



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 17, 2024 – 04:45 PM EST

PDB ID : 4IRU
Title : Crystal Structure of lepB GAP core in a transition state mimetic complex with Rab1A and ALF3
Authors : Mishra, A.K.; Delcampo, C.M.; Collins, R.E.; Roy, C.R.; Lambright, D.G.
Deposited on : 2013-01-15
Resolution : 3.20 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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

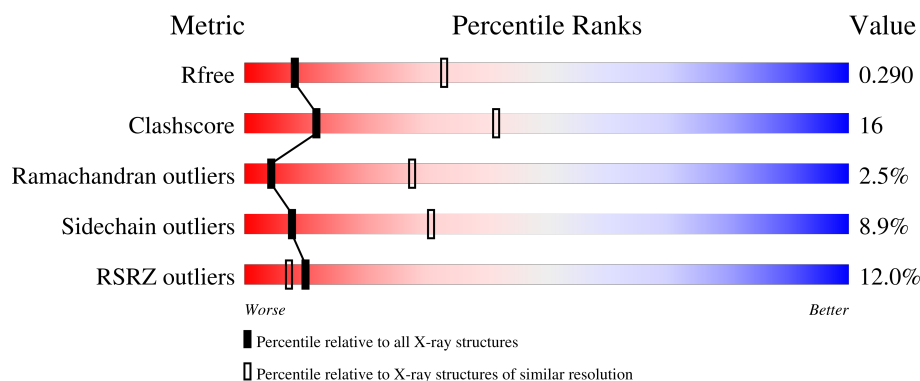
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION




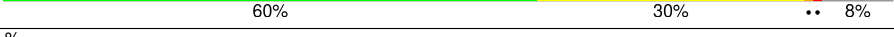
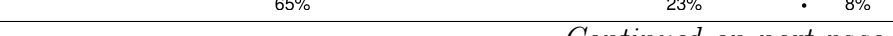
The reported resolution of this entry is 3.20 Å.

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}	164625	1370 (3.20-3.20)
Clashscore	180529	1497 (3.20-3.20)
Ramachandran outliers	177936	1479 (3.20-3.20)
Sidechain outliers	177891	1478 (3.20-3.20)
RSRZ outliers	164620	1371 (3.20-3.20)

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	299	 67% 29% . .
1	C	299	 75% 22% . .
1	E	299	 31% 53% 39% 6% . .
2	B	184	 60% 30% . . 8%
2	D	184	 65% 23% . 8%

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Mol	Chain	Length	Quality of chain
2	F	184	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ACT	C	705	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 11410 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 LepB.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	296	Total	C	N	O	S	Se	0	0	0
			2365	1526	389	443	4	3			
1	C	296	Total	C	N	O	S	Se	0	0	0
			2365	1526	389	443	4	3			
1	E	295	Total	C	N	O	S	Se	0	0	0
			2359	1523	388	441	4	3			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	325	SER	-	expression tag	UNP Q5ZSM7
C	325	SER	-	expression tag	UNP Q5ZSM7
E	325	SER	-	expression tag	UNP Q5ZSM7

- Molecule 2 is a protein called Ras-related protein Rab-1A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	170	Total	C	N	O	S	Se	0	0	0
			1362	868	222	267	2	3			
2	D	170	Total	C	N	O	S	Se	0	0	0
			1362	868	222	267	2	3			
2	F	170	Total	C	N	O	S	Se	0	0	0
			1362	868	222	267	2	3			

There are 30 discrepancies between the modelled and reference sequences:

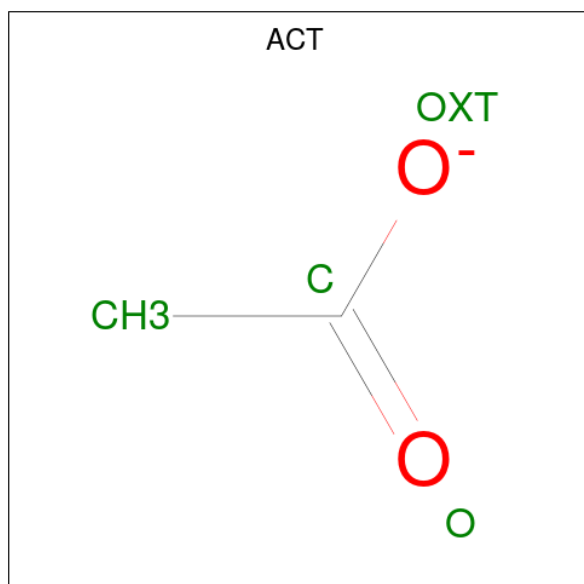
Chain	Residue	Modelled	Actual	Comment	Reference
B	-6	MSE	-	expression tag	UNP P62820
B	-5	GLY	-	expression tag	UNP P62820
B	-4	HIS	-	expression tag	UNP P62820
B	-3	HIS	-	expression tag	UNP P62820
B	-2	HIS	-	expression tag	UNP P62820

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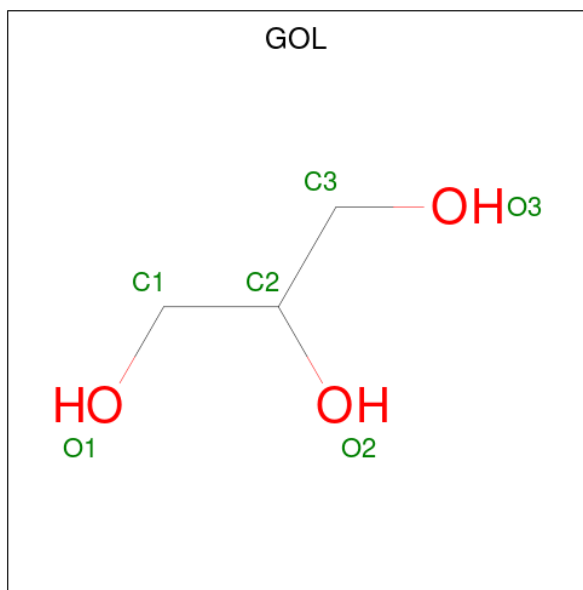
Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	HIS	-	expression tag	UNP P62820
B	0	HIS	-	expression tag	UNP P62820
B	1	HIS	-	expression tag	UNP P62820
B	2	GLY	-	expression tag	UNP P62820
B	3	SER	-	expression tag	UNP P62820
D	-6	MSE	-	expression tag	UNP P62820
D	-5	GLY	-	expression tag	UNP P62820
D	-4	HIS	-	expression tag	UNP P62820
D	-3	HIS	-	expression tag	UNP P62820
D	-2	HIS	-	expression tag	UNP P62820
D	-1	HIS	-	expression tag	UNP P62820
D	0	HIS	-	expression tag	UNP P62820
D	1	HIS	-	expression tag	UNP P62820
D	2	GLY	-	expression tag	UNP P62820
D	3	SER	-	expression tag	UNP P62820
F	-6	MSE	-	expression tag	UNP P62820
F	-5	GLY	-	expression tag	UNP P62820
F	-4	HIS	-	expression tag	UNP P62820
F	-3	HIS	-	expression tag	UNP P62820
F	-2	HIS	-	expression tag	UNP P62820
F	-1	HIS	-	expression tag	UNP P62820
F	0	HIS	-	expression tag	UNP P62820
F	1	HIS	-	expression tag	UNP P62820
F	2	GLY	-	expression tag	UNP P62820
F	3	SER	-	expression tag	UNP P62820

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	C	1	Total C O 6 3 3	0	0

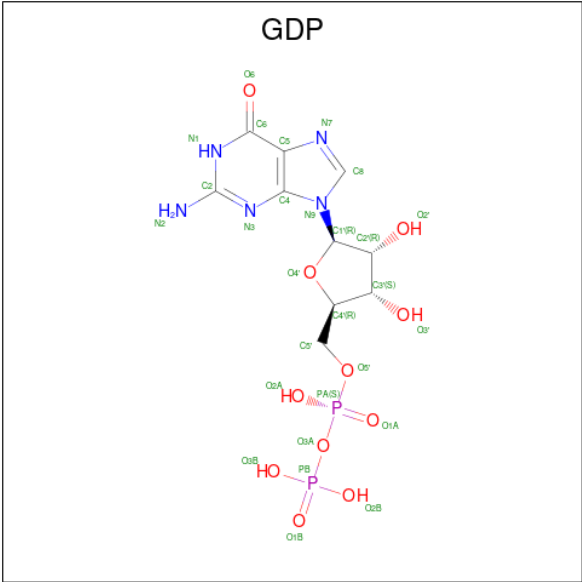
- Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	4	Total K 4 4	0	0
5	B	1	Total K 1 1	0	0
5	C	1	Total K 1 1	0	0

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

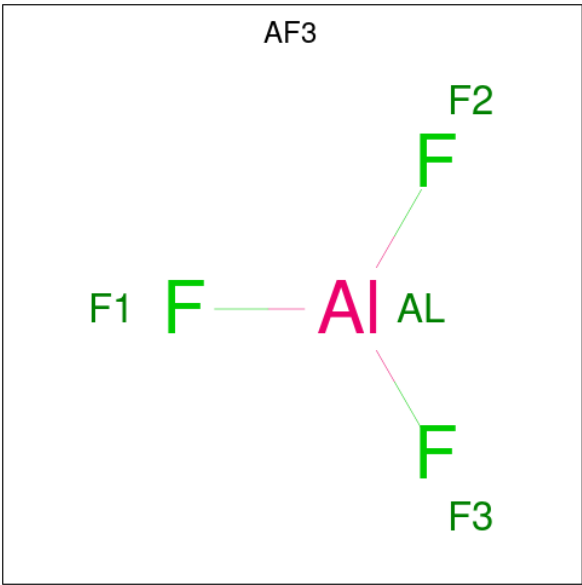
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total Mg 1 1	0	0
6	D	1	Total Mg 1 1	0	0
6	F	1	Total Mg 1 1	0	0

- Molecule 7 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
7	D	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
7	F	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 8 is ALUMINUM FLUORIDE (three-letter code: AF3) (formula: AlF₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	Al	F	0	0
			4	1	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	D	1	Total 4	Al 1	F 3	0	0
8	F	1	Total 4	Al 1	F 3	0	0

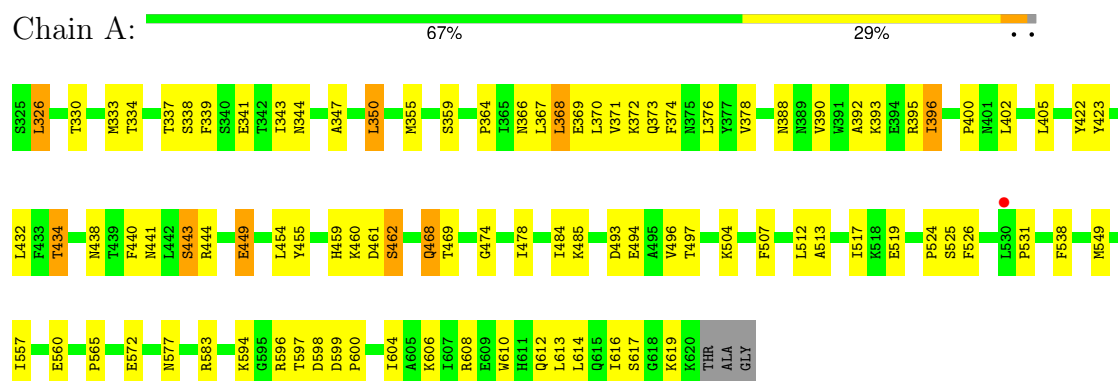
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	8	Total 8	O 8	0	0
9	B	8	Total 8	O 8	0	0
9	C	12	Total 12	O 12	0	0
9	D	3	Total 3	O 3	0	0
9	F	3	Total 3	O 3	0	0

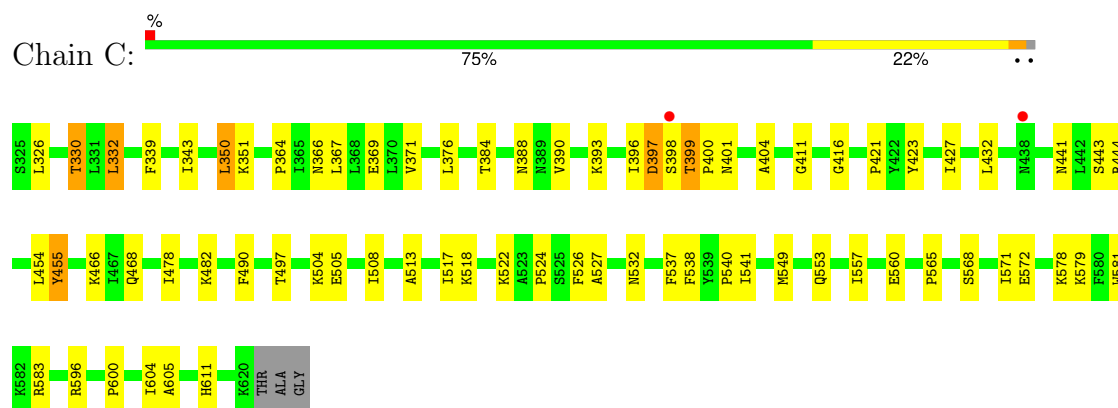
3 Residue-property plots

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.

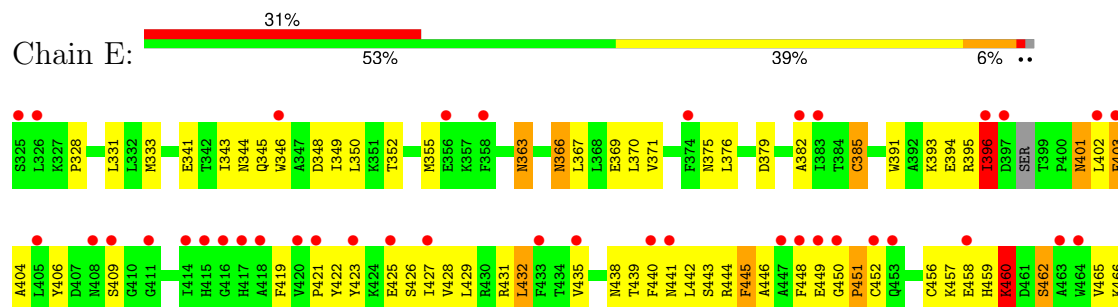
• Molecule 1: LepB

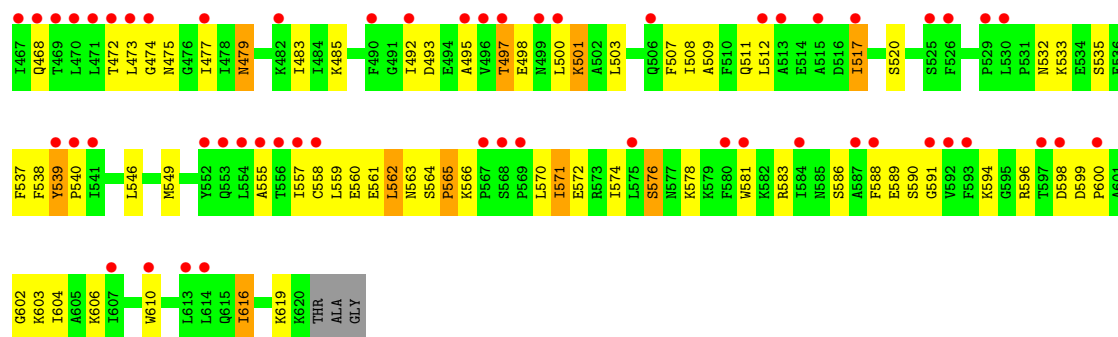


• Molecule 1: LepB



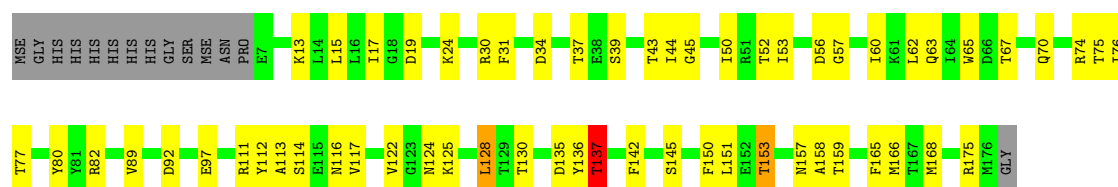
• Molecule 1: LepB





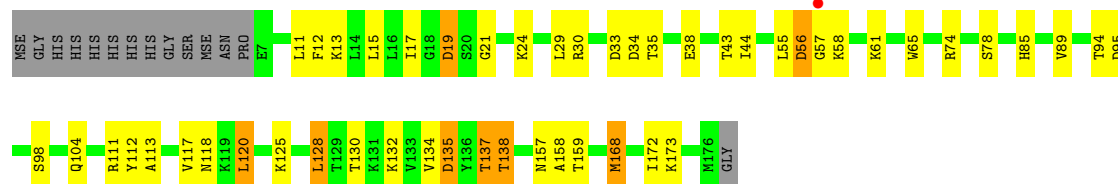
• Molecule 2: Ras-related protein Rab-1A

Chain B: 60% 30% 8%



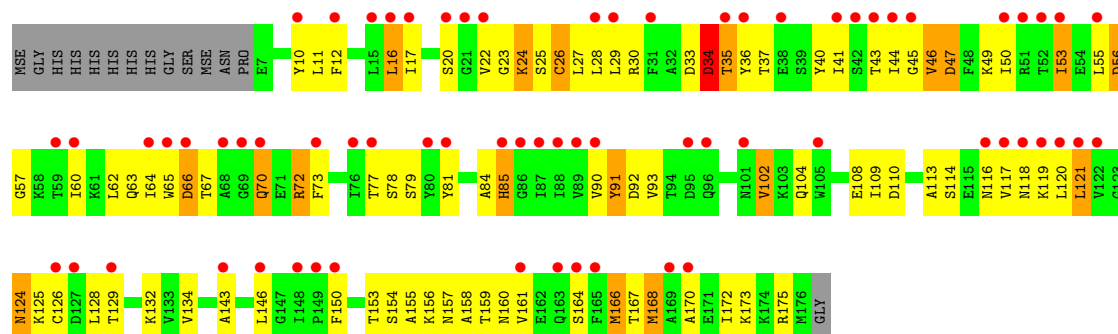
• Molecule 2: Ras-related protein Rab-1A

Chain D: 65% 23% 8%



• Molecule 2: Ras-related protein Rab-1A

Chain F: 37% 42% 40% 10% 8%



4 Data and refinement statistics

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	139.40Å 139.40Å 384.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.01 – 3.20 43.01 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (43.01-3.20) 99.9 (43.01-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.54	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.87 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.230 , 0.288 0.230 , 0.290	Depositor DCC
R_{free} test set	1602 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	54.4	Xtriage
Anisotropy	0.017	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 50.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	11410	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.16% 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: AF3, MG, ACT, GOL, GDP, K

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	0.55	0/2415	0.71	0/3262
1	C	0.55	0/2415	0.71	1/3262 (0.0%)
1	E	0.47	0/2408	0.67	1/3251 (0.0%)
2	B	0.46	0/1381	0.67	0/1859
2	D	0.42	0/1381	0.66	0/1859
2	F	0.45	0/1381	0.68	1/1859 (0.1%)
All	All	0.50	0/11381	0.69	3/15352 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	16	LEU	CA-CB-CG	5.26	127.41	115.30
1	C	332	LEU	CA-CB-CG	5.18	127.22	115.30
1	E	429	LEU	CA-CB-CG	5.06	126.94	115.30

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	2365	0	2378	50	0
1	C	2365	0	2378	44	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2359	0	2372	110	2
2	B	1362	0	1358	40	0
2	D	1362	0	1358	41	0
2	F	1362	0	1358	80	0
3	A	8	0	6	0	0
3	B	8	0	6	0	0
3	C	24	0	18	4	0
3	D	8	0	6	0	0
4	A	36	0	48	1	0
4	B	6	0	8	3	0
4	C	6	0	8	0	0
5	A	4	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
6	B	1	0	0	0	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
7	B	28	0	12	4	0
7	D	28	0	12	8	0
7	F	28	0	12	4	0
8	B	4	0	0	1	0
8	D	4	0	0	1	0
8	F	4	0	0	0	0
9	A	8	0	0	0	0
9	B	8	0	0	0	0
9	C	12	0	0	0	0
9	D	3	0	0	0	0
9	F	3	0	0	0	0
All	All	11410	0	11338	353	2

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 16.

All (353) 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:53:ILE:HD11	2:B:166:MSE:SE	1.92	1.19
1:E:456:CYS:HA	1:E:465:VAL:HG22	1.44	1.00
1:E:479:ASN:O	1:E:483:ILE:HG12	1.62	0.99
1:C:393:LYS:HG3	1:C:524:PRO:HB3	1.46	0.97
2:F:118:ASN:HD21	2:F:175:ARG:HH21	1.15	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:508:ILE:HA	1:E:511:GLN:HG2	1.48	0.93
1:E:498:GLU:O	1:E:501:LYS:HB2	1.71	0.90
2:D:56:ASP:N	2:D:57:GLY:HA2	1.89	0.88
2:B:53:ILE:CD1	2:B:166:MSE:SE	2.73	0.86
1:E:457:LYS:HA	1:E:460:LYS:HE3	1.56	0.86
1:E:509:ALA:HA	1:E:512:LEU:HG	1.59	0.85
2:D:15:LEU:HD12	2:D:65:TRP:HB2	1.60	0.83
2:F:93:VAL:HG21	2:F:126:CYS:HA	1.62	0.82
1:C:366:ASN:ND2	1:C:369:GLU:HB2	1.95	0.82
1:E:428:VAL:HA	1:E:445:PHE:CE2	2.16	0.79
2:F:56:ASP:N	2:F:57:GLY:HA2	1.97	0.79
1:E:432:LEU:HD13	1:E:445:PHE:HD2	1.47	0.78
2:B:56:ASP:N	2:B:57:GLY:HA2	1.99	0.75
1:C:596:ARG:HB2	1:C:600:PRO:HG3	1.69	0.75
2:F:114:SER:HB2	2:F:117:VAL:HG23	1.69	0.75
1:E:403:PHE:HE2	1:E:428:VAL:HG11	1.53	0.74
1:C:423:TYR:OH	1:C:560:GLU:HG3	1.88	0.73
2:F:118:ASN:ND2	2:F:175:ARG:HH21	1.86	0.73
2:B:122:VAL:HG13	2:B:153:THR:CG2	2.19	0.73
1:E:475:ASN:HB3	2:F:44:ILE:HD13	1.72	0.72
2:B:15:LEU:HD12	2:B:65:TRP:HB2	1.72	0.72
1:A:326:LEU:HD12	1:A:326:LEU:H	1.55	0.71
1:E:508:ILE:HA	1:E:511:GLN:CG	2.20	0.71
1:C:366:ASN:HD21	1:C:369:GLU:HB2	1.56	0.70
2:D:30:ARG:O	2:D:34:ASP:HA	1.90	0.70
2:F:12:PHE:HB2	2:F:62:LEU:CD2	2.20	0.70
1:C:513:ALA:O	1:C:517:ILE:HD13	1.91	0.70
2:D:13:LYS:H	2:D:85:HIS:HD2	1.40	0.70
2:F:56:ASP:H	2:F:57:GLY:HA2	1.53	0.70
1:E:402:LEU:HD12	1:E:425:GLU:OE2	1.91	0.69
1:C:427:ILE:HD12	1:C:537:PHE:HD1	1.57	0.69
1:E:462:SER:O	1:E:466:LYS:HG2	1.93	0.68
1:E:435:VAL:HG13	1:E:440:PHE:O	1.94	0.68
1:A:549:MSE:O	1:A:583:ARG:NH1	2.26	0.68
1:E:343:ILE:HG23	1:E:507:PHE:CD1	2.28	0.68
2:F:10:TYR:HB2	2:F:60:ILE:HG12	1.75	0.67
1:E:539:TYR:HB3	1:E:540:PRO:CD	2.22	0.67
2:F:154:SER:HB3	2:F:159:THR:HB	1.77	0.67
1:C:540:PRO:HA	3:C:705:ACT:C	2.24	0.67
1:E:441:ASN:HB2	2:F:41:ILE:HG23	1.78	0.66
1:A:350:LEU:HD12	1:A:504:LYS:HB2	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:535:SER:HB2	1:E:570:LEU:HD22	1.78	0.65
1:E:393:LYS:HB3	1:E:394:GLU:OE2	1.96	0.65
1:A:600:PRO:O	1:A:604:ILE:HG12	1.97	0.65
2:F:168:MSE:HG3	2:F:172:ILE:HD11	1.79	0.65
2:F:26:CYS:HG	2:F:36:TYR:HE1	1.38	0.65
1:C:366:ASN:ND2	1:C:369:GLU:CB	2.60	0.64
2:B:80:TYR:CD2	4:B:206:GOL:H32	2.32	0.64
1:A:423:TYR:OH	1:A:560:GLU:HG3	1.97	0.64
2:D:13:LYS:H	2:D:85:HIS:CD2	2.15	0.64
2:B:31:PHE:CE2	2:B:165:PHE:HB2	2.32	0.64
1:E:401:ASN:ND2	1:E:421:PRO:O	2.25	0.64
1:C:330:THR:OG1	1:C:364:PRO:HG2	1.99	0.63
2:F:12:PHE:HD1	2:F:85:HIS:HD2	1.45	0.63
2:B:150:PHE:O	2:B:151:LEU:HD12	1.99	0.63
2:D:135:ASP:O	2:D:138:THR:HG23	1.98	0.63
1:E:427:ILE:HG13	1:E:537:PHE:HA	1.80	0.62
2:F:55:LEU:O	2:F:56:ASP:HB2	1.99	0.62
2:B:142:PHE:O	2:B:145:SER:HB3	1.98	0.62
2:D:128:LEU:HD13	7:D:202:GDP:HN21	1.65	0.62
2:D:12:PHE:HA	2:D:85:HIS:CD2	2.35	0.61
1:E:555:ALA:O	1:E:559:LEU:HG	1.99	0.61
1:A:468:GLN:HG3	1:A:469:THR:N	2.15	0.61
2:D:12:PHE:HA	2:D:85:HIS:HD2	1.65	0.61
1:E:432:LEU:HD13	1:E:445:PHE:CD2	2.33	0.61
1:E:571:ILE:HA	1:E:574:ILE:HG13	1.81	0.61
1:E:578:LYS:HA	1:E:581:TRP:HB3	1.83	0.61
1:A:449:GLU:OE2	2:B:70:GLN:HG2	2.01	0.60
1:E:404:ALA:HA	1:E:419:PHE:CE2	2.36	0.60
1:E:561:GLU:HG3	1:E:571:ILE:HB	1.84	0.60
2:F:35:THR:HG22	2:F:36:TYR:N	2.16	0.60
2:B:80:TYR:HD2	4:B:206:GOL:H32	1.65	0.60
1:C:388:ASN:O	1:C:524:PRO:HD2	2.02	0.59
1:E:428:VAL:HA	1:E:445:PHE:HE2	1.64	0.59
1:E:456:CYS:HA	1:E:465:VAL:CG2	2.26	0.59
2:F:26:CYS:O	2:F:29:LEU:HB3	2.02	0.59
2:D:30:ARG:HG3	2:D:30:ARG:HH11	1.66	0.59
2:F:12:PHE:HB2	2:F:62:LEU:HD22	1.85	0.59
2:B:111:ARG:HD2	2:B:112:TYR:CZ	2.38	0.59
1:E:492:ILE:HD11	2:F:50:ILE:HD11	1.85	0.58
2:F:37:THR:HG23	2:F:37:THR:O	2.03	0.58
2:B:135:ASP:HB3	2:B:137:THR:HG23	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:399:THR:HB	1:C:404:ALA:HB3	1.84	0.58
1:E:406:TYR:HB2	1:E:451:PRO:HB3	1.86	0.58
2:F:104:GLN:O	2:F:108:GLU:HG2	2.03	0.58
2:B:114:SER:HB2	2:B:117:VAL:HG23	1.86	0.58
2:D:38:GLU:OE2	2:D:38:GLU:HA	2.04	0.58
2:F:77:THR:HG22	2:F:81:TYR:CE1	2.38	0.58
1:A:355:MSE:HE3	1:A:355:MSE:O	2.03	0.58
1:E:561:GLU:O	1:E:563:ASN:N	2.37	0.57
2:D:19:ASP:O	2:D:24:LYS:NZ	2.37	0.57
2:F:35:THR:CG2	2:F:36:TYR:N	2.67	0.57
2:F:67:THR:HB	2:F:77:THR:HG23	1.87	0.57
1:A:493:ASP:O	1:A:497:THR:HG22	2.04	0.57
2:D:128:LEU:CD1	7:D:202:GDP:N2	2.67	0.57
2:B:122:VAL:HG13	2:B:153:THR:HG21	1.86	0.57
2:F:77:THR:HG22	2:F:81:TYR:HE1	1.69	0.57
2:B:67:THR:HB	2:B:77:THR:HG22	1.87	0.56
1:E:479:ASN:O	1:E:483:ILE:CG1	2.47	0.56
1:E:503:LEU:HG	1:E:507:PHE:CE2	2.40	0.56
1:E:539:TYR:HB3	1:E:540:PRO:HD2	1.87	0.56
2:F:26:CYS:HB2	7:F:201:GDP:O2A	2.06	0.56
2:B:53:ILE:HG22	2:B:60:ILE:HB	1.88	0.56
1:E:591:GLY:O	1:E:594:LYS:HB2	2.06	0.56
2:F:22:VAL:HG22	2:F:92:ASP:HB2	1.88	0.56
2:F:120:LEU:HD21	2:F:164:SER:HB3	1.88	0.56
2:F:129:THR:HG22	2:F:132:LYS:HD2	1.89	0.55
1:C:398:SER:O	1:C:399:THR:C	2.44	0.55
2:F:25:SER:N	7:F:201:GDP:O3B	2.39	0.55
1:E:591:GLY:O	1:E:594:LYS:CB	2.55	0.55
1:E:509:ALA:CA	1:E:512:LEU:HG	2.35	0.55
2:D:33:ASP:HB2	2:D:35:THR:HG22	1.89	0.55
2:B:113:ALA:HB1	2:B:117:VAL:HG21	1.89	0.55
1:C:549:MSE:O	1:C:583:ARG:NH1	2.36	0.54
1:E:404:ALA:HA	1:E:419:PHE:HE2	1.71	0.54
1:A:368:LEU:HD12	1:A:372:LYS:HD3	1.89	0.54
2:F:22:VAL:HG12	2:F:90:VAL:HG12	1.89	0.54
1:C:351:LYS:HA	1:C:504:LYS:HE3	1.90	0.54
1:E:444:ARG:HD2	2:F:40:TYR:HB3	1.89	0.54
2:F:20:SER:OG	2:F:70:GLN:NE2	2.41	0.54
1:E:444:ARG:O	1:E:446:ALA:N	2.42	0.53
1:A:366:ASN:OD1	1:A:369:GLU:HB2	2.08	0.53
2:F:23:GLY:HA3	2:F:124:ASN:OD1	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:29:LEU:HD21	2:D:35:THR:HG23	1.90	0.53
1:E:403:PHE:CE2	1:E:428:VAL:HG11	2.37	0.53
1:A:513:ALA:O	1:A:517:ILE:HD13	2.09	0.53
1:E:343:ILE:HG23	1:E:507:PHE:HD1	1.72	0.53
1:E:366:ASN:OD1	1:E:369:GLU:HB2	2.09	0.52
1:A:400:PRO:HB3	1:A:422:TYR:CD1	2.43	0.52
2:B:175:ARG:O	2:B:175:ARG:HG2	2.08	0.52
2:F:35:THR:CG2	2:F:36:TYR:H	2.22	0.52
1:E:393:LYS:HE2	1:E:394:GLU:HG3	1.90	0.52
2:F:170:ALA:HA	2:F:173:LYS:HB3	1.91	0.52
1:E:406:TYR:O	1:E:451:PRO:HG3	2.09	0.52
2:F:156:LYS:HB2	7:F:201:GDP:N1	2.24	0.52
2:D:128:LEU:HD13	7:D:202:GDP:N2	2.24	0.52
1:E:472:THR:HG22	1:E:473:LEU:HG	1.92	0.52
2:F:109:ILE:HG23	2:F:113:ALA:HB3	1.92	0.52
2:D:111:ARG:HD2	2:D:112:TYR:CZ	2.44	0.52
2:F:113:ALA:HB1	2:F:117:VAL:HG21	1.91	0.51
1:E:331:LEU:HB3	1:E:346:TRP:CE2	2.45	0.51
1:E:441:ASN:HD22	2:F:44:ILE:H	1.57	0.51
1:A:504:LYS:O	1:A:507:PHE:HB2	2.10	0.51
1:E:517:ILE:HG22	1:E:520:SER:HB2	1.91	0.51
2:F:17:ILE:HD11	2:F:81:TYR:CE2	2.45	0.51
1:A:326:LEU:HD13	1:A:359:SER:HB2	1.92	0.51
2:D:74:ARG:O	2:D:78:SER:HB3	2.10	0.51
2:D:21:GLY:N	7:D:202:GDP:O1B	2.43	0.51
1:E:348:ASP:O	1:E:352:THR:HG22	2.10	0.51
2:F:55:LEU:HD11	2:F:166:MSE:SE	2.60	0.51
1:E:509:ALA:HA	1:E:512:LEU:CG	2.34	0.51
1:E:375:ASN:HD21	1:E:435:VAL:HB	1.75	0.51
1:A:538:PHE:CE2	1:A:557:ILE:HG23	2.46	0.51
1:E:606:LYS:O	1:E:610:TRP:CD1	2.64	0.50
2:F:168:MSE:HG3	2:F:172:ILE:CD1	2.40	0.50
2:D:120:LEU:HD12	2:D:168:MSE:HB2	1.92	0.50
2:D:29:LEU:CD2	2:D:35:THR:HG23	2.41	0.50
1:C:427:ILE:CD1	1:C:537:PHE:HD1	2.23	0.50
2:F:46:VAL:O	2:F:47:ASP:HB2	2.11	0.50
2:B:125:LYS:HG2	7:B:202:GDP:C5	2.46	0.50
1:E:367:LEU:O	1:E:370:LEU:HB3	2.12	0.50
1:E:565:PRO:C	1:E:566:LYS:HG2	2.31	0.50
1:E:363:ASN:N	1:E:363:ASN:OD1	2.45	0.50
2:F:91:TYR:HE2	2:F:150:PHE:HE1	1.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:596:ARG:HB3	1:A:598:ASP:OD1	2.12	0.49
2:F:155:ALA:HB3	7:F:201:GDP:O6	2.12	0.49
1:A:338:SER:HA	1:A:373:GLN:OE1	2.13	0.49
2:B:116:ASN:HD22	2:B:175:ARG:HE	1.60	0.49
1:E:493:ASP:O	1:E:497:THR:HG22	2.12	0.49
2:F:28:LEU:HD22	2:F:66:ASP:HB3	1.94	0.49
2:F:53:ILE:HD11	2:F:166:MSE:SE	2.62	0.49
1:A:577:ASN:OD1	1:A:577:ASN:C	2.51	0.49
2:B:67:THR:HB	2:B:77:THR:CG2	2.42	0.49
1:E:385:CYS:HB3	1:E:391:TRP:CZ2	2.48	0.49
2:D:125:LYS:HG2	7:D:202:GDP:C6	2.48	0.49
2:F:25:SER:OG	2:F:66:ASP:OD2	2.31	0.48
2:F:30:ARG:HH21	2:F:36:TYR:HB2	1.78	0.48
1:A:333:MSE:HE1	1:A:370:LEU:HA	1.94	0.48
2:D:113:ALA:HB1	2:D:117:VAL:HG21	1.95	0.48
1:E:439:THR:O	1:E:440:PHE:HB2	2.13	0.48
2:D:137:THR:OG1	2:D:138:THR:N	2.47	0.48
1:E:382:ALA:HB1	1:E:426:SER:HB3	1.95	0.48
2:F:30:ARG:HH11	2:F:158:ALA:HB2	1.79	0.48
1:A:344:ASN:O	1:A:347:ALA:HB3	2.14	0.48
2:F:63:GLN:C	2:F:64:ILE:HG13	2.33	0.48
2:D:43:THR:HB	8:D:203:AF3:F1	2.04	0.48
2:F:25:SER:OG	2:F:43:THR:OG1	2.25	0.48
2:F:81:TYR:O	2:F:84:ALA:HB3	2.12	0.48
1:A:378:VAL:HG11	1:A:434:THR:HG23	1.95	0.47
1:C:532:ASN:HD21	3:C:705:ACT:H3	1.79	0.47
1:A:371:VAL:HG21	1:A:440:PHE:CD1	2.49	0.47
1:C:367:LEU:HD11	1:C:482:LYS:HA	1.97	0.47
2:F:33:ASP:O	2:F:34:ASP:HB2	2.15	0.47
2:B:43:THR:HB	8:B:203:AF3:F1	2.04	0.47
2:F:47:ASP:O	2:F:65:TRP:CE3	2.68	0.47
1:A:330:THR:OG1	1:A:364:PRO:HG2	2.14	0.47
1:A:484:ILE:HG23	1:A:496:VAL:HG13	1.97	0.47
2:F:102:VAL:HG22	2:F:121:LEU:HD11	1.97	0.47
1:A:455:TYR:CD1	1:A:455:TYR:C	2.88	0.47
2:F:158:ALA:HA	2:F:161:VAL:HG22	1.97	0.47
2:D:58:LYS:HG3	2:D:173:LYS:NZ	2.31	0.46
1:E:428:VAL:HA	1:E:445:PHE:CZ	2.49	0.46
1:E:474:GLY:HA2	1:E:477:ILE:HD12	1.97	0.46
2:F:143:ALA:HB1	2:F:150:PHE:HB2	1.96	0.46
1:A:444:ARG:NH2	7:B:202:GDP:O1B	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:540:PRO:HA	3:C:705:ACT:O	2.15	0.46
1:E:466:LYS:HB3	1:E:517:ILE:HG12	1.97	0.46
1:E:562:LEU:HB3	1:E:603:LYS:HE2	1.97	0.46
2:F:116:ASN:HD22	2:F:175:ARG:HD2	1.81	0.46
2:F:157:ASN:O	2:F:158:ALA:HB3	2.15	0.46
1:C:396:ILE:HG13	1:C:397:ASP:OD1	2.15	0.46
2:D:55:LEU:O	2:D:56:ASP:HB2	2.15	0.46
1:E:450:GLY:O	1:E:452:CYS:N	2.48	0.46
2:F:23:GLY:O	2:F:24:LYS:C	2.54	0.46
2:F:124:ASN:HD21	2:F:155:ALA:H	1.63	0.46
1:E:350:LEU:HD22	1:E:355:MSE:SE	2.66	0.46
1:E:431:ARG:HB2	1:E:445:PHE:CG	2.51	0.46
1:E:456:CYS:HB3	1:E:465:VAL:HG13	1.96	0.46
1:A:334:THR:HB	1:A:337:THR:HG23	1.97	0.46
1:A:388:ASN:O	1:A:524:PRO:HD2	2.16	0.46
1:A:606:LYS:HD3	1:A:610:TRP:CZ2	2.51	0.46
1:C:400:PRO:HB2	1:C:421:PRO:O	2.15	0.46
1:E:341:GLU:O	1:E:345:GLN:HG3	2.16	0.46
1:A:441:ASN:HA	2:B:44:ILE:HG13	1.97	0.46
1:E:497:THR:HA	1:E:500:LEU:HD12	1.97	0.46
1:C:455:TYR:CD1	1:C:455:TYR:C	2.88	0.46
1:E:352:THR:HG23	1:E:352:THR:O	2.16	0.46
1:A:459:HIS:HB3	1:A:462:SER:HB3	1.97	0.46
1:C:416:GLY:O	1:C:596:ARG:NH1	2.45	0.45
1:E:532:ASN:HD21	1:E:540:PRO:HD3	1.81	0.45
1:C:581:TRP:CE2	1:C:611:HIS:CD2	3.04	0.45
1:E:444:ARG:C	1:E:446:ALA:N	2.70	0.45
1:E:403:PHE:O	1:E:419:PHE:CZ	2.70	0.45
2:F:27:LEU:HD21	2:F:124:ASN:ND2	2.32	0.45
2:B:128:LEU:HD11	7:B:202:GDP:N2	2.31	0.45
2:D:11:LEU:HD13	2:D:61:LYS:HD3	1.98	0.45
2:B:157:ASN:O	2:B:158:ALA:HB3	2.16	0.45
1:C:339:PHE:O	1:C:343:ILE:HG12	2.17	0.45
1:E:562:LEU:HB3	1:E:603:LYS:CE	2.47	0.45
1:A:400:PRO:HB3	1:A:422:TYR:CE1	2.51	0.45
1:A:460:LYS:O	1:A:461:ASP:HB2	2.17	0.45
1:E:404:ALA:HB2	1:E:421:PRO:HB3	1.98	0.45
2:D:85:HIS:HB3	2:D:172:ILE:HD13	1.99	0.45
2:D:118:ASN:HD22	2:D:172:ILE:HG12	1.81	0.45
1:E:331:LEU:HB3	1:E:346:TRP:NE1	2.31	0.45
1:C:441:ASN:HA	2:D:44:ILE:HG13	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:505:GLU:HA	1:C:508:ILE:HD12	1.99	0.45
1:A:443:SER:HB2	4:A:907:GOL:H2	1.99	0.45
2:B:128:LEU:CD1	7:B:202:GDP:N2	2.79	0.44
1:E:466:LYS:CB	1:E:517:ILE:HG12	2.47	0.44
1:E:602:GLY:O	1:E:606:LYS:HB2	2.16	0.44
1:E:616:ILE:H	1:E:616:ILE:HG13	1.67	0.44
2:D:158:ALA:O	2:D:159:THR:C	2.55	0.44
1:E:428:VAL:HG13	1:E:445:PHE:HE2	1.83	0.44
1:E:572:GLU:OE2	1:E:576:SER:OG	2.36	0.44
2:D:157:ASN:O	2:D:158:ALA:HB3	2.18	0.44
1:E:343:ILE:HG23	1:E:507:PHE:CE1	2.52	0.44
2:B:50:ILE:HA	2:B:62:LEU:O	2.19	0.43
1:C:423:TYR:OH	1:C:560:GLU:CG	2.62	0.43
1:E:371:VAL:HG21	1:E:440:PHE:CD1	2.53	0.43
1:E:422:TYR:HD2	1:E:549:MSE:HE1	1.83	0.43
2:D:17:ILE:HD11	2:D:89:VAL:HG22	2.00	0.43
1:C:454:LEU:HA	1:C:454:LEU:HD23	1.72	0.43
1:E:403:PHE:CD1	1:E:403:PHE:N	2.85	0.43
1:E:468:GLN:O	1:E:468:GLN:HG2	2.18	0.43
2:F:78:SER:HA	2:F:81:TYR:CD1	2.53	0.43
1:A:350:LEU:HA	1:A:350:LEU:HD22	1.65	0.43
1:A:614:LEU:HD23	1:A:614:LEU:HA	1.82	0.43
2:B:63:GLN:HE21	2:B:65:TRP:HE1	1.65	0.43
2:B:19:ASP:O	2:B:24:LYS:NZ	2.51	0.43
1:E:472:THR:O	2:F:73:PHE:HE1	2.02	0.43
1:A:390:VAL:O	1:A:393:LYS:HB2	2.19	0.43
2:D:95:ASP:OD2	2:D:98:SER:HB3	2.18	0.43
2:F:153:THR:HB	2:F:161:VAL:HG12	2.00	0.43
1:C:568:SER:O	1:C:571:ILE:HG22	2.19	0.43
1:E:333:MSE:HE3	1:E:333:MSE:HB2	1.97	0.43
1:E:385:CYS:HB3	1:E:391:TRP:CE2	2.54	0.43
1:E:441:ASN:HB2	2:F:41:ILE:CG2	2.48	0.43
1:E:441:ASN:ND2	2:F:43:THR:HA	2.34	0.43
1:C:596:ARG:CB	1:C:600:PRO:HG3	2.42	0.42
2:F:91:TYR:CE1	2:F:134:VAL:HG11	2.53	0.42
2:B:17:ILE:HD11	2:B:89:VAL:HG22	2.01	0.42
1:C:541:ILE:H	3:C:705:ACT:C	2.30	0.42
1:A:367:LEU:HD23	1:A:367:LEU:HA	1.79	0.42
2:D:13:LYS:N	2:D:85:HIS:HD2	2.12	0.42
1:E:495:ALA:HA	1:E:498:GLU:HB2	2.01	0.42
2:B:116:ASN:OD1	2:B:116:ASN:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:367:LEU:HD23	1:C:367:LEU:HA	1.95	0.42
1:C:399:THR:HA	1:C:400:PRO:HD3	1.91	0.42
2:F:16:LEU:HB2	2:F:66:ASP:HA	2.00	0.42
1:A:367:LEU:O	1:A:368:LEU:C	2.58	0.42
2:B:135:ASP:O	2:B:136:TYR:C	2.58	0.42
2:B:30:ARG:O	2:B:34:ASP:HA	2.20	0.42
2:F:153:THR:HG22	2:F:160:ASN:O	2.20	0.42
2:D:168:MSE:O	2:D:172:ILE:HG13	2.20	0.41
1:E:423:TYR:CD2	1:E:448:PHE:CZ	3.07	0.41
1:E:538:PHE:CE1	1:E:557:ILE:HG23	2.55	0.41
2:F:46:VAL:HG12	2:F:67:THR:HA	2.02	0.41
2:B:175:ARG:O	2:B:175:ARG:CG	2.68	0.41
1:C:350:LEU:HD23	1:C:350:LEU:HA	1.84	0.41
2:F:109:ILE:HG21	2:F:119:LYS:HE2	2.02	0.41
1:E:558:CYS:C	1:E:560:GLU:N	2.74	0.41
1:A:374:PHE:CE1	1:A:474:GLY:HA3	2.54	0.41
1:C:444:ARG:NH1	7:D:202:GDP:O1B	2.49	0.41
1:E:331:LEU:HD13	1:E:346:TRP:CD2	2.55	0.41
1:E:457:LYS:HA	1:E:460:LYS:CE	2.38	0.41
1:A:326:LEU:HD12	1:A:326:LEU:N	2.30	0.41
1:E:435:VAL:HA	1:E:441:ASN:O	2.20	0.41
1:E:599:ASP:CG	1:E:602:GLY:HA3	2.40	0.41
1:A:392:ALA:HA	1:A:395:ARG:HD2	2.03	0.41
1:E:459:HIS:O	1:E:465:VAL:HG21	2.21	0.41
1:A:341:GLU:HA	1:A:344:ASN:HB3	2.03	0.41
2:B:44:ILE:HG22	2:B:45:GLY:N	2.36	0.41
1:C:371:VAL:HG22	1:C:478:ILE:HD13	2.03	0.41
1:C:604:ILE:O	1:C:605:ALA:C	2.58	0.41
2:D:125:LYS:HG2	7:D:202:GDP:C5	2.56	0.41
2:B:124:ASN:HA	2:B:153:THR:O	2.21	0.41
1:C:466:LYS:O	1:C:517:ILE:HD11	2.21	0.41
2:D:74:ARG:HD3	2:D:74:ARG:HA	1.93	0.41
1:E:422:TYR:CD2	1:E:549:MSE:HE1	2.56	0.41
1:E:561:GLU:CB	1:E:571:ILE:HB	2.51	0.41
2:F:12:PHE:HB2	2:F:62:LEU:HD21	2.00	0.41
2:F:125:LYS:HB3	2:F:128:LEU:HD13	2.03	0.41
2:F:168:MSE:HE2	2:F:168:MSE:HB2	2.00	0.41
1:C:401:ASN:OD1	1:C:401:ASN:C	2.59	0.41
1:C:490:PHE:N	1:C:490:PHE:CD1	2.89	0.41
1:E:589:GLU:O	1:E:590:SER:C	2.59	0.41
2:F:172:ILE:HG23	2:F:175:ARG:HH22	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:128:LEU:HD11	7:D:202:GDP:N2	2.35	0.40
1:E:561:GLU:O	1:E:564:SER:N	2.27	0.40
2:B:13:LYS:HD2	4:B:206:GOL:O2	2.22	0.40
1:A:371:VAL:HG22	1:A:478:ILE:HD13	2.03	0.40
1:A:608:ARG:O	1:A:612:GLN:HG3	2.21	0.40
1:A:613:LEU:O	1:A:616:ILE:HB	2.21	0.40
2:B:76:ILE:O	2:B:77:THR:C	2.59	0.40
1:C:411:GLY:HA2	1:C:553:GLN:HE21	1.87	0.40
1:C:390:VAL:O	1:C:393:LYS:HB2	2.21	0.40
1:C:538:PHE:CE2	1:C:557:ILE:HG23	2.57	0.40
2:D:132:LYS:HE2	2:D:134:VAL:O	2.22	0.40
1:E:343:ILE:CG2	1:E:507:PHE:HD1	2.33	0.40
1:E:423:TYR:HE1	1:E:560:GLU:HG2	1.86	0.40
1:E:442:LEU:HD11	2:F:72:ARG:HH22	1.86	0.40
1:A:339:PHE:O	1:A:343:ILE:HG12	2.22	0.40
1:A:371:VAL:HG21	1:A:440:PHE:HD1	1.85	0.40
1:A:599:ASP:O	1:A:600:PRO:C	2.60	0.40
2:B:74:ARG:O	2:B:75:THR:C	2.60	0.40
1:E:558:CYS:O	1:E:560:GLU:N	2.54	0.40
2:F:128:LEU:O	2:F:132:LYS:HB2	2.22	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:395:ARG:O	1:E:395:ARG:O[6_555]	1.49	0.71
1:E:396:ILE:O	1:E:396:ILE:O[6_555]	2.17	0.03

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	294/299 (98%)	267 (91%)	23 (8%)	4 (1%)	9	40
1	C	294/299 (98%)	273 (93%)	19 (6%)	2 (1%)	19	54
1	E	291/299 (97%)	231 (79%)	44 (15%)	16 (6%)	1	11
2	B	168/184 (91%)	150 (89%)	16 (10%)	2 (1%)	11	43
2	D	168/184 (91%)	149 (89%)	16 (10%)	3 (2%)	7	35
2	F	168/184 (91%)	132 (79%)	28 (17%)	8 (5%)	2	14
All	All	1383/1449 (95%)	1202 (87%)	146 (11%)	35 (2%)	4	28

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	445	PHE
1	E	596	ARG
1	E	598	ASP
2	F	24	LYS
2	F	46	VAL
2	F	47	ASP
2	F	56	ASP
1	E	451	PRO
1	E	539	TYR
1	E	562	LEU
1	E	600	PRO
2	F	34	ASP
1	A	402	LEU
1	A	531	PRO
1	A	565	PRO
2	B	137	THR
2	D	56	ASP
1	E	619	LYS
2	F	45	GLY
2	B	159	THR
1	C	527	ALA
2	D	19	ASP
2	D	130	THR
1	E	409	SER
1	E	460	LYS
1	E	501	LYS
2	F	35	THR
2	F	168	MSE
1	A	396	ILE
1	E	328	PRO

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Mol	Chain	Res	Type
1	E	576	SER
1	C	399	THR
1	E	565	PRO
1	E	396	ILE
1	E	349	ILE

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	259/257 (101%)	234 (90%)	25 (10%)	6	27
1	C	259/257 (101%)	240 (93%)	19 (7%)	11	41
1	E	258/257 (100%)	230 (89%)	28 (11%)	5	23
2	B	150/156 (96%)	139 (93%)	11 (7%)	11	41
2	D	150/156 (96%)	142 (95%)	8 (5%)	19	52
2	F	150/156 (96%)	132 (88%)	18 (12%)	4	19
All	All	1226/1239 (99%)	1117 (91%)	109 (9%)	8	31

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	326	LEU
1	A	350	LEU
1	A	368	LEU
1	A	376	LEU
1	A	396	ILE
1	A	405	LEU
1	A	432	LEU
1	A	434	THR
1	A	438	ASN
1	A	443	SER
1	A	449	GLU
1	A	454	LEU
1	A	462	SER

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Mol	Chain	Res	Type
1	A	468	GLN
1	A	485	LYS
1	A	494	GLU
1	A	512	LEU
1	A	519	GLU
1	A	525	SER
1	A	526	PHE
1	A	572	GLU
1	A	594	LYS
1	A	597	THR
1	A	617	SER
1	A	619	LYS
2	B	37	THR
2	B	39	SER
2	B	52	THR
2	B	82	ARG
2	B	92	ASP
2	B	97	GLU
2	B	128	LEU
2	B	130	THR
2	B	137	THR
2	B	153	THR
2	B	168	MSE
1	C	326	LEU
1	C	330	THR
1	C	332	LEU
1	C	350	LEU
1	C	376	LEU
1	C	384	THR
1	C	397	ASP
1	C	432	LEU
1	C	443	SER
1	C	455	TYR
1	C	468	GLN
1	C	497	THR
1	C	518	LYS
1	C	522	LYS
1	C	526	PHE
1	C	565	PRO
1	C	572	GLU
1	C	578	LYS
1	C	579	LYS

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Mol	Chain	Res	Type
2	D	94	THR
2	D	104	GLN
2	D	120	LEU
2	D	128	LEU
2	D	135	ASP
2	D	137	THR
2	D	138	THR
2	D	168	MSE
1	E	344	ASN
1	E	363	ASN
1	E	366	ASN
1	E	376	LEU
1	E	379	ASP
1	E	385	CYS
1	E	396	ILE
1	E	401	ASN
1	E	403	PHE
1	E	432	LEU
1	E	438	ASN
1	E	443	SER
1	E	449	GLU
1	E	458	GLU
1	E	460	LYS
1	E	462	SER
1	E	479	ASN
1	E	485	LYS
1	E	497	THR
1	E	517	ILE
1	E	533	LYS
1	E	546	LEU
1	E	571	ILE
1	E	583	ARG
1	E	586	SER
1	E	588	PHE
1	E	604	ILE
1	E	616	ILE
2	F	11	LEU
2	F	26	CYS
2	F	34	ASP
2	F	49	LYS
2	F	53	ILE
2	F	66	ASP

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Mol	Chain	Res	Type
2	F	70	GLN
2	F	72	ARG
2	F	79	SER
2	F	85	HIS
2	F	91	TYR
2	F	102	VAL
2	F	110	ASP
2	F	121	LEU
2	F	124	ASN
2	F	146	LEU
2	F	166	MSE
2	F	167	THR

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

Mol	Chain	Res	Type
1	A	459	HIS
2	B	63	GLN
1	C	366	ASN
2	D	85	HIS
2	D	118	ASN
2	D	157	ASN
2	D	160	ASN
1	E	441	ASN
1	E	475	ASN
1	E	532	ASN
1	E	553	GLN
2	F	70	GLN
2	F	118	ASN
2	F	124	ASN
2	F	163	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 35 ligands modelled in this entry, 9 are monoatomic - leaving 26 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	ACT	C	701	-	3,3,3	0.87	0	3,3,3	0.92	0
8	AF3	F	202	-	0,3,3	-	-	-		
3	ACT	A	902	5	3,3,3	0.92	0	3,3,3	0.45	0
4	GOL	A	907	-	5,5,5	0.43	0	5,5,5	0.29	0
4	GOL	A	904	-	5,5,5	0.37	0	5,5,5	0.46	0
8	AF3	D	203	-	0,3,3	-	-	-		
4	GOL	A	906	-	5,5,5	0.66	0	5,5,5	0.84	0
4	GOL	A	903	-	5,5,5	0.52	0	5,5,5	0.88	0
7	GDP	B	202	6	25,30,30	1.21	3 (12%)	30,47,47	1.16	3 (10%)
3	ACT	C	706	-	3,3,3	0.86	0	3,3,3	0.76	0
3	ACT	C	704	-	3,3,3	0.82	0	3,3,3	0.98	0
3	ACT	B	205	-	3,3,3	0.83	0	3,3,3	0.97	0
7	GDP	D	202	6	25,30,30	1.26	4 (16%)	30,47,47	1.25	5 (16%)
4	GOL	B	206	-	5,5,5	0.55	0	5,5,5	0.42	0
4	GOL	A	908	-	5,5,5	0.32	0	5,5,5	0.34	0
3	ACT	C	702	-	3,3,3	0.87	0	3,3,3	0.78	0
7	GDP	F	201	6	25,30,30	1.23	4 (16%)	30,47,47	1.15	2 (6%)
4	GOL	C	707	-	5,5,5	0.51	0	5,5,5	0.17	0
3	ACT	A	901	-	3,3,3	0.90	0	3,3,3	0.81	0
8	AF3	B	203	-	0,3,3	-	-	-		
3	ACT	C	705	-	3,3,3	0.83	0	3,3,3	0.74	0
3	ACT	D	204	-	3,3,3	0.81	0	3,3,3	0.75	0
3	ACT	C	703	-	3,3,3	0.82	0	3,3,3	0.90	0
3	ACT	D	205	-	3,3,3	0.73	0	3,3,3	1.12	0
3	ACT	B	204	-	3,3,3	0.82	0	3,3,3	0.86	0
4	GOL	A	905	-	5,5,5	0.50	0	5,5,5	0.54	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
4	GOL	A	906	-	-	2/4/4/4	-
7	GDP	F	201	6	-	0/12/32/32	0/3/3/3
4	GOL	C	707	-	-	2/4/4/4	-
4	GOL	A	903	-	-	2/4/4/4	-
7	GDP	D	202	6	-	2/12/32/32	0/3/3/3
4	GOL	B	206	-	-	3/4/4/4	-
4	GOL	A	904	-	-	3/4/4/4	-
4	GOL	A	908	-	-	1/4/4/4	-
4	GOL	A	907	-	-	2/4/4/4	-
7	GDP	B	202	6	-	0/12/32/32	0/3/3/3
4	GOL	A	905	-	-	1/4/4/4	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	F	201	GDP	PA-O3A	3.62	1.63	1.59
7	D	202	GDP	PA-O3A	2.79	1.62	1.59
7	B	202	GDP	C6-N1	-2.78	1.33	1.37
7	D	202	GDP	C6-N1	-2.52	1.33	1.37
7	B	202	GDP	O4'-C1'	2.40	1.44	1.40
7	B	202	GDP	PA-O3A	2.27	1.61	1.59
7	D	202	GDP	O4'-C1'	2.19	1.43	1.40
7	F	201	GDP	O4'-C1'	2.15	1.43	1.40
7	F	201	GDP	C6-N1	-2.13	1.34	1.37
7	F	201	GDP	C5-C4	2.05	1.48	1.43
7	D	202	GDP	C5-C4	2.03	1.48	1.43

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	202	GDP	C8-N7-C5	3.11	107.84	102.55
7	B	202	GDP	C8-N7-C5	2.99	107.65	102.55
7	F	201	GDP	C8-N7-C5	2.96	107.59	102.55
7	F	201	GDP	C5-C6-N1	2.30	118.46	114.07
7	D	202	GDP	C2-N1-C6	-2.30	120.90	125.11
7	D	202	GDP	C4'-O4'-C1'	2.16	111.91	109.92
7	D	202	GDP	O3B-PB-O1B	2.10	119.03	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	202	GDP	C2-N1-C6	-2.06	121.34	125.11
7	B	202	GDP	O3B-PB-O1B	2.04	118.79	110.83
7	D	202	GDP	C5-C6-N1	2.00	117.89	114.07

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	907	GOL	C1-C2-C3-O3
4	A	907	GOL	O2-C2-C3-O3
4	B	206	GOL	O1-C1-C2-C3
4	A	904	GOL	O2-C2-C3-O3
4	C	707	GOL	O2-C2-C3-O3
4	A	903	GOL	O1-C1-C2-C3
4	A	904	GOL	C1-C2-C3-O3
4	A	905	GOL	C1-C2-C3-O3
4	A	906	GOL	C1-C2-C3-O3
4	C	707	GOL	C1-C2-C3-O3
4	A	903	GOL	O1-C1-C2-O2
4	B	206	GOL	O1-C1-C2-O2
4	A	906	GOL	O2-C2-C3-O3
7	D	202	GDP	O4'-C4'-C5'-O5'
7	D	202	GDP	C3'-C4'-C5'-O5'
4	A	904	GOL	O1-C1-C2-O2
4	B	206	GOL	C1-C2-C3-O3
4	A	908	GOL	O1-C1-C2-O2

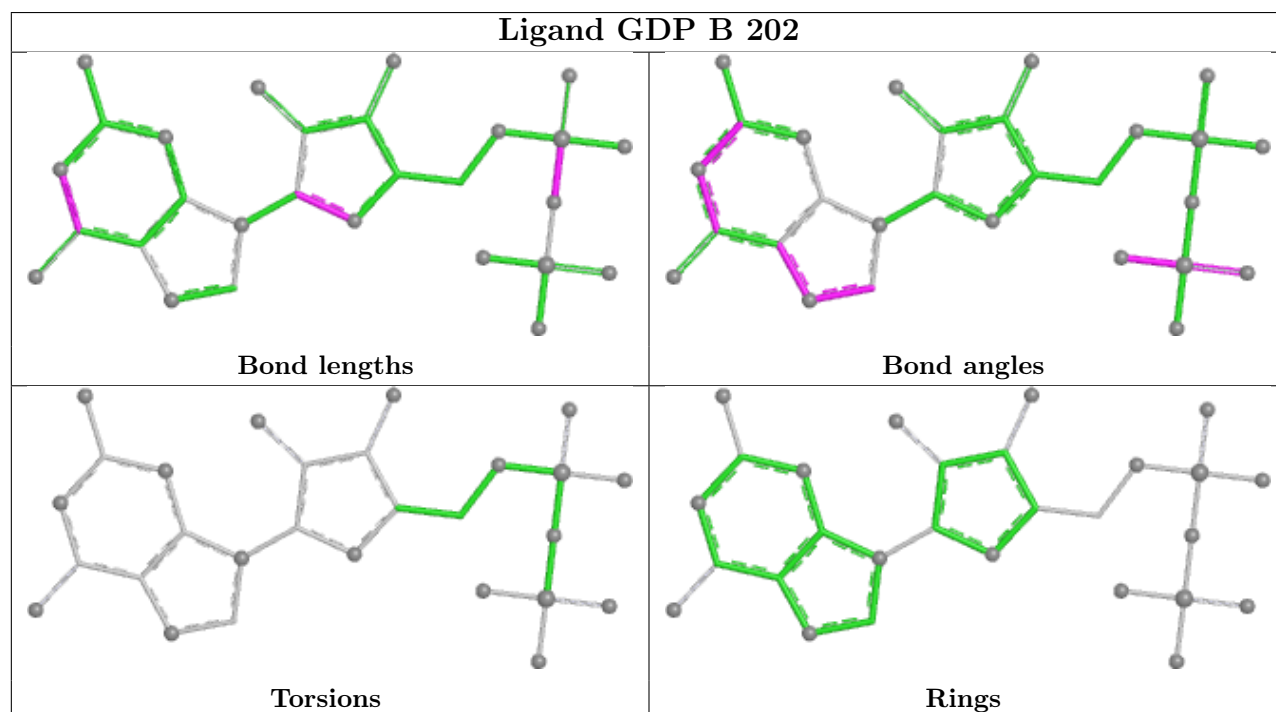
There are no ring outliers.

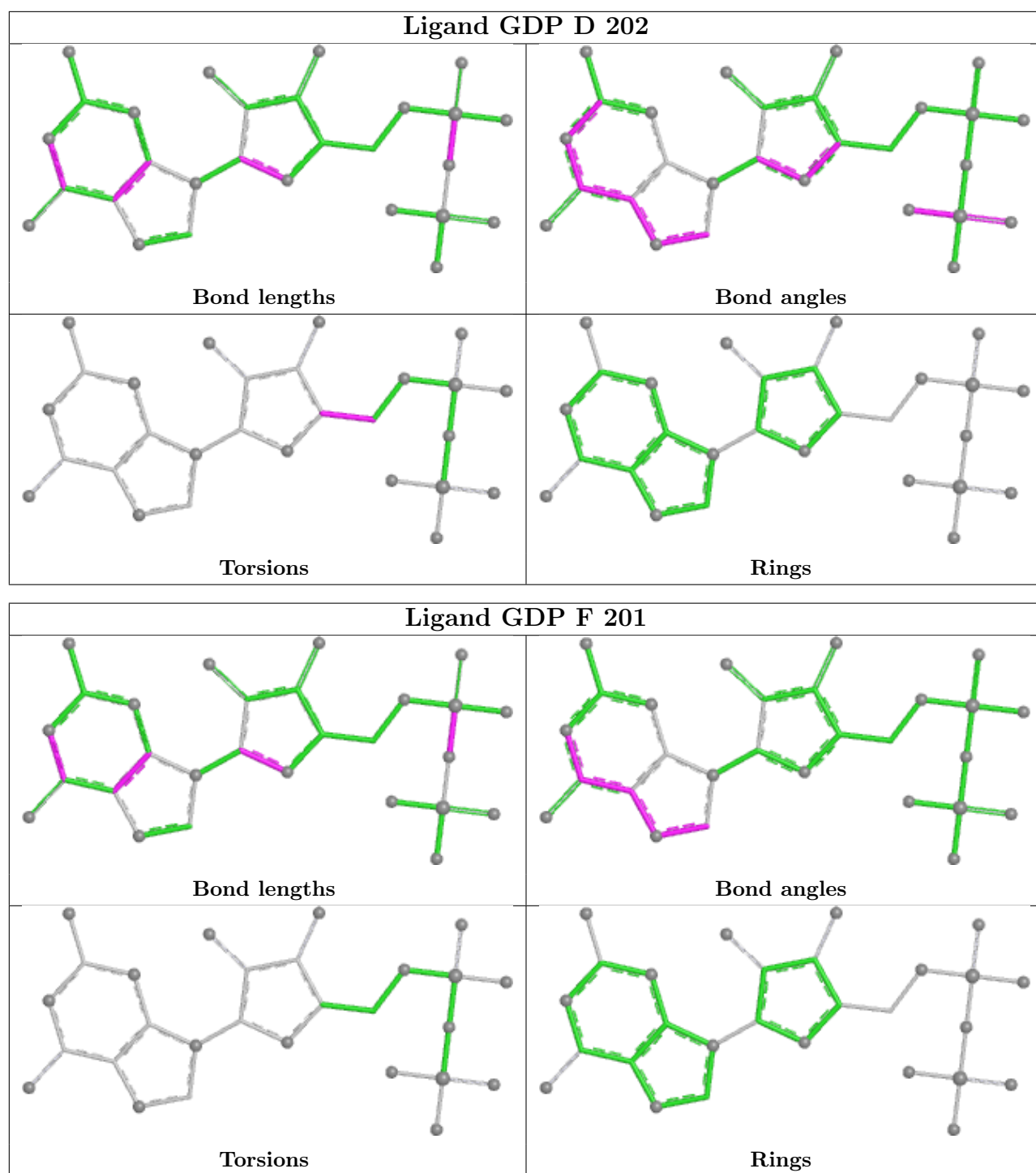
8 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	907	GOL	1	0
8	D	203	AF3	1	0
7	B	202	GDP	4	0
7	D	202	GDP	8	0
4	B	206	GOL	3	0
7	F	201	GDP	4	0
8	B	203	AF3	1	0
3	C	705	ACT	4	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	A	293/299 (97%)	-0.45	1 (0%) 90 84	15, 36, 87, 158	0
1	C	293/299 (97%)	-0.47	2 (0%) 84 73	14, 36, 76, 112	0
1	E	292/299 (97%)	1.61	94 (32%) 1 1	55, 116, 178, 213	0
2	B	167/184 (90%)	-0.32	0 100 100	17, 46, 96, 128	0
2	D	167/184 (90%)	-0.16	1 (0%) 85 76	22, 57, 100, 127	0
2	F	167/184 (90%)	1.90	68 (40%) 1 1	59, 133, 185, 213	0
All	All	1379/1449 (95%)	0.32	166 (12%) 10 7	14, 57, 162, 213	0

All (166) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	592	VAL	10.3
2	F	165	PHE	9.4
1	E	473	LEU	8.0
1	E	554	LEU	7.6
2	F	149	PRO	7.0
2	F	148	ILE	6.5
1	E	449	GLU	6.2
1	E	464	TRP	5.9
2	F	150	PHE	5.6
2	F	120	LEU	5.2
2	F	45	GLY	5.1
2	F	164	SER	5.1
2	F	53	ILE	4.8
1	E	416	GLY	4.8
1	E	452	CYS	4.7
1	E	467	ILE	4.5
1	E	588	PHE	4.5
1	E	433	PHE	4.4
2	F	68	ALA	4.3

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Mol	Chain	Res	Type	RSRZ
2	F	21	GLY	4.3
2	F	121	LEU	4.2
1	E	610	TRP	4.2
2	F	105	TRP	4.1
2	F	76	ILE	4.0
1	E	567	PRO	4.0
2	F	81	TYR	3.7
1	E	593	PHE	3.6
2	F	119	LYS	3.6
2	F	161	VAL	3.6
2	F	86	GLY	3.6
1	E	411	GLY	3.5
1	E	482	LYS	3.5
1	E	607	ILE	3.5
2	F	87	ILE	3.4
1	E	517	ILE	3.4
1	E	555	ALA	3.4
2	F	80	TYR	3.3
1	E	584	ILE	3.3
1	E	440	PHE	3.3
1	E	474	GLY	3.3
2	F	31	PHE	3.3
2	F	16	LEU	3.2
2	F	64	ILE	3.2
2	F	52	THR	3.2
2	F	66	ASP	3.1
1	E	471	LEU	3.1
1	E	472	THR	3.1
1	E	591	GLY	3.1
1	E	405	LEU	3.1
2	F	43	THR	3.1
1	E	587	ALA	3.1
1	E	469	THR	3.0
1	E	553	GLN	3.0
2	F	122	VAL	3.0
1	E	418	ALA	3.0
2	F	118	ASN	3.0
1	E	575	LEU	3.0
1	E	414	ILE	3.0
1	E	600	PRO	3.0
2	F	50	ILE	3.0
2	F	42	SER	2.9

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Mol	Chain	Res	Type	RSRZ
2	F	146	LEU	2.9
1	E	558	CYS	2.9
2	F	60	ILE	2.9
1	E	552	TYR	2.9
2	D	57	GLY	2.9
2	F	38	GLU	2.9
2	F	126	CYS	2.9
1	E	397	ASP	2.9
1	E	499	ASN	2.8
1	E	470	LEU	2.8
2	F	55	LEU	2.8
1	E	453	GLN	2.8
1	E	409	SER	2.8
1	E	614	LEU	2.8
2	F	88	ILE	2.8
2	F	70	GLN	2.8
1	E	613	LEU	2.7
2	F	35	THR	2.7
2	F	69	GLY	2.7
1	E	529	PRO	2.7
1	E	598	ASP	2.7
2	F	95	ASP	2.7
2	F	73	PHE	2.7
1	E	568	SER	2.7
1	E	425	GLU	2.7
1	E	512	LEU	2.7
2	F	127	ASP	2.7
1	E	541	ILE	2.7
2	F	29	LEU	2.6
1	E	448	PHE	2.6
1	E	496	VAL	2.6
2	F	15	LEU	2.6
1	E	556	THR	2.6
1	E	557	ILE	2.6
1	E	463	ALA	2.6
2	F	143	ALA	2.6
1	E	417	HIS	2.6
1	E	477	ILE	2.5
2	F	22	VAL	2.5
1	E	447	ALA	2.5
2	F	20	SER	2.5
1	E	490	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
2	F	28	LEU	2.5
2	F	85	HIS	2.5
2	F	129	THR	2.5
2	F	65	TRP	2.5
1	E	569	PRO	2.5
2	F	44	ILE	2.5
2	F	170	ALA	2.5
1	E	423	TYR	2.4
1	E	530	LEU	2.4
2	F	36	TYR	2.4
1	E	497	THR	2.4
2	F	17	ILE	2.4
2	F	12	PHE	2.4
1	E	450	GLY	2.4
2	F	41	ILE	2.3
2	F	89	VAL	2.3
2	F	77	THR	2.3
1	E	421	PRO	2.3
1	E	420	VAL	2.3
1	E	468	GLN	2.3
2	F	163	GLN	2.3
1	E	382	ALA	2.3
1	E	515	ALA	2.3
1	E	581	TRP	2.2
1	E	526	PHE	2.2
1	E	435	VAL	2.2
2	F	90	VAL	2.2
1	E	402	LEU	2.2
1	E	427	ILE	2.2
2	F	96	GLN	2.2
1	E	326	LEU	2.2
1	E	396	ILE	2.2
1	E	415	HIS	2.2
2	F	101	ASN	2.2
1	E	383	ILE	2.2
1	E	492	ILE	2.2
1	E	325	SER	2.2
1	E	539	TYR	2.2
1	E	358	PHE	2.1
1	E	374	PHE	2.1
1	E	403	PHE	2.1
2	F	117	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
2	F	116	ASN	2.1
1	E	356	GLU	2.1
2	F	10	TYR	2.1
1	E	506	GLN	2.1
1	E	580	PHE	2.1
1	A	530	LEU	2.1
1	E	495	ALA	2.1
2	F	59	THR	2.1
1	C	398	SER	2.1
1	E	525	SER	2.1
1	E	408	ASN	2.1
1	E	441	ASN	2.1
1	E	500	LEU	2.1
1	E	540	PRO	2.1
1	E	458	GLU	2.1
1	E	597	THR	2.0
1	C	438	ASN	2.0
2	F	169	ALA	2.0
2	F	51	ARG	2.0
1	E	346	TRP	2.0
1	E	513	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	ACT	C	706	4/4	0.61	0.23	98,100,102,103	0
3	ACT	C	704	4/4	0.66	0.21	65,75,79,79	0

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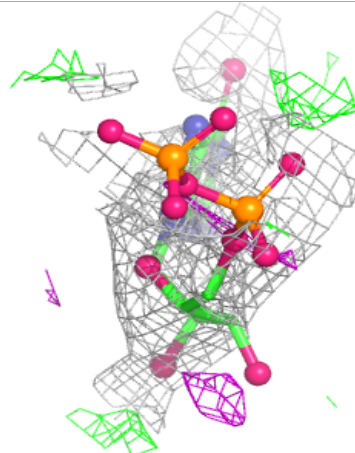
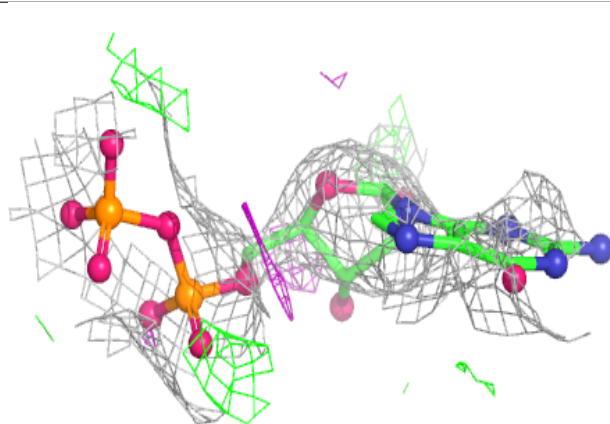
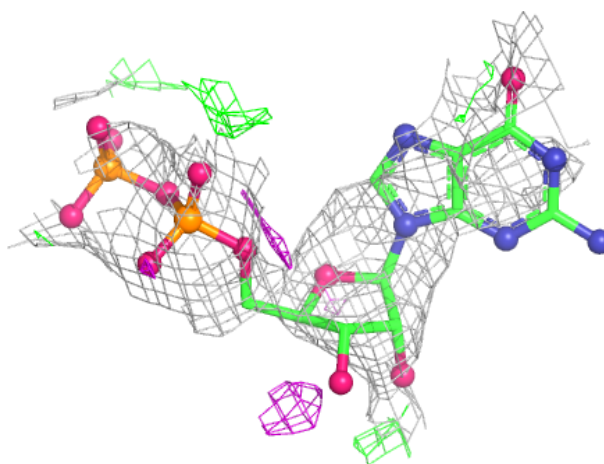
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	ACT	B	204	4/4	0.80	0.23	84,87,89,94	0
3	ACT	D	205	4/4	0.80	0.23	64,69,71,73	0
4	GOL	A	905	6/6	0.80	0.18	94,97,102,104	0
7	GDP	F	201	28/28	0.82	0.16	84,111,172,173	0
3	ACT	C	703	4/4	0.84	0.29	82,88,90,94	0
4	GOL	A	903	6/6	0.84	0.10	44,50,51,52	0
3	ACT	A	901	4/4	0.84	0.16	51,54,56,57	0
3	ACT	C	701	4/4	0.84	0.23	59,61,65,67	0
4	GOL	C	707	6/6	0.85	0.20	73,79,85,86	0
4	GOL	A	906	6/6	0.85	0.14	43,47,51,53	0
5	K	A	912	1/1	0.86	0.14	85,85,85,85	0
4	GOL	A	908	6/6	0.86	0.23	88,96,97,99	0
3	ACT	A	902	4/4	0.87	0.15	66,68,72,76	0
8	AF3	F	202	4/4	0.87	0.09	56,60,61,66	0
3	ACT	C	702	4/4	0.88	0.15	60,63,65,65	0
4	GOL	B	206	6/6	0.88	0.19	58,74,76,77	0
5	K	A	911	1/1	0.89	0.12	90,90,90,90	0
4	GOL	A	907	6/6	0.90	0.21	80,94,97,98	0
3	ACT	B	205	4/4	0.91	0.15	63,66,68,75	0
5	K	A	909	1/1	0.92	0.08	85,85,85,85	0
4	GOL	A	904	6/6	0.93	0.14	61,68,73,78	0
5	K	B	207	1/1	0.93	0.06	52,52,52,52	0
3	ACT	C	705	4/4	0.93	0.33	88,88,94,100	0
3	ACT	D	204	4/4	0.93	0.13	64,66,69,72	0
5	K	A	910	1/1	0.95	0.06	101,101,101,101	0
5	K	C	708	1/1	0.95	0.08	72,72,72,72	0
7	GDP	D	202	28/28	0.98	0.06	22,29,38,41	0
6	MG	B	201	1/1	0.98	0.05	32,32,32,32	0
8	AF3	B	203	4/4	0.98	0.06	31,32,33,33	0
7	GDP	B	202	28/28	0.98	0.06	19,32,43,47	0
6	MG	F	200	1/1	0.99	0.06	45,45,45,45	0
8	AF3	D	203	4/4	0.99	0.06	29,30,30,30	0
6	MG	D	201	1/1	0.99	0.03	36,36,36,36	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.

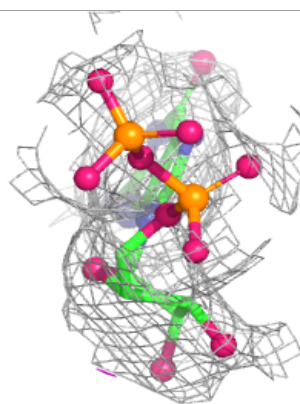
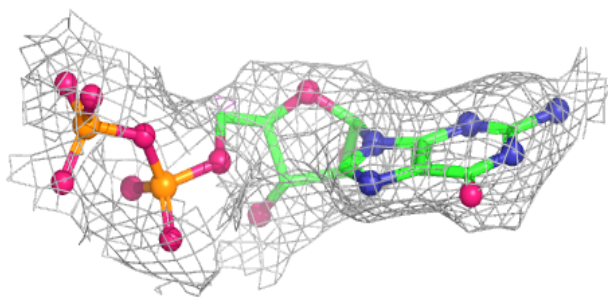
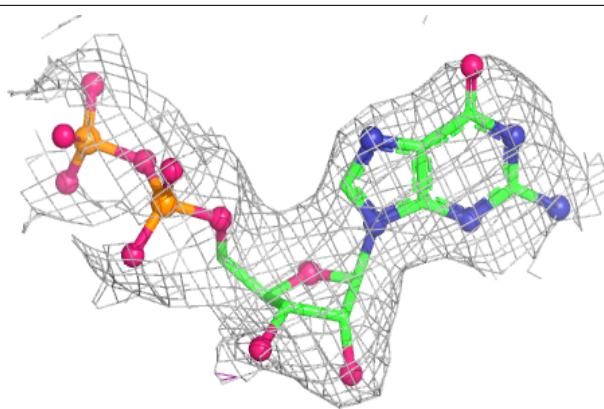
Electron density around GDP F 201:

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

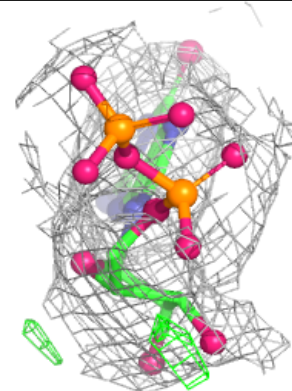
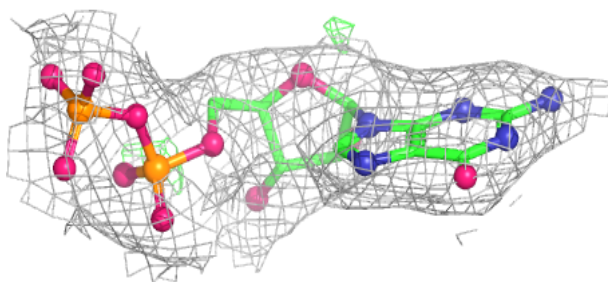
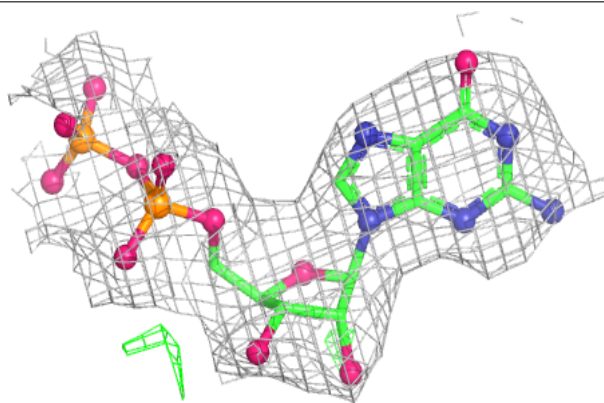


Electron density around GDP D 202:

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

**Electron density around GDP B 202:**

$2mF_o-DF_c$ (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.