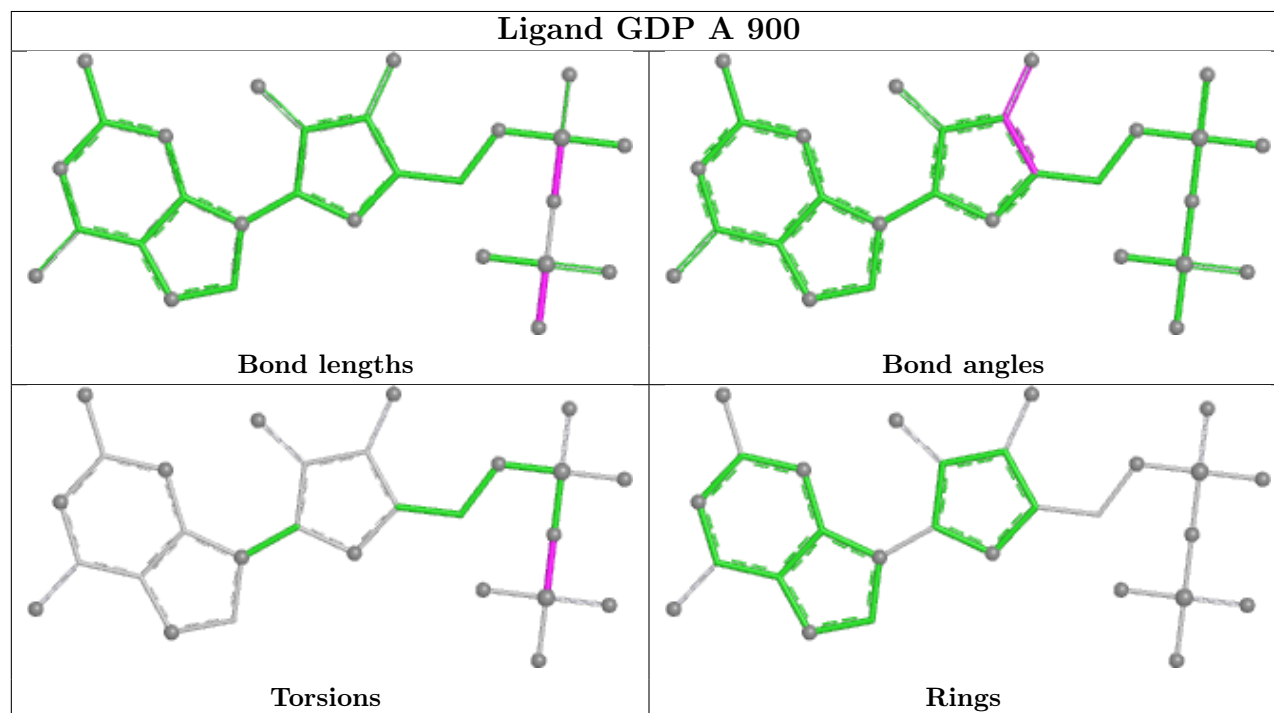
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	900	GDP	1	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.



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	655/691 (94%)	-0.27	7 (1%) 78 70	17, 44, 81, 141	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	503	GLY	2.9
1	A	320	PRO	2.4
1	A	434	GLU	2.3
1	A	617	MET	2.3
1	A	68	ALA	2.1
1	A	685	GLU	2.1
1	A	465	ARG	2.1

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.

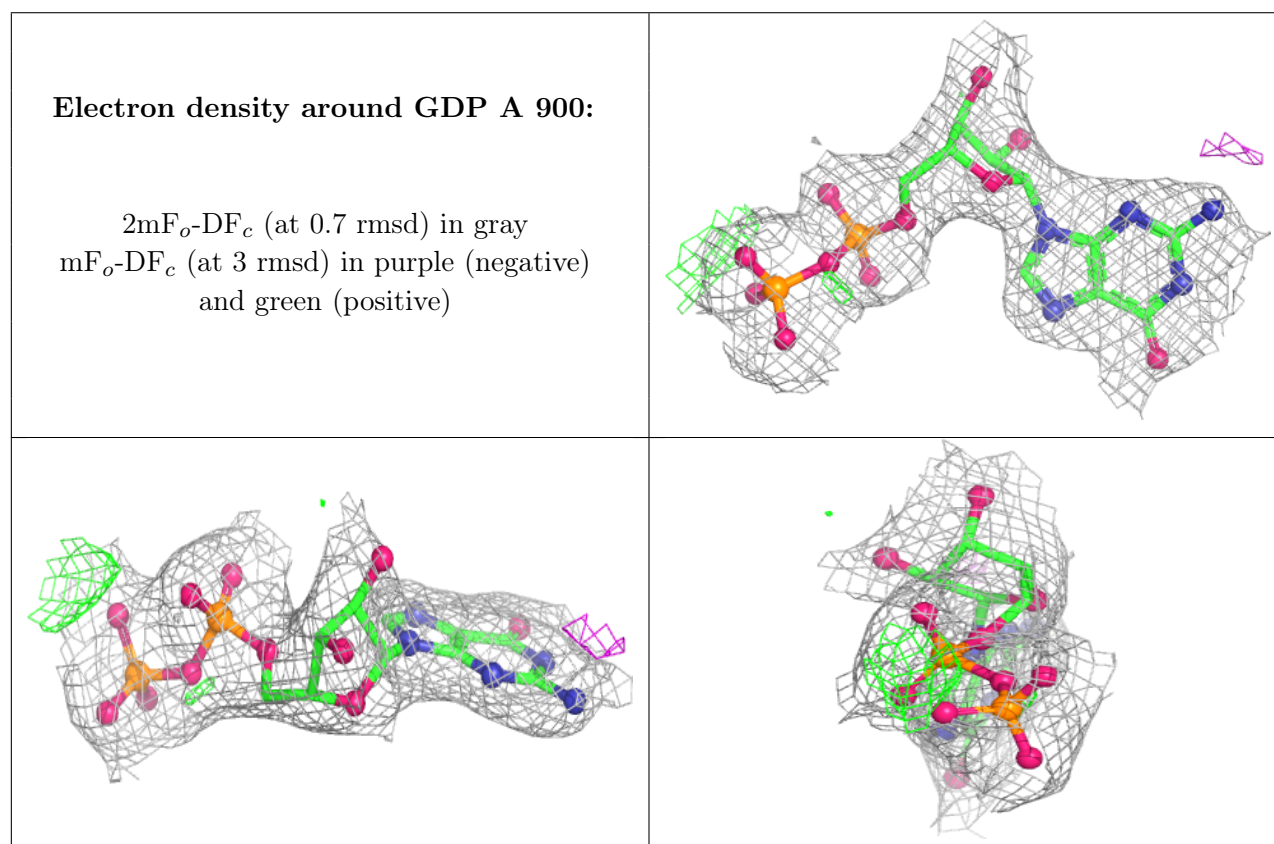
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MG	A	950	1/1	0.83	0.27	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GDP	A	900	28/28	0.97	0.06	32,32,32,32	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.