



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 09:47 AM UTC

PDB ID : 9T38 / pdb_00009t38
Title : Rhs2-CT endonuclease toxin in complex with cognate immunity protein RhsI2 and EF-Tu
Authors : Pankov, G.; Hunter, W.N.; Coulthurst, S.J.
Deposited on : 2025-10-27
Resolution : 2.45 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

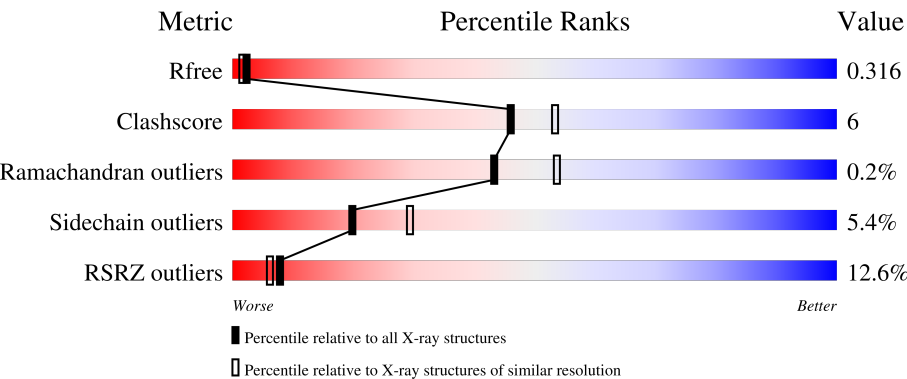
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

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	C	394	<div><div>12%</div><div>83%</div><div>13%</div><div>..</div></div>
1	F	394	<div><div>10%</div><div>83%</div><div>13%</div><div>..</div></div>
2	B	162	<div><div>20%</div><div>77%</div><div>14%</div><div>.. 5%</div></div>
2	E	162	<div><div>14%</div><div>77%</div><div>14%</div><div>.. .</div></div>
3	A	162	<div><div>7%</div><div>62%</div><div>10%</div><div>27%</div></div>

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Mol	Chain	Length	Quality of chain
3	D	162	<div><div></div><div>7%</div><div>66%</div><div>6%</div><div>28%</div></div>

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 10491 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 Tu 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	384	Total	C	N	O	S	0	0	0
			2954	1867	508	566	13			
1	F	384	Total	C	N	O	S	0	1	0
			2958	1869	508	568	13			

- Molecule 2 is a protein called Immunity protein RhsI2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	154	Total	C	N	O	S	0	0	0
			1248	808	204	231	5			
2	E	155	Total	C	N	O	S	0	0	0
			1257	814	206	232	5			

- Molecule 3 is a protein called Rhs-family protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	119	Total	C	N	O	S	0	0	0
			939	586	182	167	4			
3	D	117	Total	C	N	O	S	0	0	0
			913	568	177	164	4			

There are 42 discrepancies between the modelled and reference sequences:

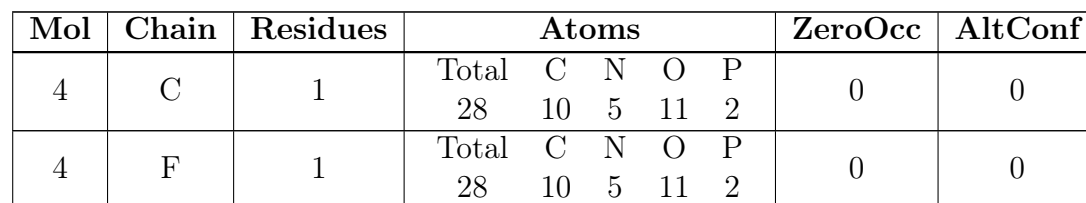
Chain	Residue	Modelled	Actual	Comment	Reference
A	1269	MET	-	initiating methionine	UNP A0ABC9II69
A	1270	GLY	-	expression tag	UNP A0ABC9II69
A	1271	SER	-	expression tag	UNP A0ABC9II69
A	1272	SER	-	expression tag	UNP A0ABC9II69
A	1273	HIS	-	expression tag	UNP A0ABC9II69
A	1274	HIS	-	expression tag	UNP A0ABC9II69
A	1275	HIS	-	expression tag	UNP A0ABC9II69
A	1276	HIS	-	expression tag	UNP A0ABC9II69


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Chain	Residue	Modelled	Actual	Comment	Reference
A	1277	HIS	-	expression tag	UNP A0ABC9II69
A	1278	HIS	-	expression tag	UNP A0ABC9II69
A	1279	SER	-	expression tag	UNP A0ABC9II69
A	1280	SER	-	expression tag	UNP A0ABC9II69
A	1281	GLY	-	expression tag	UNP A0ABC9II69
A	1282	GLU	-	expression tag	UNP A0ABC9II69
A	1283	ASN	-	expression tag	UNP A0ABC9II69
A	1284	LEU	-	expression tag	UNP A0ABC9II69
A	1285	TYR	-	expression tag	UNP A0ABC9II69
A	1286	PHE	-	expression tag	UNP A0ABC9II69
A	1287	GLN	-	expression tag	UNP A0ABC9II69
A	1288	GLY	-	expression tag	UNP A0ABC9II69
A	1289	GLY	-	expression tag	UNP A0ABC9II69
D	1269	MET	-	initiating methionine	UNP A0ABC9II69
D	1270	GLY	-	expression tag	UNP A0ABC9II69
D	1271	SER	-	expression tag	UNP A0ABC9II69
D	1272	SER	-	expression tag	UNP A0ABC9II69
D	1273	HIS	-	expression tag	UNP A0ABC9II69
D	1274	HIS	-	expression tag	UNP A0ABC9II69
D	1275	HIS	-	expression tag	UNP A0ABC9II69
D	1276	HIS	-	expression tag	UNP A0ABC9II69
D	1277	HIS	-	expression tag	UNP A0ABC9II69
D	1278	HIS	-	expression tag	UNP A0ABC9II69
D	1279	SER	-	expression tag	UNP A0ABC9II69
D	1280	SER	-	expression tag	UNP A0ABC9II69
D	1281	GLY	-	expression tag	UNP A0ABC9II69
D	1282	GLU	-	expression tag	UNP A0ABC9II69
D	1283	ASN	-	expression tag	UNP A0ABC9II69
D	1284	LEU	-	expression tag	UNP A0ABC9II69
D	1285	TYR	-	expression tag	UNP A0ABC9II69
D	1286	PHE	-	expression tag	UNP A0ABC9II69
D	1287	GLN	-	expression tag	UNP A0ABC9II69
D	1288	GLY	-	expression tag	UNP A0ABC9II69
D	1289	GLY	-	expression tag	UNP A0ABC9II69

- Molecule 4 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂) (labeled as "Ligand of Interest" by depositor).



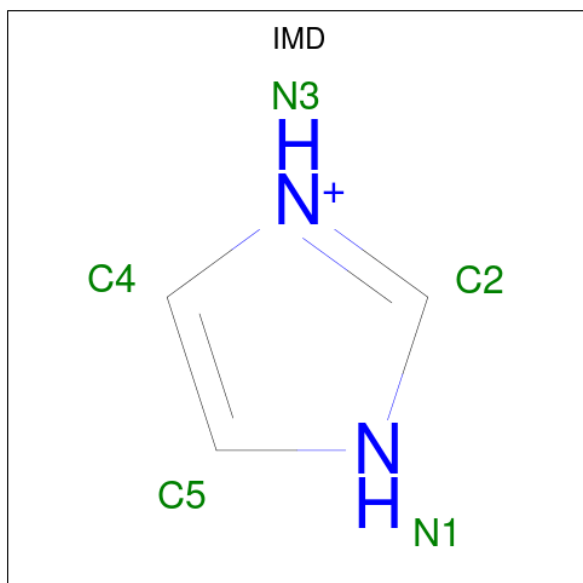
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total 4	C 2	O 2	0	0
5	F	1	Total 4	C 2	O 2	0	0

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	1	Total	Mg	0	0
			1	1		
6	F	1	Total	Mg	0	0
			1	1		

- Molecule 7 is IMIDAZOLE (CCD ID: IMD) (formula: C₃H₅N₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	C	N	0	0
			5	3	2		
7	F	1	Total	C	N	0	0
			5	3	2		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	C	38	Total	O	0	0
			38	38		
8	B	16	Total	O	0	0
			16	16		
8	A	17	Total	O	0	0
			17	17		
8	F	43	Total	O	0	0
			43	43		
8	E	11	Total	O	0	0
			11	11		

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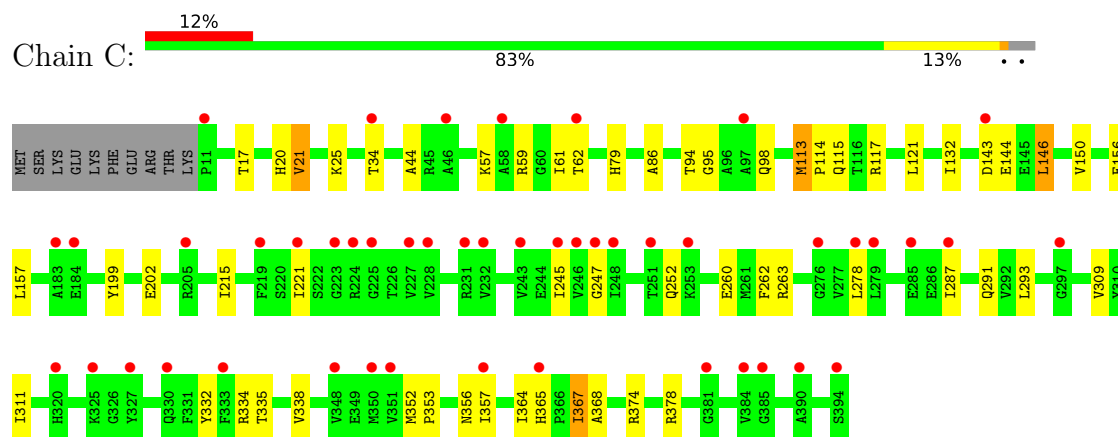
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	D	21	Total	O	0	0
			21	21		

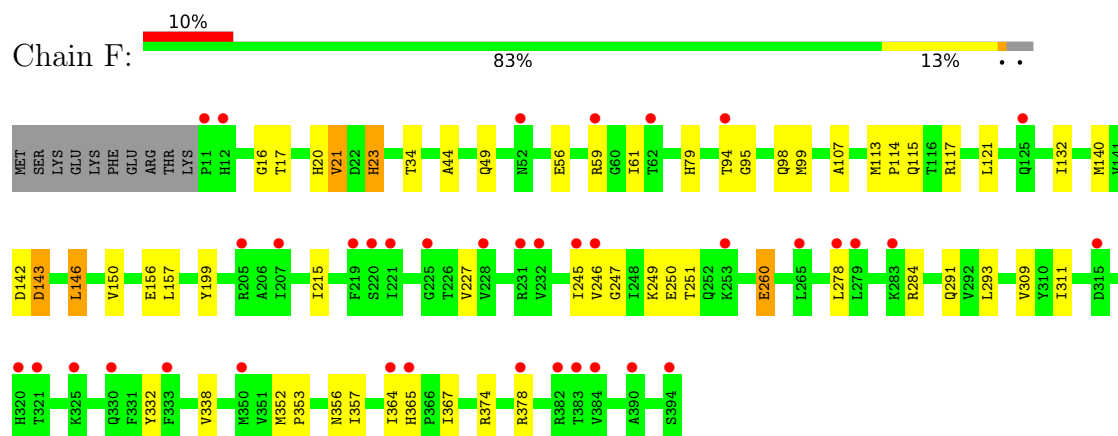
3 Residue-property plots [i](#)

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.

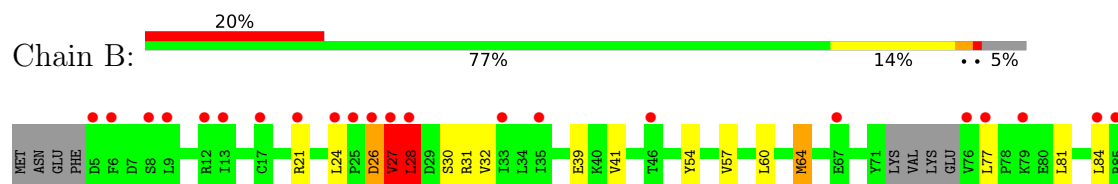
• Molecule 1: Elongation factor Tu 2

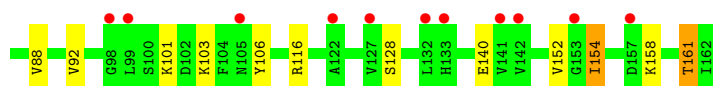


• Molecule 1: Elongation factor Tu 2

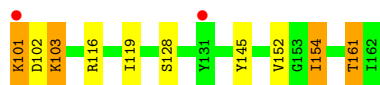
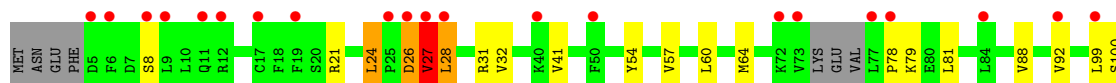
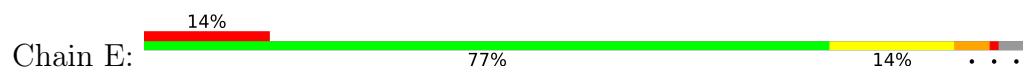


• Molecule 2: Immunity protein RhsI2

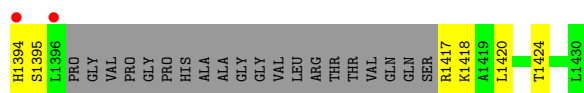
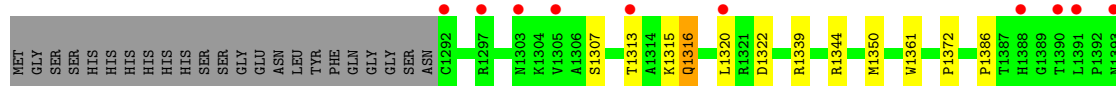




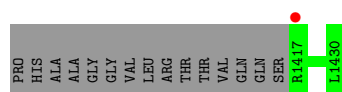
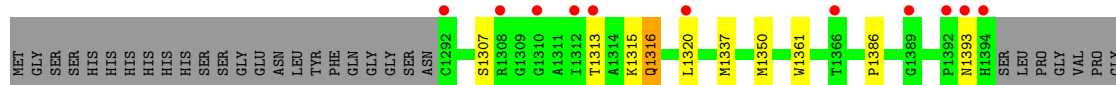
• Molecule 2: Immunity protein RhsI2



• Molecule 3: Rhs-family protein



• Molecule 3: Rhs-family protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	61.60Å 110.57Å 113.86Å 90.00° 102.39° 90.00°	Depositor
Resolution (Å)	60.24 – 2.45 60.24 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.9 (60.24-2.45) 99.9 (60.24-2.45)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.270 , 0.314 0.274 , 0.316	Depositor DCC
R_{free} test set	2724 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	51.5	Xtriage
Anisotropy	0.068	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 33.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	10491	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.32% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: IMD, GDP, EDO, MG

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	C	0.94	0/3009	1.09	0/4074
1	F	0.92	0/3017	1.10	0/4085
2	B	0.89	0/1280	1.13	0/1731
2	E	0.91	1/1289 (0.1%)	1.13	0/1742
3	A	0.91	0/961	1.21	0/1303
3	D	0.92	0/934	1.22	0/1268
All	All	0.92	1/10490 (0.0%)	1.13	0/14203

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	79	LYS	C-N	-7.45	1.23	1.33

There are no bond angle outliers.

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	C	2954	0	2960	36	0
1	F	2958	0	2960	39	0
2	B	1248	0	1218	21	0
2	E	1257	0	1231	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	939	0	939	9	0
3	D	913	0	898	4	0
4	C	28	0	12	1	0
4	F	28	0	12	0	0
5	C	4	0	6	0	0
5	F	4	0	6	0	0
6	C	1	0	0	0	0
6	F	1	0	0	0	0
7	C	5	0	5	0	0
7	F	5	0	5	0	0
8	A	17	0	0	2	0
8	B	16	0	0	0	0
8	C	38	0	0	1	0
8	D	21	0	0	1	0
8	E	11	0	0	0	0
8	F	43	0	0	3	0
All	All	10491	0	10252	120	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 6.

All (120) 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)
2:B:21:ARG:HD3	2:B:26:ASP:OD2	1.68	0.93
1:C:59:ARG:HH11	1:C:94:THR:HG23	1.38	0.85
1:F:59:ARG:HH11	1:F:94:THR:HG23	1.40	0.84
1:C:338:VAL:HG21	1:C:367:ILE:HD11	1.65	0.78
2:B:21:ARG:CD	2:B:26:ASP:OD2	2.33	0.77
1:F:338:VAL:HG21	1:F:367:ILE:HD11	1.65	0.76
2:E:21:ARG:HD2	2:E:24:LEU:HD23	1.66	0.76
1:C:59:ARG:NH1	1:C:94:THR:HG23	2.04	0.72
1:F:61:ILE:HD12	1:F:94:THR:HG21	1.73	0.71
1:F:59:ARG:NH1	1:F:94:THR:HG23	2.06	0.70
1:C:143:ASP:OD1	1:C:146:LEU:HG	1.92	0.69
1:F:247:GLY:HA3	1:F:291:GLN:HG2	1.76	0.67
1:C:61:ILE:HD12	1:C:94:THR:HG21	1.77	0.66
4:C:401:GDP:O2'	3:A:1344:ARG:NH1	2.28	0.66
1:C:150:VAL:HG23	2:B:64:MET:HE1	1.76	0.65
1:F:20:HIS:CE1	1:F:113:MET:HE3	2.31	0.65
1:F:49:GLN:NE2	8:F:502:HOH:O	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:34:THR:HG22	1:C:44:ALA:HB1	1.79	0.63
1:F:150:VAL:HG23	2:E:64:MET:HE1	1.80	0.63
1:C:143:ASP:OD2	1:C:146:LEU:HD23	1.99	0.63
2:B:81:LEU:HA	2:B:84:LEU:HD12	1.80	0.62
2:E:32:VAL:HG13	2:E:161:THR:HG23	1.82	0.62
1:C:150:VAL:HG23	2:B:64:MET:CE	2.32	0.59
2:E:54:TYR:O	2:E:57:VAL:HG12	2.02	0.59
1:F:23:HIS:HD2	8:F:509:HOH:O	1.86	0.58
1:F:34:THR:HG22	1:F:44:ALA:HB1	1.85	0.58
2:B:54:TYR:O	2:B:57:VAL:HG12	2.03	0.57
1:F:117:ARG:HG2	1:F:157:LEU:HD11	1.87	0.56
2:B:27:VAL:O	2:B:28:LEU:HB2	2.05	0.56
2:B:32:VAL:HG13	2:B:161:THR:HG23	1.87	0.56
1:C:17:THR:HG23	1:C:79:HIS:CE1	2.41	0.56
1:C:20:HIS:HE1	8:A:1511:HOH:O	1.87	0.55
1:C:221:ILE:HD12	1:C:278:LEU:HD21	1.88	0.55
1:F:311:ILE:HD12	1:F:311:ILE:N	2.22	0.55
2:B:77:LEU:HD12	2:B:77:LEU:H	1.72	0.54
1:F:260:GLU:O	1:F:260:GLU:HG3	2.08	0.54
1:C:311:ILE:HD12	1:C:311:ILE:N	2.22	0.54
2:E:27:VAL:O	2:E:28:LEU:HB2	2.06	0.54
1:C:247:GLY:HA3	1:C:291:GLN:HG2	1.89	0.54
1:F:23:HIS:CD2	8:F:509:HOH:O	2.59	0.53
1:C:113:MET:HB3	1:C:114:PRO:CD	2.38	0.53
2:E:81:LEU:HD21	2:E:128:SER:HA	1.90	0.52
1:F:17:THR:HG23	1:F:79:HIS:CE1	2.44	0.52
2:B:41:VAL:HG11	2:B:152:VAL:HG21	1.93	0.51
2:E:41:VAL:HG11	2:E:152:VAL:HG21	1.93	0.51
2:B:31:ARG:HA	2:B:158:LYS:HD3	1.91	0.51
3:A:1350:MET:HE3	3:A:1361:TRP:CD1	2.45	0.51
1:C:334:ARG:NH2	1:C:368:ALA:O	2.43	0.51
1:F:113:MET:HB3	1:F:114:PRO:CD	2.41	0.51
1:F:146:LEU:O	2:E:64:MET:HE1	2.11	0.51
1:C:21:VAL:HG13	8:A:1506:HOH:O	2.11	0.50
2:E:60:LEU:HD21	2:E:154:ILE:HD13	1.93	0.50
2:B:60:LEU:HD21	2:B:154:ILE:HD13	1.92	0.50
3:D:1307:SER:HB2	3:D:1386:PRO:HB2	1.94	0.50
1:C:215:ILE:HD11	1:C:293:LEU:HD12	1.94	0.50
2:E:78:PRO:O	2:E:81:LEU:N	2.45	0.50
1:C:20:HIS:HA	1:C:115:GLN:HB2	1.94	0.49
1:C:262:PHE:O	8:C:501:HOH:O	2.20	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:215:ILE:HD11	1:F:293:LEU:HD12	1.94	0.49
1:F:20:HIS:HA	1:F:115:GLN:HB2	1.93	0.49
1:F:246:VAL:HG13	1:F:251:THR:HG22	1.95	0.49
1:F:246:VAL:HA	1:F:251:THR:HG22	1.96	0.48
1:C:113:MET:HB3	1:C:114:PRO:HD2	1.94	0.48
1:F:352:MET:HE3	1:F:353:PRO:HD2	1.95	0.48
1:C:57:LYS:HE3	1:C:62:THR:HG22	1.95	0.48
1:F:332:TYR:CD2	1:F:378:ARG:NH1	2.81	0.48
1:C:352:MET:HE3	1:C:353:PRO:HD2	1.95	0.47
1:C:332:TYR:CD2	1:C:378:ARG:NH1	2.82	0.47
2:E:99:LEU:O	2:E:101:LYS:HE3	2.14	0.47
1:C:245:ILE:HB	1:C:252:GLN:HB2	1.97	0.47
1:F:246:VAL:HG13	1:F:251:THR:CG2	2.45	0.47
2:B:39:GLU:HG3	2:B:106:TYR:CE2	2.50	0.47
1:F:113:MET:HB3	1:F:114:PRO:HD2	1.97	0.47
1:F:95:GLY:O	1:F:374:ARG:NH1	2.44	0.47
3:D:1350:MET:HE3	3:D:1361:TRP:CD1	2.50	0.46
1:F:132:ILE:HD11	1:F:199:TYR:HB3	1.98	0.46
1:C:95:GLY:O	1:C:374:ARG:NH1	2.44	0.45
2:E:88:VAL:O	2:E:92:VAL:HG23	2.16	0.45
1:F:309:VAL:O	1:F:356:ASN:HA	2.16	0.45
1:C:117:ARG:HG2	1:C:157:LEU:HD11	1.99	0.45
1:C:98:GLN:HG2	1:C:374:ARG:HH21	1.81	0.45
2:B:26:ASP:N	2:B:26:ASP:OD1	2.49	0.45
2:B:88:VAL:O	2:B:92:VAL:HG23	2.16	0.44
2:E:26:ASP:OD1	2:E:26:ASP:N	2.49	0.44
3:A:1313:THR:HG23	3:A:1316:GLN:H	1.82	0.44
1:F:245:ILE:HD12	1:F:245:ILE:N	2.33	0.44
2:E:32:VAL:HG13	2:E:161:THR:CG2	2.46	0.44
1:C:309:VAL:O	1:C:356:ASN:HA	2.17	0.44
1:F:227:VAL:HG23	1:F:278:LEU:HD23	1.99	0.44
2:E:21:ARG:HH11	2:E:24:LEU:HB3	1.83	0.44
3:D:1313:THR:HG23	3:D:1316:GLN:H	1.82	0.43
2:B:28:LEU:HD12	2:B:32:VAL:HG21	2.01	0.43
1:C:245:ILE:HD13	1:C:287:ILE:CD1	2.49	0.43
2:B:28:LEU:HA	2:B:28:LEU:HD13	1.75	0.43
1:F:21:VAL:HG13	8:D:1509:HOH:O	2.19	0.43
1:C:20:HIS:HD2	1:C:115:GLN:H	1.67	0.43
3:A:1420:LEU:HD13	3:A:1424:THR:HG21	2.01	0.43
3:A:1372:PRO:HG2	3:A:1394:HIS:O	2.18	0.42
2:E:100:SER:OG	2:E:103:LYS:HG2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:98:GLN:HG2	1:F:374:ARG:HH21	1.84	0.42
1:F:23:HIS:CD2	1:F:107:ALA:H	2.38	0.41
2:B:81:LEU:HD21	2:B:128:SER:HA	2.01	0.41
1:C:132:ILE:HD11	1:C:199:TYR:HB3	2.03	0.41
1:C:262:PHE:O	1:C:263:ARG:HG2	2.20	0.41
3:A:1350:MET:HE3	3:A:1361:TRP:NE1	2.36	0.41
3:A:1307:SER:HB2	3:A:1386:PRO:HB2	2.03	0.41
1:F:143[A]:ASP:CG	1:F:146:LEU:HG	2.46	0.41
1:C:263:ARG:HA	1:F:284:ARG:NH2	2.36	0.41
2:B:21:ARG:HD2	2:B:26:ASP:OD2	2.17	0.41
2:E:21:ARG:HA	2:E:24:LEU:HD22	2.03	0.41
1:C:146:LEU:HD13	2:B:64:MET:HG3	2.03	0.41
3:A:1394:HIS:CD2	3:A:1395:SER:H	2.39	0.41
1:F:20:HIS:HD2	1:F:115:GLN:H	1.67	0.41
1:C:86:ALA:HB2	3:A:1322:ASP:HB3	2.03	0.41
2:E:28:LEU:HD13	2:E:28:LEU:HA	1.75	0.40
1:F:140:MET:HE2	3:D:1337:MET:SD	2.61	0.40
2:E:119:ILE:HD12	2:E:145:TYR:CD1	2.57	0.40
2:B:32:VAL:HG13	2:B:161:THR:CG2	2.50	0.40
1:F:16:GLY:HA3	1:F:99:MET:HE2	2.04	0.40
1:F:249:LYS:O	1:F:250:GLU:C	2.65	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	C	382/394 (97%)	366 (96%)	16 (4%)	0	100	100
1	F	383/394 (97%)	369 (96%)	14 (4%)	0	100	100
2	B	150/162 (93%)	140 (93%)	8 (5%)	2 (1%)	9	9
2	E	151/162 (93%)	142 (94%)	8 (5%)	1 (1%)	18	24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	115/162 (71%)	110 (96%)	5 (4%)	0	100	100
3	D	113/162 (70%)	111 (98%)	2 (2%)	0	100	100
All	All	1294/1436 (90%)	1238 (96%)	53 (4%)	3 (0%)	43	54

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	27	VAL
2	E	27	VAL
2	B	28	LEU

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	C	316/327 (97%)	302 (96%)	14 (4%)	25	37
1	F	317/327 (97%)	304 (96%)	13 (4%)	27	40
2	B	137/145 (94%)	125 (91%)	12 (9%)	9	10
2	E	138/145 (95%)	126 (91%)	12 (9%)	9	11
3	A	100/133 (75%)	94 (94%)	6 (6%)	17	26
3	D	95/133 (71%)	91 (96%)	4 (4%)	26	39
All	All	1103/1210 (91%)	1042 (94%)	61 (6%)	20	28

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	21	VAL
1	C	25	LYS
1	C	113	MET
1	C	121	LEU
1	C	144	GLU
1	C	146	LEU
1	C	156	GLU

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Mol	Chain	Res	Type
1	C	202	GLU
1	C	260	GLU
1	C	335	THR
1	C	357	ILE
1	C	364	ILE
1	C	365	HIS
1	C	367	ILE
2	B	24	LEU
2	B	26	ASP
2	B	27	VAL
2	B	28	LEU
2	B	30	SER
2	B	64	MET
2	B	101	LYS
2	B	103	LYS
2	B	116	ARG
2	B	140	GLU
2	B	154	ILE
2	B	161	THR
3	A	1315	LYS
3	A	1316	GLN
3	A	1320	LEU
3	A	1339	ARG
3	A	1417	ARG
3	A	1418	LYS
1	F	21	VAL
1	F	23	HIS
1	F	56	GLU
1	F	121	LEU
1	F	142	ASP
1	F	143[A]	ASP
1	F	143[B]	ASP
1	F	146	LEU
1	F	156	GLU
1	F	260	GLU
1	F	357	ILE
1	F	364	ILE
1	F	365	HIS
2	E	8	SER
2	E	24	LEU
2	E	26	ASP
2	E	27	VAL

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Mol	Chain	Res	Type
2	E	28	LEU
2	E	31	ARG
2	E	101	LYS
2	E	102	ASP
2	E	103	LYS
2	E	116	ARG
2	E	154	ILE
2	E	161	THR
3	D	1315	LYS
3	D	1316	GLN
3	D	1320	LEU
3	D	1393	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	20	HIS
1	C	49	GLN
1	C	64	ASN
1	C	274	ASN
2	B	89	ASN
2	B	105	ASN
3	A	1346	GLN
3	A	1394	HIS
1	F	20	HIS
1	F	23	HIS
1	F	49	GLN
1	F	274	ASN
2	E	89	ASN
2	E	105	ASN
3	D	1346	GLN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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	$\# Z > 2$
7	IMD	F	404	-	5,5,5	0.20	0	5,5,5	0.53	0
4	GDP	C	401	6	29,30,30	1.14	5 (17%)	45,47,47	1.26	4 (8%)
5	EDO	C	402	-	3,3,3	0.13	0	2,2,2	0.25	0
4	GDP	F	401	6	29,30,30	1.25	4 (13%)	45,47,47	1.76	5 (11%)
5	EDO	F	402	-	3,3,3	0.11	0	2,2,2	0.20	0
7	IMD	C	404	-	5,5,5	0.24	0	5,5,5	0.57	0

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
7	IMD	F	404	-	-	-	0/1/1/1
4	GDP	C	401	6	-	1/16/32/32	0/3/3/3
5	EDO	C	402	-	-	1/1/1/1	-
4	GDP	F	401	6	-	1/16/32/32	0/3/3/3
5	EDO	F	402	-	-	0/1/1/1	-
7	IMD	C	404	-	-	-	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	401	GDP	C6-N1	-2.97	1.33	1.38
4	C	401	GDP	C5-C4	2.81	1.46	1.38
4	F	401	GDP	C5-C4	2.78	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	401	GDP	C4-N9	-2.60	1.31	1.38
4	C	401	GDP	C2'-C3'	-2.36	1.47	1.53
4	F	401	GDP	C5-N7	-2.34	1.34	1.39
4	F	401	GDP	C4-N9	-2.19	1.32	1.38
4	C	401	GDP	C5-N7	-2.18	1.34	1.39
4	C	401	GDP	C6-N1	-2.13	1.34	1.38

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	401	GDP	C5-C4-N3	-5.90	119.00	128.39
4	F	401	GDP	C2-N3-C4	4.84	120.64	112.30
4	C	401	GDP	O3'-C3'-C2'	-4.44	97.59	111.82
4	F	401	GDP	N9-C4-N3	4.18	134.32	125.95
4	F	401	GDP	C6-C5-N7	3.60	136.83	130.29
4	F	401	GDP	C4-C5-N7	-2.85	106.15	110.67
4	C	401	GDP	N9-C4-N3	2.68	131.31	125.95
4	C	401	GDP	C6-C5-N7	2.60	135.03	130.29
4	C	401	GDP	C8-N9-C4	2.52	110.75	106.03

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	F	401	GDP	PA-O3A-PB-O1B
5	C	402	EDO	O1-C1-C2-O2
4	C	401	GDP	PA-O3A-PB-O1B

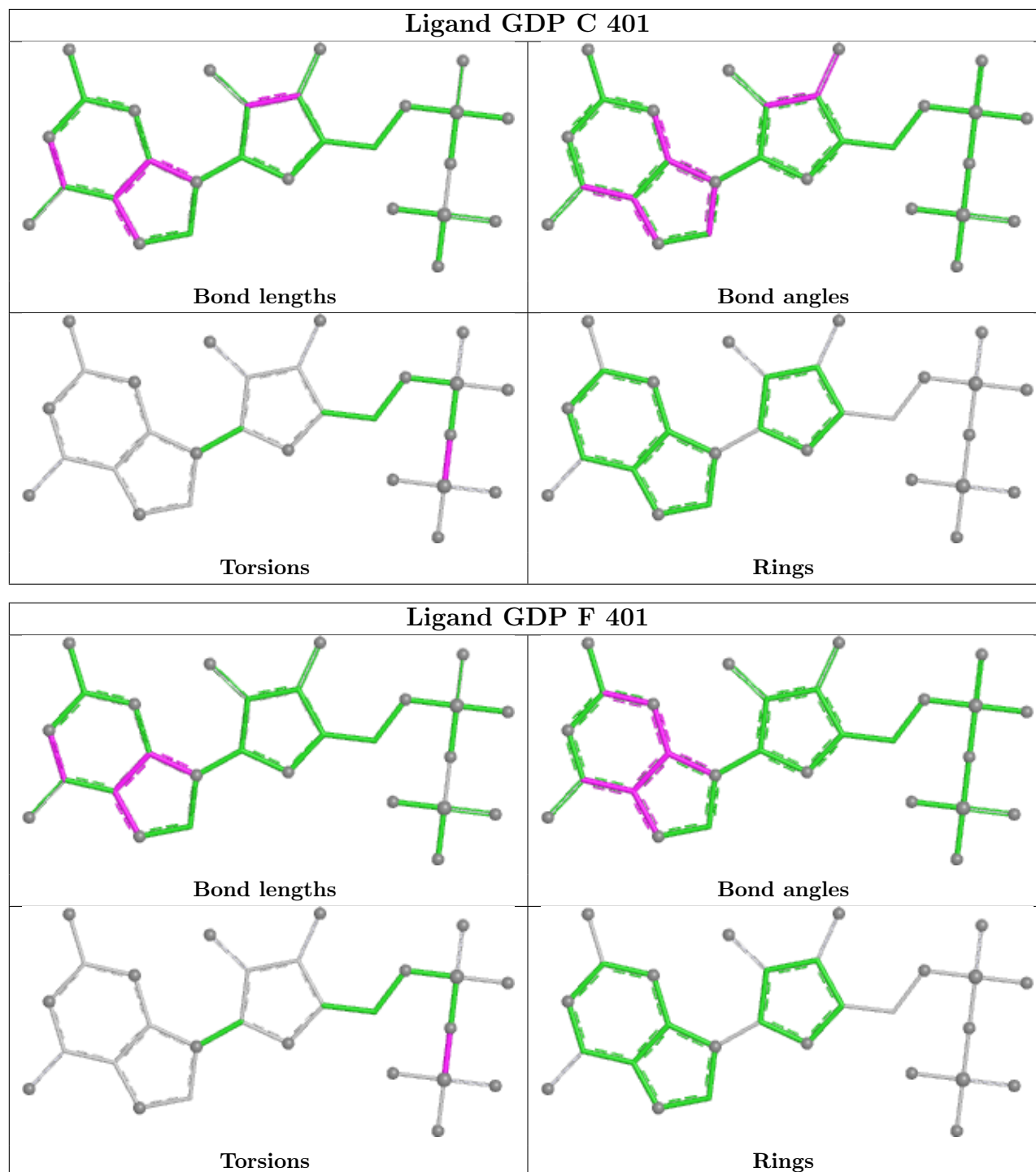
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	401	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

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	C	384/394 (97%)	1.06	47 (12%) 8 7	34, 63, 94, 112	0
1	F	384/394 (97%)	1.00	38 (9%) 13 10	33, 61, 90, 107	1 (0%)
2	B	154/162 (95%)	1.36	33 (21%) 2 2	39, 63, 90, 102	0
2	E	155/162 (95%)	1.20	23 (14%) 5 4	33, 61, 89, 99	0
3	A	119/162 (73%)	0.88	12 (10%) 12 10	34, 51, 84, 106	0
3	D	117/162 (72%)	1.01	12 (10%) 12 9	33, 51, 79, 103	0
All	All	1313/1436 (91%)	1.08	165 (12%) 8 6	33, 59, 91, 112	1 (0%)

All (165) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	77	LEU	5.4
2	E	73	VAL	4.4
2	B	27	VAL	4.4
2	B	67	GLU	4.3
1	F	62	THR	3.8
1	C	221	ILE	3.8
1	C	11	PRO	3.7
3	A	1394	HIS	3.6
1	F	11	PRO	3.6
2	B	77	LEU	3.5
1	F	390	ALA	3.5
3	A	1396	LEU	3.4
3	D	1394	HIS	3.4
1	F	246	VAL	3.3
3	D	1292	CYS	3.3
2	B	25	PRO	3.2
2	B	28	LEU	3.2
2	E	27	VAL	3.2
2	E	78	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	62	THR	3.2
1	C	247	GLY	3.2
2	B	76	VAL	3.2
1	C	297	GLY	3.1
1	C	251	THR	3.1
1	C	46	ALA	3.0
3	D	1308	ARG	3.0
2	B	26	ASP	3.0
1	F	12	HIS	3.0
1	F	394	SER	2.9
3	D	1392	PRO	2.9
1	F	265	LEU	2.9
2	B	132	LEU	2.9
2	B	133	HIS	2.8
3	D	1320	LEU	2.8
1	F	330	GLN	2.8
1	C	224	ARG	2.8
1	C	385	GLY	2.8
2	B	142	VAL	2.8
2	E	92	VAL	2.8
1	C	97	ALA	2.8
2	E	26	ASP	2.8
2	B	8	SER	2.7
1	C	279	LEU	2.7
1	F	279	LEU	2.7
1	C	325	LYS	2.7
2	E	72	LYS	2.7
3	A	1390	THR	2.7
1	F	382	ARG	2.7
1	F	220	SER	2.7
1	C	333	PHE	2.7
2	E	11	GLN	2.7
3	D	1310	GLY	2.6
2	E	28	LEU	2.6
2	B	141	VAL	2.6
3	A	1305	VAL	2.6
3	A	1313	THR	2.6
1	C	205	ARG	2.5
1	F	245	ILE	2.5
2	B	9	LEU	2.5
3	A	1391	LEU	2.5
1	C	232	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	12	ARG	2.5
1	C	184	GLU	2.5
2	B	157	ASP	2.5
2	B	13	ILE	2.5
1	C	278	LEU	2.5
2	B	24	LEU	2.5
2	B	6	PHE	2.5
1	C	58	ALA	2.5
3	A	1320	LEU	2.4
1	F	365	HIS	2.4
2	E	50	PHE	2.4
3	A	1303	ASN	2.4
2	E	131	TYR	2.4
1	C	246	VAL	2.4
1	C	384	VAL	2.4
1	C	381	GLY	2.4
1	C	219	PHE	2.4
1	C	350	MET	2.4
2	E	25	PRO	2.3
1	C	225	GLY	2.3
3	D	1389	GLY	2.3
1	F	278	LEU	2.3
2	B	33	ILE	2.3
3	A	1388	HIS	2.3
1	C	253	LYS	2.3
1	C	34	THR	2.3
2	E	12	ARG	2.3
2	B	79	LYS	2.3
2	B	105	ASN	2.3
1	F	378	ARG	2.3
2	B	85	ARG	2.3
2	B	98	GLY	2.3
1	C	357	ILE	2.3
2	E	99	LEU	2.3
2	E	8	SER	2.3
1	C	248	ILE	2.3
1	C	287	ILE	2.3
2	E	6	PHE	2.3
1	C	243	VAL	2.3
1	C	351	VAL	2.3
3	A	1292	CYS	2.3
3	A	1393	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
3	D	1417	ARG	2.3
1	C	223	GLY	2.2
1	C	276	GLY	2.2
1	C	320	HIS	2.2
1	F	221	ILE	2.2
1	F	350	MET	2.2
1	F	364	ILE	2.2
1	C	327	TYR	2.2
2	B	46	THR	2.2
1	F	59	ARG	2.2
1	F	384	VAL	2.2
1	C	183	ALA	2.2
1	C	365	HIS	2.2
1	F	253	LYS	2.2
2	E	101	LYS	2.2
2	B	17	CYS	2.2
3	D	1366	THR	2.2
3	D	1312	ILE	2.2
1	F	333	PHE	2.2
1	C	390	ALA	2.2
1	F	320	HIS	2.2
2	E	19	PHE	2.2
1	F	232	VAL	2.1
1	F	225	GLY	2.1
2	B	153	GLY	2.1
1	C	245	ILE	2.1
1	F	207	ILE	2.1
1	C	285	GLU	2.1
2	B	5	ASP	2.1
2	E	40	LYS	2.1
1	C	348	VAL	2.1
2	B	127	VAL	2.1
2	B	122	ALA	2.1
1	F	52	ASN	2.1
3	D	1393	ASN	2.1
2	E	17	CYS	2.1
1	F	283	LYS	2.1
1	F	315	ASP	2.1
1	C	231	ARG	2.1
1	F	231	ARG	2.1
2	B	21	ARG	2.1
1	F	94	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	325	LYS	2.1
1	C	330	GLN	2.0
1	C	227	VAL	2.0
1	F	228	VAL	2.0
2	B	99	LEU	2.0
2	E	9	LEU	2.0
3	D	1313	THR	2.0
1	C	143	ASP	2.0
1	F	125	GLN	2.0
1	C	228	VAL	2.0
1	F	205	ARG	2.0
1	F	219	PHE	2.0
3	A	1297	ARG	2.0
2	B	84	LEU	2.0
2	E	84	LEU	2.0
1	F	321	THR	2.0
1	F	383	THR	2.0
2	B	35	ILE	2.0
2	E	5	ASP	2.0
1	C	394	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 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.

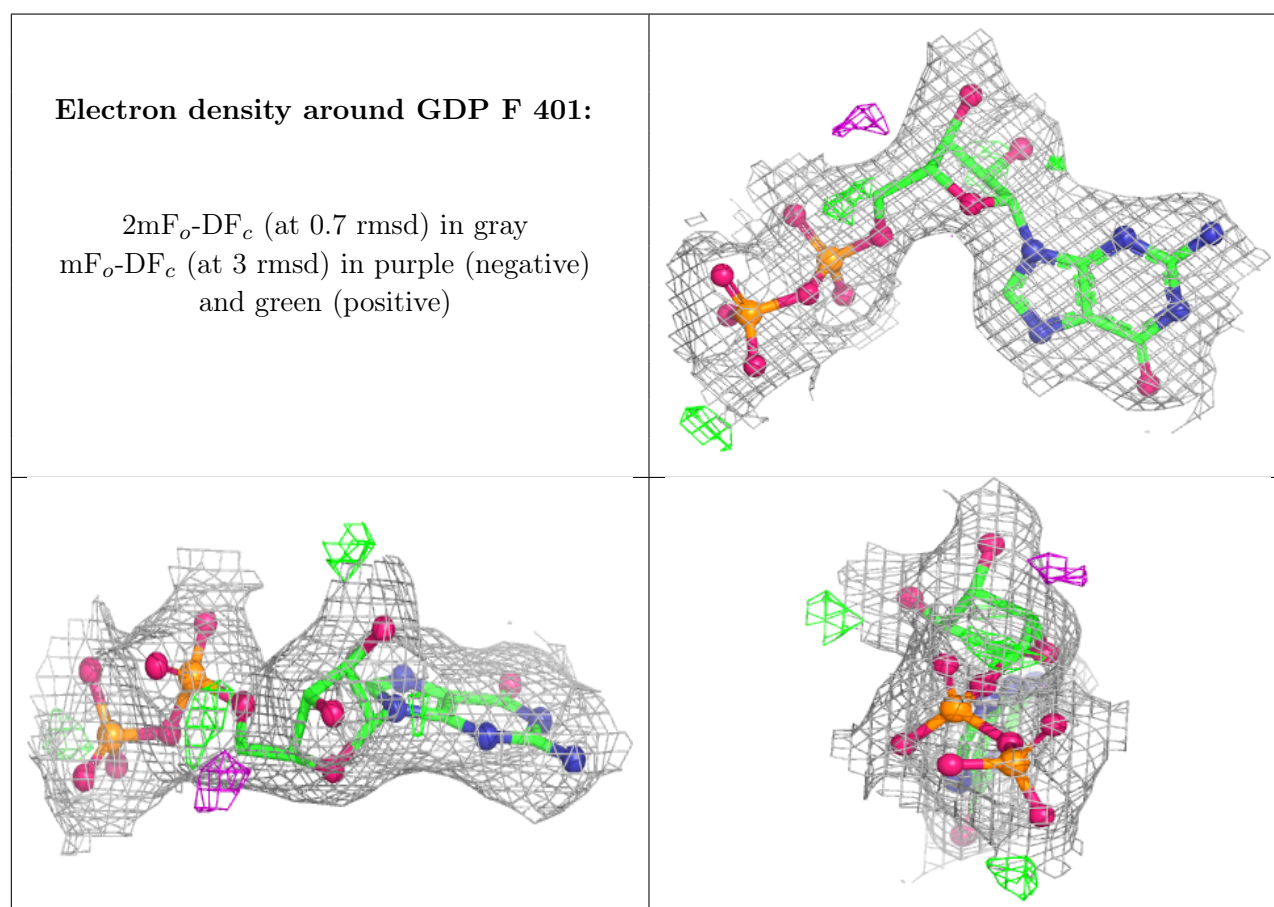
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	IMD	C	404	5/5	0.80	0.14	53,55,59,63	0
7	IMD	F	404	5/5	0.81	0.16	55,56,58,58	0
5	EDO	C	402	4/4	0.84	0.15	54,60,61,61	0

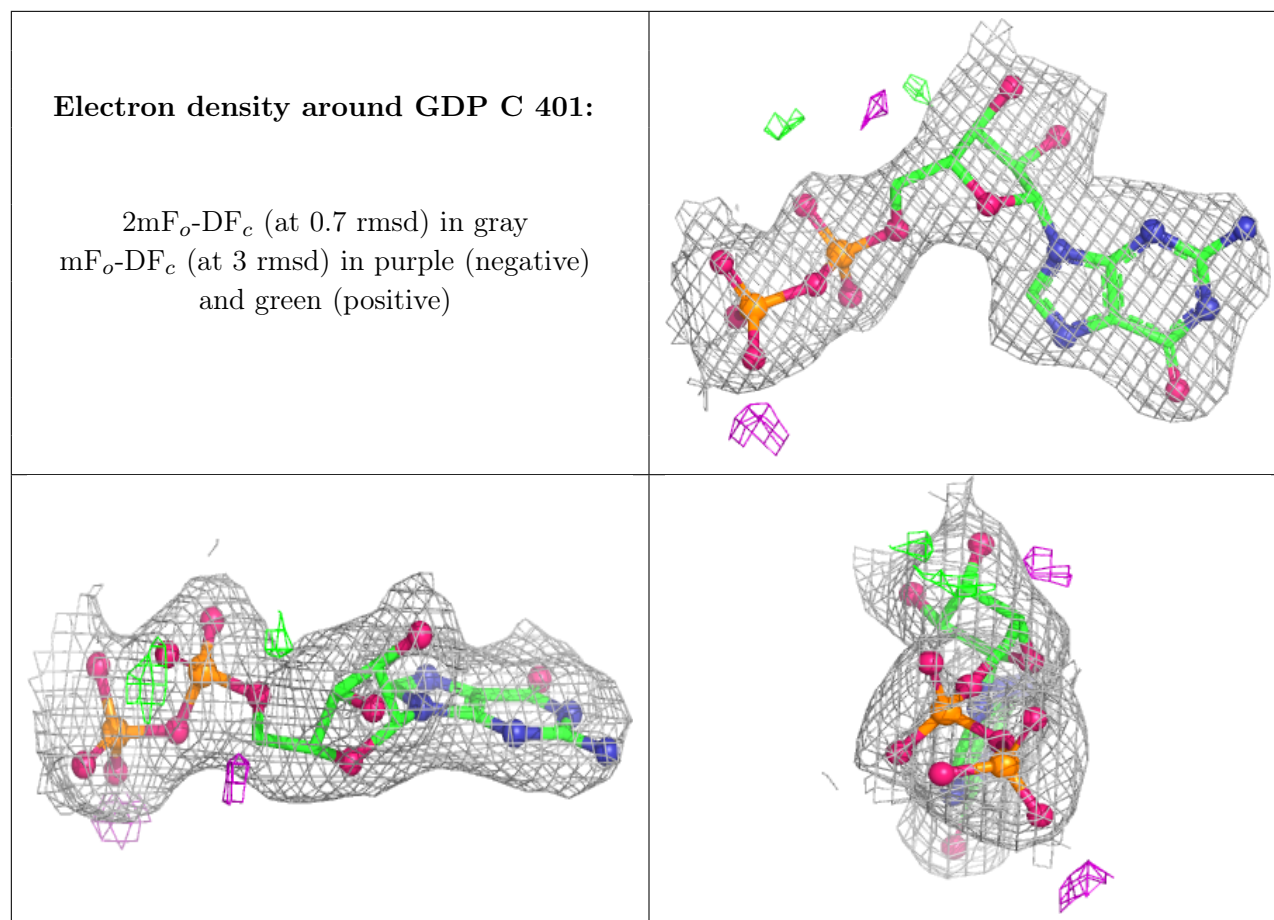
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	EDO	F	402	4/4	0.89	0.12	51,52,53,54	0
4	GDP	F	401	28/28	0.93	0.09	31,37,44,46	0
4	GDP	C	401	28/28	0.95	0.08	31,40,43,46	0
6	MG	C	403	1/1	0.97	0.04	36,36,36,36	0
6	MG	F	403	1/1	0.99	0.04	26,26,26,26	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 ⓘ

There are no such residues in this entry.