



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:26 PM UTC

PDB ID : 2G1T / pdb_00002g1t
Title : A Src-like Inactive Conformation in the Abl Tyrosine Kinase Domain
Authors : Levinson, N.M.; Kuchment, O.
Deposited on : 2006-02-14
Resolution : 1.80 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

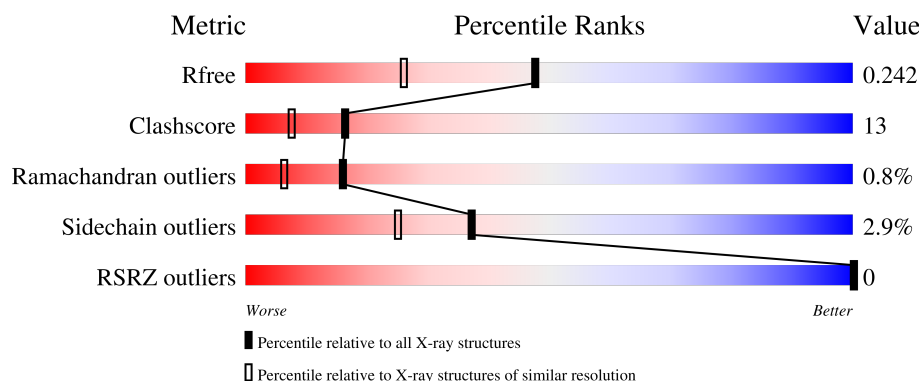
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	287	
1	B	287	
1	C	287	
1	D	287	
2	E	13	

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Mol	Chain	Length	Quality of chain
2	F	13	62%8%8%23%
2	G	13	46%8%46%
2	H	13	54%8%38%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10249 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 Proto-oncogene tyrosine-protein kinase ABL1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	271	Total	C	N	O	S	0	0	0
			2210	1424	359	410	17			
1	B	273	Total	C	N	O	S	0	0	0
			2225	1433	362	413	17			
1	C	276	Total	C	N	O	S	0	0	0
			2249	1446	364	422	17			
1	D	277	Total	C	N	O	S	0	0	0
			2253	1449	368	418	18			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	226	GLY	-	cloning artifact	UNP P00519
A	227	HIS	-	cloning artifact	UNP P00519
A	228	MET	-	cloning artifact	UNP P00519
B	226	GLY	-	cloning artifact	UNP P00519
B	227	HIS	-	cloning artifact	UNP P00519
B	228	MET	-	cloning artifact	UNP P00519
C	226	GLY	-	cloning artifact	UNP P00519
C	227	HIS	-	cloning artifact	UNP P00519
C	228	MET	-	cloning artifact	UNP P00519
D	226	GLY	-	cloning artifact	UNP P00519
D	227	HIS	-	cloning artifact	UNP P00519
D	228	MET	-	cloning artifact	UNP P00519

- Molecule 2 is a protein called ATP-Peptide Conjugate.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	8	Total	C	N	O	0	0	0
			66	44	8	14			
2	F	10	Total	C	N	O	0	0	0
			76	50	10	16			

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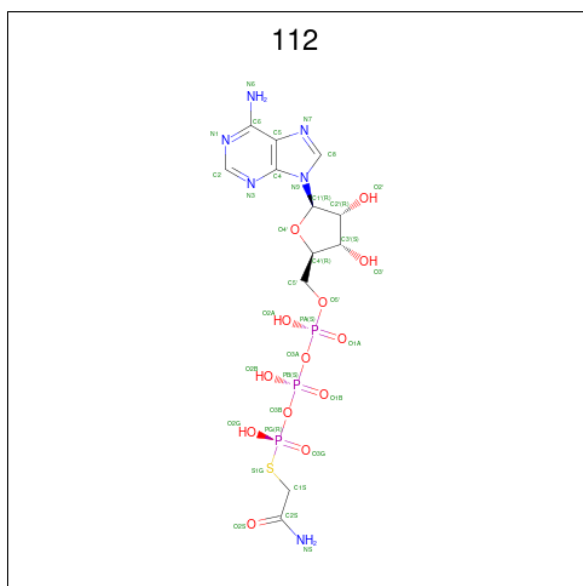
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	G	7	Total	C	N	O	0	0	0
			57	39	7	11			
2	H	8	Total	C	N	O	0	0	0
			70	46	8	16			

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		

- Molecule 4 is THIOPHOSPHORIC ACID O-((ADENOSYL-PHOSPHO)PHOSPHO)-S-AC ETAMIDYL-DIESTER (CCD ID: 112) (formula: C₁₂H₁₉N₆O₁₃P₃S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	E	1	Total	C	N	O	P	S	0	0
			35	12	6	13	3	1		
4	F	1	Total	C	N	O	P	S	0	0
			35	12	6	13	3	1		
4	G	1	Total	C	N	O	P	S	0	0
			35	12	6	13	3	1		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	H	1	Total	C	N	O	P	S	0	0
			35	12	6	13	3	1		

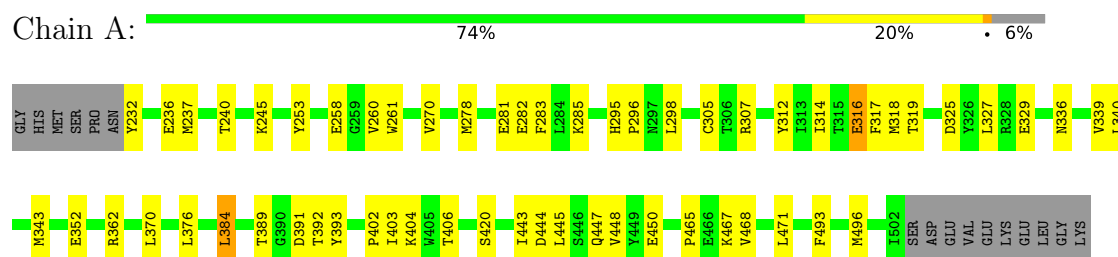
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	244	Total	O	0	0
			244	244		
5	B	197	Total	O	0	0
			197	197		
5	C	172	Total	O	0	0
			172	172		
5	D	209	Total	O	0	0
			209	209		
5	E	19	Total	O	0	0
			19	19		
5	F	29	Total	O	0	0
			29	29		
5	G	15	Total	O	0	0
			15	15		
5	H	14	Total	O	0	0
			14	14		

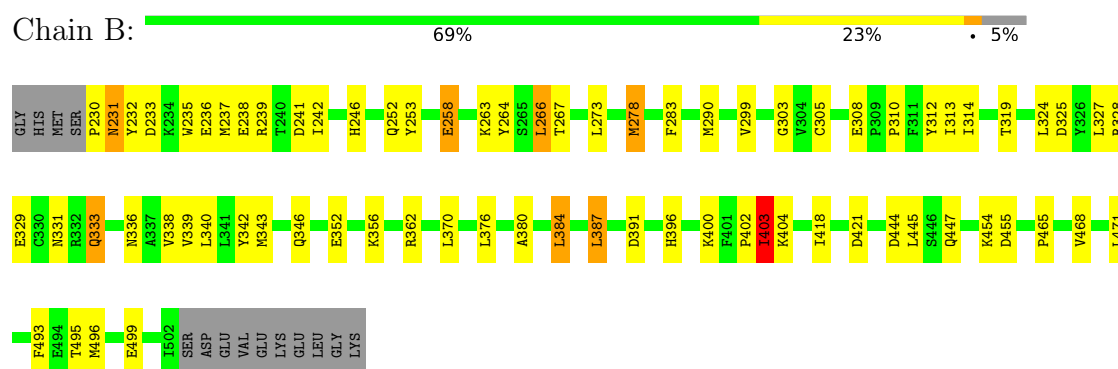
3 Residue-property plots

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.

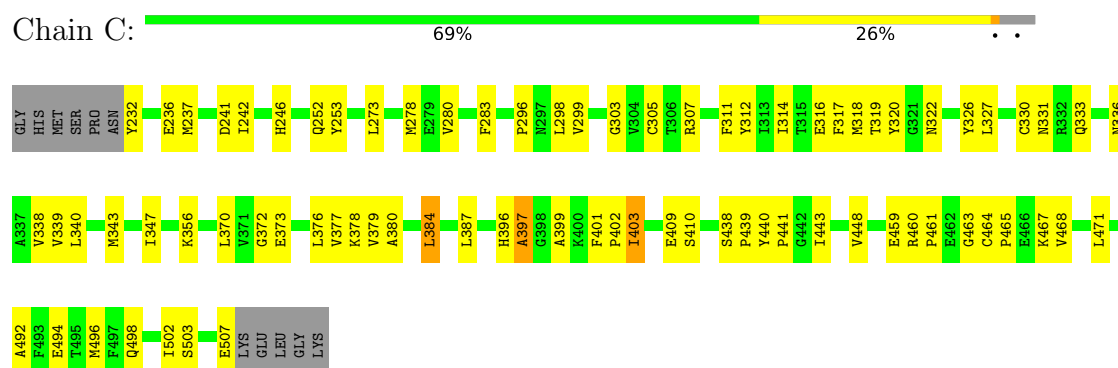
- Molecule 1: Proto-oncogene tyrosine-protein kinase ABL1



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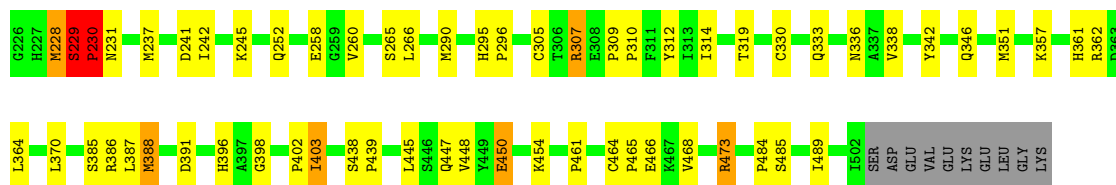


- Molecule 1: Proto-oncogene tyrosine-protein kinase ABL1



- Molecule 1: Proto-oncogene tyrosine-protein kinase ABL1

Chain D:  76% 18% ...



- Molecule 2: ATP-Peptide Conjugate

Chain E:  62% 38%

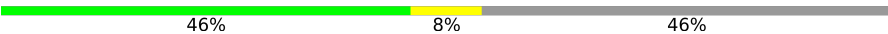


- Molecule 2: ATP-Peptide Conjugate

Chain F:  62% 8% 8% 23%



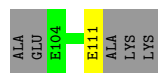
- Molecule 2: ATP-Peptide Conjugate

Chain G:  46% 8% 46%



- Molecule 2: ATP-Peptide Conjugate

Chain H:  54% 8% 38%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	62.59Å 78.44Å 141.61Å 90.00° 90.11° 90.00°	Depositor
Resolution (Å)	50.00 – 1.80 50.00 – 1.83	Depositor EDS
% Data completeness (in resolution range)	92.6 (50.00-1.80) 97.0 (50.00-1.83)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 1.83Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.219 , 0.244 0.214 , 0.242	Depositor DCC
R_{free} test set	11279 reflections (9.30%)	wwPDB-VP
Wilson B-factor (Å ²)	21.8	Xtriage
Anisotropy	0.824	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 31.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.084 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10249	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.08% 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: MG, 112

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	0.38	0/2267	0.92	9/3068 (0.3%)
1	B	0.38	1/2283 (0.0%)	0.90	5/3090 (0.2%)
1	C	0.36	0/2306	0.87	4/3121 (0.1%)
1	D	0.41	0/2312	0.89	8/3129 (0.3%)
2	E	0.40	0/67	0.76	0/88
2	F	0.38	0/77	0.77	0/102
2	G	0.35	0/58	0.95	0/76
2	H	0.34	0/71	0.67	0/93
All	All	0.38	1/9441 (0.0%)	0.89	26/12767 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	278	MET	SD-CE	-5.33	1.66	1.79

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	402	PRO	N-CA-C	-8.68	94.47	112.36
1	B	402	PRO	N-CA-C	-8.52	94.81	112.36
1	A	319	THR	N-CA-C	7.56	121.43	111.75
1	A	448	VAL	N-CA-C	7.46	117.54	110.30
1	C	319	THR	N-CA-C	7.32	121.12	111.75
1	B	319	THR	N-CA-C	7.06	120.79	111.75
1	D	229	SER	N-CA-C	7.02	125.33	109.81
1	C	402	PRO	N-CA-C	-6.83	98.28	112.36
1	D	319	THR	N-CA-C	6.53	120.34	112.38
1	D	333	GLN	N-CA-C	-6.16	104.11	111.69
1	A	403	ILE	N-CA-C	6.10	122.02	109.34
1	B	403	ILE	N-CA-C	6.06	121.94	109.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	448	VAL	N-CA-C	6.00	116.17	110.53
1	B	333	GLN	N-CA-C	-5.88	104.95	111.36
1	D	258	GLU	N-CA-C	-5.78	101.07	110.20
1	A	258	GLU	N-CA-C	-5.65	101.27	110.20
1	D	330	CYS	N-CA-C	5.63	117.33	110.41
1	D	403	ILE	N-CA-C	5.56	120.91	109.34
1	A	389	THR	N-CA-C	-5.39	104.95	112.45
1	D	402	PRO	N-CA-C	-5.27	97.36	113.27
1	C	403	ILE	N-CA-C	5.26	120.28	109.34
1	A	406	THR	N-CA-C	5.21	117.24	108.96
1	D	448	VAL	N-CA-C	5.15	115.36	110.42
1	B	258	GLU	N-CA-C	-5.10	102.15	110.20
1	A	420	SER	N-CA-C	-5.07	105.94	111.82
1	A	352	GLU	N-CA-C	-5.05	105.77	111.28

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	2210	0	2163	36	0
1	B	2225	0	2177	72	0
1	C	2249	0	2193	79	0
1	D	2253	0	2200	53	0
2	E	66	0	54	0	0
2	F	76	0	58	3	0
2	G	57	0	45	1	0
2	H	70	0	55	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	E	35	0	14	0	0
4	F	35	0	14	0	0
4	G	35	0	14	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	35	0	15	1	0
5	A	244	0	0	3	0
5	B	197	0	0	2	0
5	C	172	0	0	1	0
5	D	209	0	0	3	0
5	E	19	0	0	0	0
5	F	29	0	0	0	0
5	G	15	0	0	0	0
5	H	14	0	0	1	0
All	All	10249	0	9002	239	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 13.

All (239) 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:D:307:ARG:HH11	1:D:307:ARG:HB2	1.08	1.15
1:C:471:LEU:HD11	1:C:496:MET:HE1	1.42	1.01
1:D:473:ARG:HH11	1:D:473:ARG:HB3	1.33	0.94
1:C:316:GLU:HG3	1:C:318:MET:HE3	1.50	0.94
1:D:307:ARG:HH11	1:D:307:ARG:CB	1.87	0.86
1:D:484:PRO:HG2	1:D:489:ILE:HD11	1.58	0.86
1:D:307:ARG:HB2	1:D:307:ARG:NH1	1.93	0.84
1:B:327:LEU:HD21	1:B:343:MET:HE1	1.60	0.84
1:A:340:LEU:HA	1:A:343:MET:HE2	1.60	0.83
1:C:237:MET:HE1	1:C:314:ILE:HB	1.60	0.83
1:A:316:GLU:HG3	1:A:318:MET:HE3	1.60	0.82
1:D:237:MET:HE2	1:D:242:ILE:HD11	1.63	0.80
1:A:404:LYS:HE3	1:A:445:LEU:HD23	1.65	0.78
1:C:317:PHE:O	1:C:318:MET:HE2	1.85	0.77
1:A:316:GLU:CG	1:A:318:MET:HE3	2.15	0.74
1:B:278:MET:CE	1:B:283:PHE:HD1	1.99	0.74
1:C:327:LEU:HD21	1:C:343:MET:HE1	1.69	0.74
1:C:278:MET:CE	1:C:283:PHE:HD1	2.03	0.72
1:C:237:MET:HE2	1:C:303:GLY:HA3	1.72	0.71
1:B:324:LEU:O	1:B:328:ARG:HG2	1.89	0.71
1:D:229:SER:O	1:D:230:PRO:C	2.31	0.70
1:B:273:LEU:HD13	1:B:313:ILE:HD13	1.74	0.69
1:B:237:MET:HE1	1:B:314:ILE:HB	1.73	0.69
1:C:278:MET:HE1	1:C:283:PHE:HD1	1.57	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:278:MET:HE3	1:C:283:PHE:HB2	1.74	0.68
1:D:336:ASN:OD1	1:D:338:VAL:HG12	1.93	0.68
1:B:237:MET:HE2	1:B:303:GLY:HA3	1.75	0.68
1:D:484:PRO:CG	1:D:489:ILE:HD11	2.24	0.68
1:B:312:TYR:C	1:B:313:ILE:HD12	2.20	0.67
1:A:447:GLN:HG2	1:C:459:GLU:OE2	1.95	0.67
1:C:237:MET:HE1	1:C:314:ILE:CB	2.24	0.67
1:A:443:ILE:HD13	1:C:441:PRO:O	1.95	0.67
1:C:336:ASN:OD1	1:C:339:VAL:HG23	1.96	0.66
1:D:445:LEU:HD12	1:D:445:LEU:H	1.60	0.65
1:C:237:MET:HE2	1:C:303:GLY:C	2.21	0.65
1:C:340:LEU:HA	1:C:343:MET:HE2	1.77	0.65
1:D:485:SER:O	1:D:489:ILE:HD13	1.96	0.64
1:D:473:ARG:HB3	1:D:473:ARG:NH1	2.11	0.64
1:A:327:LEU:HD21	1:A:343:MET:HE1	1.78	0.64
1:A:318:MET:HE2	1:A:318:MET:HA	1.78	0.64
1:B:305:CYS:HB2	1:B:312:TYR:HB2	1.79	0.64
1:A:391:ASP:O	1:A:391:ASP:OD1	2.16	0.63
1:B:238:GLU:HB2	1:B:241:ASP:OD1	1.98	0.63
1:A:317:PHE:O	1:A:318:MET:HE2	1.97	0.63
1:B:352:GLU:O	1:B:356:LYS:HG3	1.98	0.63
5:A:1691:HOH:O	1:D:228:MET:HG3	1.99	0.63
1:C:376:LEU:HD11	1:C:378:LYS:HG3	1.80	0.62
1:D:242:ILE:N	1:D:242:ILE:HD12	2.14	0.62
1:C:237:MET:HE2	1:C:303:GLY:CA	2.29	0.62
1:C:336:ASN:OD1	1:C:338:VAL:HG12	2.01	0.61
1:D:245:LYS:HE3	1:D:260:VAL:CG2	2.31	0.61
1:D:461:PRO:HG2	1:D:464:CYS:HB2	1.83	0.61
1:C:252:GLN:HG3	2:G:107:PHE:CZ	2.36	0.60
1:C:336:ASN:CG	1:C:338:VAL:HG12	2.25	0.60
1:B:230:PRO:O	1:B:231:ASN:HB3	2.02	0.59
1:B:242:ILE:N	1:B:242:ILE:HD12	2.15	0.59
1:B:278:MET:HE3	1:B:283:PHE:HD1	1.66	0.59
1:C:305:CYS:HB2	1:C:312:TYR:HB2	1.85	0.59
1:C:443:ILE:N	1:C:443:ILE:HD12	2.17	0.59
1:A:232:TYR:HB2	1:A:236:GLU:OE2	2.03	0.58
1:D:237:MET:CE	1:D:242:ILE:HD11	2.33	0.58
1:A:305:CYS:HB2	1:A:312:TYR:HB2	1.86	0.58
1:C:237:MET:HE1	1:C:314:ILE:CG1	2.34	0.57
1:D:245:LYS:HE3	1:D:260:VAL:HG23	1.85	0.57
1:B:278:MET:HE3	1:B:283:PHE:CD1	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:495:THR:O	1:B:499:GLU:HG2	2.04	0.57
1:B:444:ASP:HB3	1:B:447:GLN:HE21	1.70	0.57
1:B:493:PHE:HA	1:B:496:MET:HE3	1.86	0.57
1:B:471:LEU:HD12	1:B:496:MET:HE1	1.86	0.57
1:B:313:ILE:HD12	1:B:313:ILE:N	2.19	0.56
1:C:465:PRO:HG2	1:C:468:VAL:CG2	2.35	0.56
1:C:278:MET:HE1	1:C:387:LEU:O	2.06	0.56
1:A:278:MET:HE2	1:A:283:PHE:N	2.21	0.56
1:B:314:ILE:N	1:B:314:ILE:HD12	2.20	0.56
1:C:347:ILE:HD11	1:C:377:VAL:CG1	2.36	0.56
1:D:362:ARG:HD3	1:D:385:SER:OG	2.06	0.56
1:B:339:VAL:O	1:B:343:MET:HG3	2.05	0.56
1:C:326:TYR:O	1:C:330:CYS:HB3	2.06	0.56
1:B:237:MET:HE2	1:B:303:GLY:CA	2.36	0.55
1:C:242:ILE:HD12	1:C:242:ILE:N	2.20	0.55
1:B:278:MET:HE3	1:B:283:PHE:HB2	1.87	0.55
1:D:314:ILE:N	1:D:314:ILE:HD12	2.20	0.55
1:C:299:VAL:HG21	1:C:380:ALA:HB2	1.88	0.55
1:C:376:LEU:HD13	1:C:376:LEU:C	2.32	0.55
1:C:331:ASN:OD1	1:C:333:GLN:HB2	2.07	0.54
1:D:229:SER:O	1:D:231:ASN:N	2.40	0.54
1:C:307:ARG:HG3	1:C:307:ARG:HH11	1.72	0.54
1:B:231:ASN:C	1:B:231:ASN:HD22	2.15	0.54
1:B:237:MET:CE	1:B:314:ILE:HD13	2.37	0.54
1:B:325:ASP:HB3	1:B:329:GLU:OE2	2.07	0.54
1:B:263:LYS:HE3	1:B:264:TYR:CZ	2.43	0.54
1:A:325:ASP:O	1:A:329:GLU:HG3	2.07	0.53
1:C:322:ASN:HA	1:C:370:LEU:HD23	1.89	0.53
1:C:347:ILE:HD11	1:C:377:VAL:HG11	1.91	0.53
1:C:503:SER:O	1:C:507:GLU:HG3	2.08	0.53
1:B:273:LEU:CD1	1:B:313:ILE:HD13	2.39	0.53
1:C:314:ILE:HD12	1:C:314:ILE:N	2.24	0.53
1:C:343:MET:O	1:C:347:ILE:HG12	2.09	0.53
1:A:237:MET:HE2	1:A:261:TRP:CZ2	2.43	0.53
1:B:239:ARG:HG3	1:B:239:ARG:HH11	1.74	0.53
1:B:237:MET:HE2	1:B:303:GLY:C	2.34	0.53
1:B:237:MET:HE1	1:B:314:ILE:CB	2.39	0.52
1:D:252:GLN:HG2	5:H:1413:HOH:O	2.09	0.52
1:B:396:HIS:NE2	2:F:109:GLU:HG3	2.24	0.52
1:B:278:MET:HE3	1:B:283:PHE:CB	2.39	0.52
1:A:278:MET:HE3	1:A:282:GLU:HG2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:447:GLN:HA	1:D:447:GLN:NE2	2.25	0.51
1:C:340:LEU:HD23	1:C:343:MET:HE2	1.92	0.51
1:B:336:ASN:OD1	1:B:338:VAL:HG12	2.11	0.51
1:A:465:PRO:HG2	1:A:468:VAL:CG2	2.41	0.50
1:B:241:ASP:HB2	1:B:242:ILE:HD12	1.93	0.50
1:B:336:ASN:OD1	1:B:339:VAL:HG23	2.12	0.50
1:C:356:LYS:HE2	5:C:1763:HOH:O	2.11	0.50
1:B:253:TYR:CD2	1:B:384:LEU:HD13	2.47	0.50
1:C:317:PHE:C	1:C:318:MET:HE2	2.36	0.49
1:C:336:ASN:ND2	1:C:338:VAL:HG12	2.27	0.49
1:D:357:LYS:HE3	5:D:1950:HOH:O	2.12	0.49
1:C:461:PRO:HG2	1:C:464:CYS:HB2	1.93	0.49
1:B:331:ASN:OD1	1:B:333:GLN:HB2	2.13	0.49
1:C:278:MET:CE	1:C:283:PHE:CD1	2.92	0.49
1:D:241:ASP:C	1:D:242:ILE:HD12	2.38	0.49
1:C:237:MET:CE	1:C:314:ILE:HD13	2.42	0.48
1:D:447:GLN:HA	1:D:447:GLN:HE21	1.78	0.48
1:D:473:ARG:HH11	1:D:473:ARG:CB	2.16	0.48
1:B:266:LEU:HD22	1:B:267:THR:O	2.13	0.48
1:C:494:GLU:O	1:C:498:GLN:HG3	2.13	0.48
1:D:450:GLU:O	1:D:454:LYS:HG2	2.12	0.48
1:B:230:PRO:HB3	1:B:232:TYR:CE2	2.49	0.48
1:C:280:VAL:HG22	1:C:311:PHE:CZ	2.49	0.48
1:D:445:LEU:H	1:D:445:LEU:CD1	2.26	0.48
1:C:241:ASP:C	1:C:242:ILE:HD12	2.38	0.48
1:C:298:LEU:HD23	1:C:379:VAL:HB	1.95	0.47
1:A:340:LEU:HD23	1:A:343:MET:HE2	1.97	0.47
1:B:278:MET:HE1	1:B:387:LEU:HA	1.97	0.47
1:B:356:LYS:HE2	5:B:1797:HOH:O	2.14	0.47
1:C:278:MET:HE3	1:C:283:PHE:CD1	2.50	0.47
1:C:439:PRO:O	1:C:440:TYR:C	2.58	0.47
1:D:241:ASP:HB2	1:D:242:ILE:HD12	1.96	0.46
1:D:351:MET:HE2	1:D:364:LEU:HD22	1.96	0.46
1:B:471:LEU:CD1	1:B:496:MET:HE1	2.45	0.46
1:D:307:ARG:HH11	1:D:307:ARG:CG	2.28	0.46
1:D:450:GLU:OE1	1:D:450:GLU:HA	2.15	0.46
1:B:340:LEU:HD23	1:B:343:MET:HE2	1.96	0.46
1:B:299:VAL:HG21	1:B:380:ALA:HB2	1.97	0.46
1:B:352:GLU:HG2	1:B:356:LYS:HE3	1.97	0.46
1:C:441:PRO:O	1:C:443:ILE:HD12	2.15	0.46
1:D:362:ARG:NH1	5:D:1839:HOH:O	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:263:LYS:HE3	1:B:264:TYR:CE1	2.50	0.46
1:B:340:LEU:HA	1:B:343:MET:HE2	1.98	0.46
1:B:454:LYS:O	1:B:455:ASP:HB2	2.14	0.46
1:A:467:LYS:HD2	1:A:467:LYS:N	2.31	0.45
1:A:392:THR:HG22	1:A:393:TYR:CE2	2.51	0.45
1:C:299:VAL:HG13	1:C:316:GLU:HG2	1.98	0.45
1:C:399:ALA:HB3	1:C:401:PHE:CZ	2.51	0.45
1:C:241:ASP:HB2	1:C:242:ILE:HD12	1.99	0.45
1:B:237:MET:HE3	1:B:314:ILE:HD13	1.98	0.45
1:A:281:GLU:O	1:A:285:LYS:HG3	2.17	0.45
1:B:465:PRO:HG2	1:B:468:VAL:CG2	2.46	0.45
1:C:336:ASN:OD1	1:C:338:VAL:CG1	2.64	0.45
1:A:339:VAL:O	1:A:343:MET:HG3	2.17	0.45
1:D:228:MET:HB2	5:D:1987:HOH:O	2.15	0.45
1:D:229:SER:HB2	1:D:230:PRO:HD3	1.98	0.45
1:A:336:ASN:OD1	1:A:339:VAL:HG23	2.17	0.44
1:B:231:ASN:C	1:B:231:ASN:ND2	2.75	0.44
1:B:252:GLN:HG3	2:F:107:PHE:CZ	2.52	0.44
1:C:278:MET:CE	1:C:387:LEU:O	2.65	0.44
1:C:409:GLU:HG2	1:C:410:SER:N	2.33	0.44
4:H:1401:112:H8	4:H:1401:112:H5'2	2.00	0.44
1:A:253:TYR:CD1	1:A:384:LEU:HD13	2.53	0.44
1:C:316:GLU:OE2	1:C:318:MET:HE1	2.18	0.44
1:A:295:HIS:CG	1:A:296:PRO:HD2	2.53	0.44
1:B:237:MET:HE1	1:B:314:ILE:CG1	2.48	0.44
1:D:229:SER:O	1:D:231:ASN:CG	2.61	0.44
1:D:290:MET:SD	1:D:387:LEU:HD11	2.58	0.44
1:B:237:MET:HE1	1:B:314:ILE:HD13	2.00	0.44
1:C:253:TYR:CD1	1:C:384:LEU:HD13	2.53	0.43
1:A:240:THR:HG23	5:A:1663:HOH:O	2.17	0.43
1:C:232:TYR:O	1:C:236:GLU:HG3	2.18	0.43
1:C:376:LEU:HD13	1:C:377:VAL:N	2.33	0.43
1:A:245:LYS:HE3	1:A:260:VAL:HG23	1.99	0.43
1:C:376:LEU:CD1	1:C:378:LYS:HG3	2.47	0.43
1:D:229:SER:O	1:D:231:ASN:ND2	2.51	0.43
1:D:447:GLN:HE21	1:D:447:GLN:CA	2.32	0.43
1:A:444:ASP:HB2	1:A:447:GLN:HG3	2.00	0.43
1:B:231:ASN:ND2	1:B:233:ASP:OD2	2.51	0.43
1:A:232:TYR:O	1:A:236:GLU:HG3	2.18	0.43
1:D:305:CYS:HB2	1:D:312:TYR:HB2	2.01	0.43
1:B:246:HIS:HE1	1:B:258:GLU:OE2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:342:TYR:O	1:B:346:GLN:HG3	2.19	0.43
1:C:467:LYS:HD3	1:C:496:MET:HG2	2.00	0.43
1:D:245:LYS:HE3	1:D:260:VAL:HG21	2.00	0.43
1:C:320:TYR:HD2	1:C:372:GLY:O	2.02	0.42
1:C:460:ARG:HD2	1:C:464:CYS:O	2.19	0.42
1:A:270:VAL:HG22	1:A:314:ILE:HD12	2.00	0.42
1:A:493:PHE:HA	1:A:496:MET:HE3	2.00	0.42
1:C:396:HIS:O	1:C:397:ALA:C	2.62	0.42
1:B:232:TYR:O	1:B:236:GLU:HG3	2.19	0.42
1:C:307:ARG:HG3	1:C:307:ARG:NH1	2.34	0.42
1:B:239:ARG:HG3	1:B:239:ARG:NH1	2.34	0.42
1:B:239:ARG:NH2	1:B:308:GLU:O	2.52	0.42
1:B:404:LYS:HE3	1:B:445:LEU:HD23	2.00	0.42
1:D:398:GLY:CA	2:H:111:GLU:HA	2.50	0.42
1:A:278:MET:HE2	1:A:282:GLU:C	2.45	0.42
1:C:440:TYR:C	1:C:443:ILE:HD13	2.45	0.42
1:C:492:ALA:O	1:C:496:MET:HE3	2.19	0.42
1:D:445:LEU:HD12	1:D:445:LEU:N	2.29	0.42
1:A:316:GLU:HG3	1:A:318:MET:CE	2.41	0.42
1:D:342:TYR:O	1:D:346:GLN:HG3	2.20	0.42
1:B:273:LEU:HD22	1:B:313:ILE:HD11	2.02	0.42
1:B:403:ILE:HB	1:B:445:LEU:HD22	2.02	0.41
1:C:438:SER:HA	1:C:439:PRO:HD3	1.88	0.41
1:C:465:PRO:HG2	1:C:468:VAL:HG23	2.01	0.41
1:B:239:ARG:NH2	1:B:310:PRO:O	2.53	0.41
1:D:229:SER:HB2	1:D:230:PRO:CD	2.50	0.41
1:B:313:ILE:N	1:B:313:ILE:CD1	2.84	0.41
1:B:313:ILE:C	1:B:314:ILE:HD12	2.46	0.41
1:C:498:GLN:O	1:C:502:ILE:HG12	2.20	0.41
1:D:465:PRO:HG2	1:D:468:VAL:CG2	2.50	0.41
1:C:296:PRO:O	1:C:378:LYS:HE2	2.19	0.41
1:D:387:LEU:C	1:D:388:MET:HG2	2.45	0.41
1:D:295:HIS:CG	1:D:296:PRO:HD2	2.55	0.41
1:A:307:ARG:HE	1:A:307:ARG:HB2	1.73	0.41
1:B:235:TRP:HB2	1:B:303:GLY:HA2	2.03	0.41
1:C:278:MET:HE3	1:C:283:PHE:CB	2.48	0.41
1:A:295:HIS:HB3	1:A:298:LEU:HD12	2.02	0.41
1:A:450:GLU:HG2	5:A:1715:HOH:O	2.21	0.41
1:C:318:MET:HE2	1:C:318:MET:HA	2.03	0.41
1:D:336:ASN:OD1	1:D:338:VAL:CG1	2.64	0.41
1:D:438:SER:HA	1:D:439:PRO:HD3	1.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:232:TYR:HB3	1:B:235:TRP:CE2	2.56	0.41
1:C:232:TYR:HB2	1:C:236:GLU:CD	2.45	0.41
1:D:361:HIS:O	1:D:362:ARG:CB	2.69	0.40
1:C:246:HIS:CD2	1:C:246:HIS:H	2.39	0.40
1:B:418:ILE:O	1:B:421:ASP:HB2	2.21	0.40
1:C:347:ILE:HD11	1:C:377:VAL:HG12	2.03	0.40
1:D:309:PRO:HA	1:D:310:PRO:C	2.46	0.40
1:B:290:MET:HE3	5:B:1710:HOH:O	2.22	0.40
1:B:400:LYS:HA	2:F:109:GLU:HA	2.03	0.40
1:C:468:VAL:O	1:C:471:LEU:HB2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	269/287 (94%)	260 (97%)	9 (3%)	0	100	100
1	B	271/287 (94%)	261 (96%)	8 (3%)	2 (1%)	18	8
1	C	274/287 (96%)	265 (97%)	6 (2%)	3 (1%)	11	3
1	D	275/287 (96%)	262 (95%)	9 (3%)	4 (2%)	8	2
2	E	6/13 (46%)	6 (100%)	0	0	100	100
2	F	8/13 (62%)	8 (100%)	0	0	100	100
2	G	5/13 (38%)	5 (100%)	0	0	100	100
2	H	6/13 (46%)	6 (100%)	0	0	100	100
All	All	1114/1200 (93%)	1073 (96%)	32 (3%)	9 (1%)	16	6

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	397	ALA
1	D	229	SER
1	B	231	ASN
1	D	228	MET
1	D	230	PRO
1	C	403	ILE
1	B	403	ILE
1	D	403	ILE
1	C	463	GLY

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	237/251 (94%)	231 (98%)	6 (2%)	42	30
1	B	239/251 (95%)	232 (97%)	7 (3%)	37	25
1	C	242/251 (96%)	239 (99%)	3 (1%)	63	57
1	D	242/251 (96%)	230 (95%)	12 (5%)	22	10
2	E	6/10 (60%)	6 (100%)	0	100	100
2	F	6/10 (60%)	5 (83%)	1 (17%)	2	0
2	G	5/10 (50%)	5 (100%)	0	100	100
2	H	7/10 (70%)	7 (100%)	0	100	100
All	All	984/1044 (94%)	955 (97%)	29 (3%)	37	25

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	316	GLU
1	A	362	ARG
1	A	370	LEU
1	A	376	LEU
1	A	384	LEU
1	A	471	LEU
1	B	266	LEU

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Mol	Chain	Res	Type
1	B	362	ARG
1	B	370	LEU
1	B	376	LEU
1	B	384	LEU
1	B	387	LEU
1	B	391	ASP
1	C	273	LEU
1	C	373	GLU
1	C	384	LEU
1	D	230	PRO
1	D	265	SER
1	D	266	LEU
1	D	307	ARG
1	D	370	LEU
1	D	386	ARG
1	D	388	MET
1	D	391	ASP
1	D	396	HIS
1	D	450	GLU
1	D	466	GLU
1	D	473	ARG
2	F	109	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	491	GLN
1	B	231	ASN
1	B	246	HIS
1	B	300	GLN
1	B	358	ASN
1	B	375	HIS
1	B	447	GLN
1	C	358	ASN
1	C	447	GLN
1	D	375	HIS
1	D	447	GLN

5.3.3 RNA ⓘ

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 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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
4	112	H	1401	2,3	34,37,37	3.74	13 (38%)	46,57,57	1.83	16 (34%)
4	112	E	1101	2,3	34,37,37	3.92	14 (41%)	46,57,57	1.78	17 (36%)
4	112	G	1301	2,3	34,37,37	3.84	13 (38%)	46,57,57	1.82	17 (36%)
4	112	F	1201	2,3	34,37,37	3.83	13 (38%)	46,57,57	1.73	17 (36%)

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	112	H	1401	2,3	-	0/23/44/44	0/3/3/3
4	112	E	1101	2,3	-	0/23/44/44	0/3/3/3
4	112	G	1301	2,3	-	0/23/44/44	0/3/3/3
4	112	F	1201	2,3	-	0/23/44/44	0/3/3/3

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	1101	112	C1S-S1G	-15.77	1.64	1.84
4	F	1201	112	C1S-S1G	-15.52	1.65	1.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	1301	112	C1S-S1G	-15.43	1.65	1.84
4	H	1401	112	C1S-S1G	-14.37	1.66	1.84
4	G	1301	112	PA-O3A	9.08	1.69	1.59
4	F	1201	112	PA-O3A	8.99	1.69	1.59
4	H	1401	112	PB-O3A	-8.44	1.50	1.59
4	E	1101	112	PB-O3A	-8.12	1.50	1.59
4	E	1101	112	PA-O3A	7.95	1.68	1.59
4	H	1401	112	PA-O3A	7.77	1.67	1.59
4	F	1201	112	PB-O3A	-6.56	1.52	1.59
4	G	1301	112	PB-O3A	-6.46	1.52	1.59
4	E	1101	112	C4-N3	4.89	1.43	1.34
4	H	1401	112	C4-N3	4.71	1.43	1.34
4	G	1301	112	C4-N3	4.40	1.42	1.34
4	F	1201	112	C4-N3	4.34	1.42	1.34
4	G	1301	112	PG-O2G	-4.33	1.45	1.56
4	E	1101	112	PG-O2G	-4.32	1.45	1.56
4	F	1201	112	PG-O2G	-4.21	1.46	1.56
4	E	1101	112	PB-O3B	-4.14	1.55	1.59
4	G	1301	112	C6-N6	4.04	1.44	1.34
4	H	1401	112	PG-O2G	-4.03	1.46	1.56
4	G	1301	112	C5-C4	3.94	1.46	1.39
4	F	1201	112	C6-N6	3.92	1.44	1.34
4	F	1201	112	PB-O3B	-3.89	1.55	1.59
4	E	1101	112	C5-C4	3.84	1.45	1.39
4	F	1201	112	C5-C4	3.82	1.45	1.39
4	H	1401	112	C5-C4	3.64	1.45	1.39
4	E	1101	112	C6-N6	3.61	1.43	1.34
4	H	1401	112	C6-N6	3.57	1.43	1.34
4	H	1401	112	C2-N1	3.48	1.40	1.33
4	H	1401	112	PB-O3B	-3.36	1.55	1.59
4	G	1301	112	C2-N1	3.34	1.39	1.33
4	E	1101	112	C2-N1	3.31	1.39	1.33
4	F	1201	112	C2-N1	3.04	1.39	1.33
4	H	1401	112	C8-N9	2.93	1.42	1.37
4	G	1301	112	C2-N3	2.77	1.38	1.33
4	G	1301	112	PB-O3B	-2.76	1.56	1.59
4	H	1401	112	O5'-C5'	-2.72	1.34	1.44
4	G	1301	112	C8-N9	2.66	1.42	1.37
4	E	1101	112	C8-N9	2.61	1.42	1.37
4	G	1301	112	C1'-N9	2.56	1.53	1.46
4	F	1201	112	O5'-C5'	-2.53	1.35	1.44
4	G	1301	112	O5'-C5'	-2.53	1.35	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	1101	112	O5'-C5'	-2.51	1.35	1.44
4	H	1401	112	C1'-N9	2.44	1.53	1.46
4	E	1101	112	C1'-N9	2.41	1.53	1.46
4	F	1201	112	C1'-N9	2.41	1.53	1.46
4	F	1201	112	C8-N9	2.40	1.41	1.37
4	H	1401	112	C2-N3	2.35	1.38	1.33
4	F	1201	112	C2-N3	2.20	1.37	1.33
4	E	1101	112	C2-N3	2.11	1.37	1.33
4	E	1101	112	C3'-C4'	-2.02	1.47	1.53

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	1301	112	N9-C8-N7	4.24	119.94	113.94
4	H	1401	112	N9-C8-N7	4.17	119.86	113.94
4	F	1201	112	N9-C8-N7	4.15	119.83	113.94
4	G	1301	112	C4-N9-C8	-4.11	101.42	105.74
4	E	1101	112	N9-C8-N7	4.04	119.67	113.94
4	H	1401	112	C4-N9-C8	-3.88	101.67	105.74
4	F	1201	112	O3A-PB-O1B	-3.84	99.15	110.70
4	F	1201	112	C4-N9-C8	-3.82	101.73	105.74
4	H	1401	112	O3A-PB-O1B	-3.77	99.35	110.70
4	E	1101	112	O3A-PB-O1B	-3.74	99.46	110.70
4	G	1301	112	O3A-PB-O1B	-3.63	99.77	110.70
4	E	1101	112	C4-N9-C8	-3.63	101.93	105.74
4	H	1401	112	O2A-PA-O5'	3.12	121.69	107.57
4	E	1101	112	O2A-PA-O5'	3.09	121.57	107.57
4	G	1301	112	O2A-PA-O5'	3.00	121.15	107.57
4	H	1401	112	O2A-PA-O3A	-2.92	99.38	107.27
4	G	1301	112	O2A-PA-O3A	-2.87	99.52	107.27
4	E	1101	112	O3A-PA-O1A	2.81	119.17	110.70
4	H	1401	112	O3A-PA-O1A	2.80	119.12	110.70
4	F	1201	112	O2A-PA-O5'	2.79	120.20	107.57
4	E	1101	112	O2A-PA-O3A	-2.74	99.87	107.27
4	G	1301	112	C1'-N9-C8	2.66	133.00	127.09
4	H	1401	112	O2S-C2S-NS	-2.58	115.65	122.53
4	H	1401	112	O2A-PA-O1A	2.56	124.35	112.44
4	F	1201	112	C1'-N9-C8	2.54	132.74	127.09
4	E	1101	112	C6-C5-C4	-2.53	113.72	117.18
4	H	1401	112	C1'-N9-C8	2.49	132.62	127.09
4	G	1301	112	O2A-PA-O1A	2.49	124.01	112.44
4	H	1401	112	O5'-PA-O1A	-2.46	99.20	108.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	1401	112	C4-C5-N7	2.45	113.39	110.58
4	G	1301	112	O3A-PA-O1A	2.45	118.08	110.70
4	F	1201	112	O2S-C2S-NS	-2.44	116.02	122.53
4	F	1201	112	C6-C5-C4	-2.43	113.86	117.18
4	F	1201	112	C5-N7-C8	-2.43	99.63	103.45
4	E	1101	112	O2S-C2S-NS	-2.42	116.06	122.53
4	H	1401	112	N3-C2-N1	-2.41	124.94	128.58
4	H	1401	112	C5-N7-C8	-2.40	99.68	103.45
4	E	1101	112	C5-N7-C8	-2.40	99.68	103.45
4	E	1101	112	N3-C2-N1	-2.39	124.97	128.58
4	E	1101	112	C1'-N9-C8	2.39	132.39	127.09
4	G	1301	112	O2S-C2S-NS	-2.38	116.17	122.53
4	F	1201	112	O2A-PA-O1A	2.37	123.49	112.44
4	E	1101	112	O2A-PA-O1A	2.36	123.43	112.44
4	G	1301	112	N3-C2-N1	-2.35	125.02	128.58
4	G	1301	112	C5-N7-C8	-2.34	99.77	103.45
4	F	1201	112	O2A-PA-O3A	-2.34	100.96	107.27
4	E	1101	112	C5'-C4'-C3'	-2.33	106.83	115.21
4	F	1201	112	O3A-PA-O1A	2.31	117.65	110.70
4	G	1301	112	O2G-PG-O3B	-2.29	101.10	107.27
4	G	1301	112	C4-C5-N7	2.28	113.19	110.58
4	E	1101	112	C4-C5-N7	2.25	113.16	110.58
4	E	1101	112	O4'-C4'-C3'	2.23	109.57	105.15
4	E	1101	112	O5'-PA-O1A	-2.21	100.18	108.94
4	H	1401	112	C5'-C4'-C3'	-2.19	107.32	115.21
4	G	1301	112	C5'-C4'-C3'	-2.19	107.33	115.21
4	H	1401	112	C6-C5-C4	-2.19	114.19	117.18
4	G	1301	112	O5'-PA-O1A	-2.18	100.29	108.94
4	H	1401	112	O2G-PG-O3B	-2.18	101.38	107.27
4	F	1201	112	N3-C2-N1	-2.14	125.34	128.58
4	F	1201	112	O4'-C4'-C3'	2.13	109.38	105.15
4	G	1301	112	O4'-C4'-C3'	2.12	109.36	105.15
4	F	1201	112	C5'-C4'-C3'	-2.12	107.58	115.21
4	E	1101	112	O2G-PG-O3B	-2.09	101.64	107.27
4	G	1301	112	C6-C5-C4	-2.07	114.35	117.18
4	F	1201	112	C4-C5-N7	2.06	112.94	110.58
4	F	1201	112	O5'-PA-O1A	-2.03	100.87	108.94
4	F	1201	112	O2G-PG-O3B	-2.03	101.79	107.27

There are no chirality outliers.

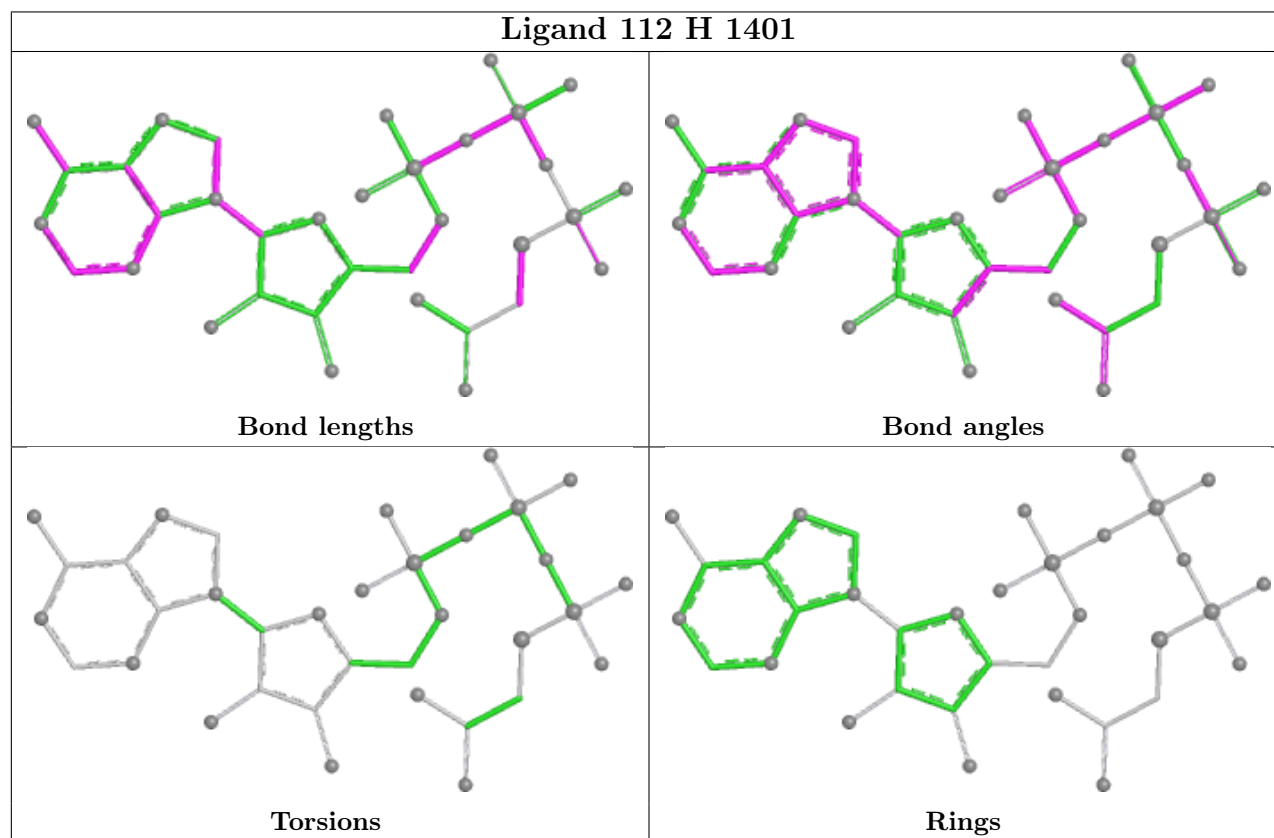
There are no torsion outliers.

There are no ring outliers.

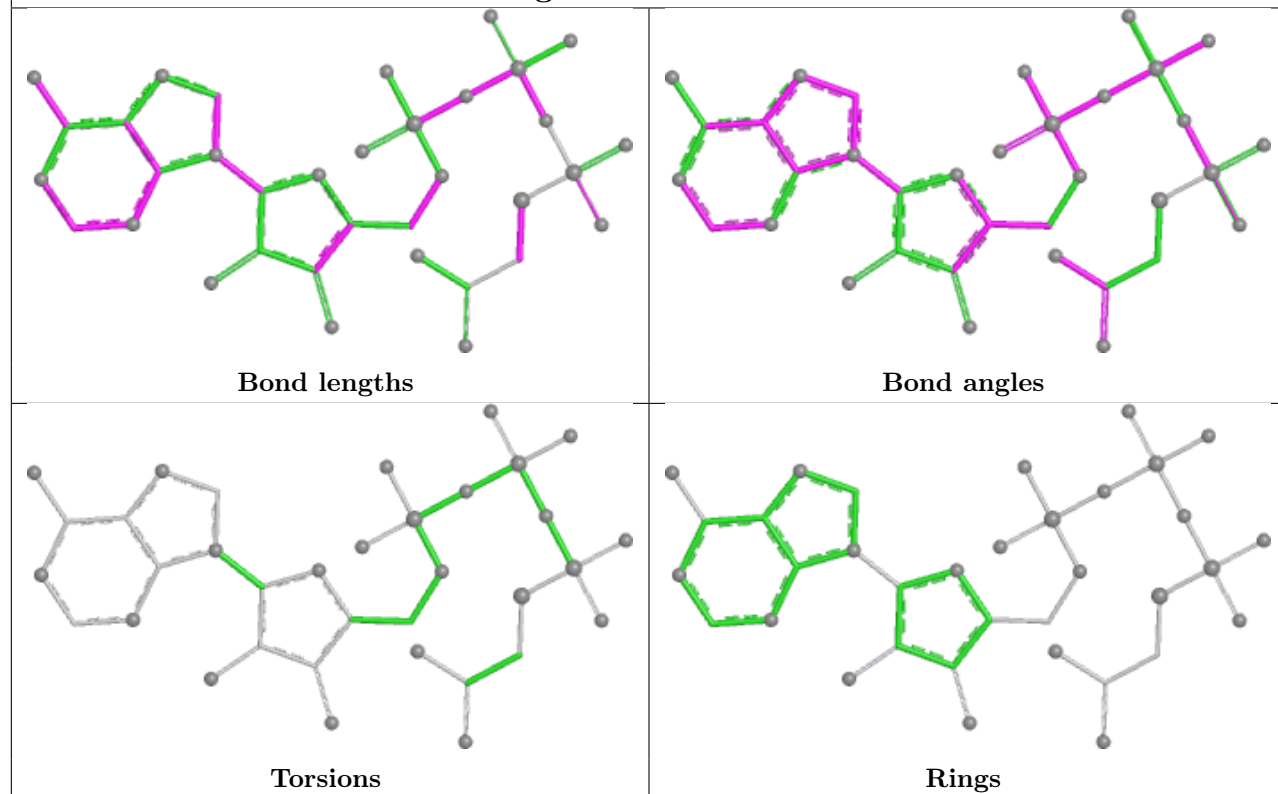
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	1401	112	1	0

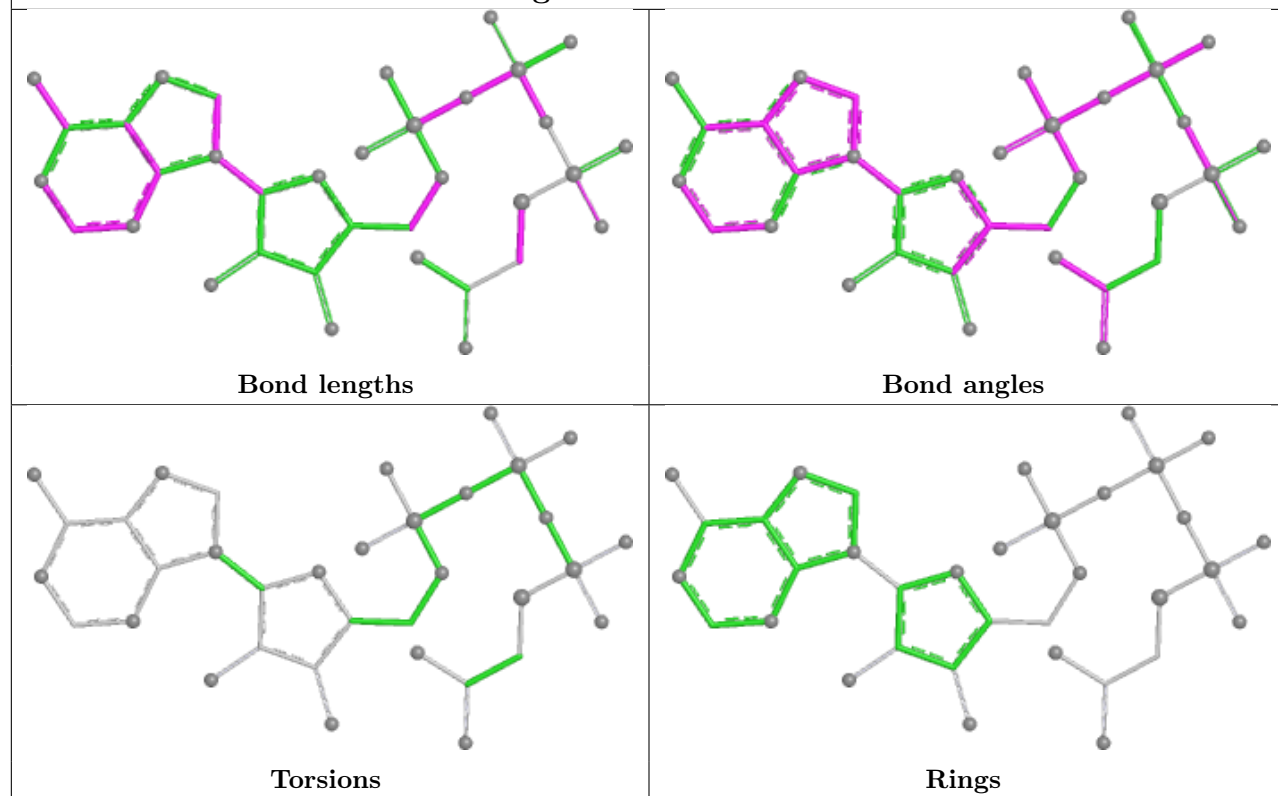
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

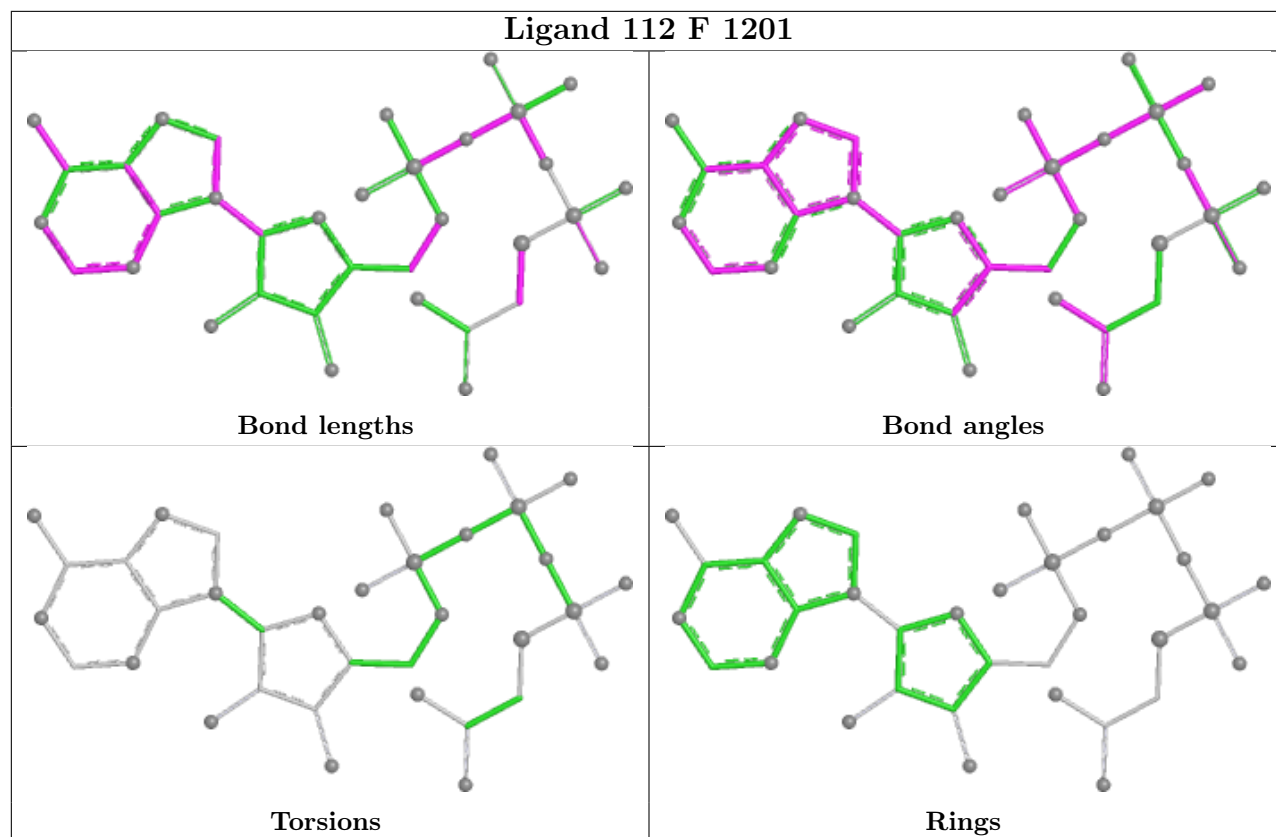


Ligand 112 E 1101



Ligand 112 G 1301





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	271/287 (94%)	-1.40	0 100 100	13, 23, 43, 66	0
1	B	273/287 (95%)	-1.33	0 100 100	13, 27, 45, 70	0
1	C	276/287 (96%)	-1.31	0 100 100	18, 28, 49, 66	0
1	D	277/287 (96%)	-1.38	0 100 100	15, 24, 45, 70	0
2	E	8/13 (61%)	-1.27	0 100 100	22, 28, 37, 39	0
2	F	10/13 (76%)	-1.27	0 100 100	23, 33, 44, 44	0
2	G	7/13 (53%)	-1.17	0 100 100	28, 30, 45, 45	0
2	H	8/13 (61%)	-1.30	0 100 100	23, 44, 48, 51	0
All	All	1130/1200 (94%)	-1.35	0 100 100	13, 26, 46, 70	0

There are no RSRZ outliers to report.

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](#)

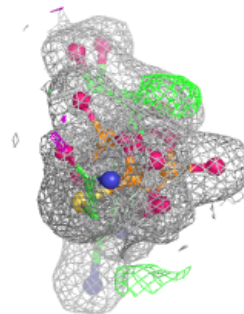
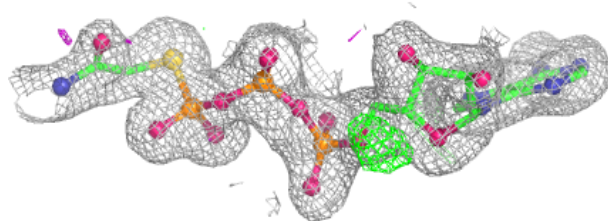
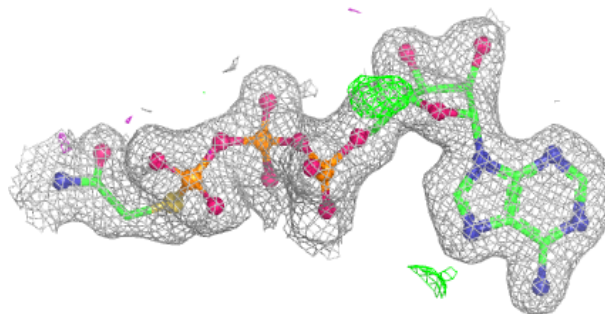
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MG	A	1501	1/1	1.00	0.01	17,17,17,17	0
3	MG	B	1601	1/1	1.00	0.01	21,21,21,21	0
3	MG	C	1701	1/1	1.00	0.01	20,20,20,20	0
3	MG	D	1801	1/1	1.00	0.02	20,20,20,20	0
4	112	E	1101	35/35	1.00	0.02	15,21,28,30	0
4	112	F	1201	35/35	1.00	0.02	20,24,27,30	0
4	112	G	1301	35/35	1.00	0.02	18,24,28,29	0
4	112	H	1401	35/35	1.00	0.02	15,19,26,27	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.

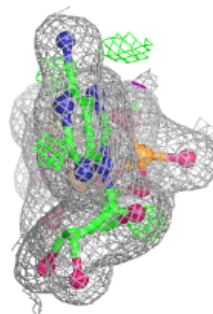
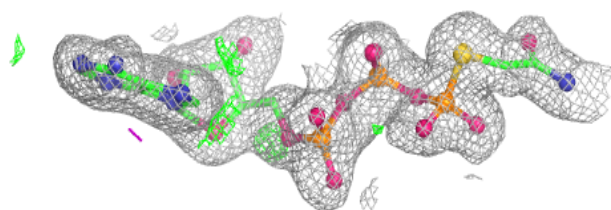
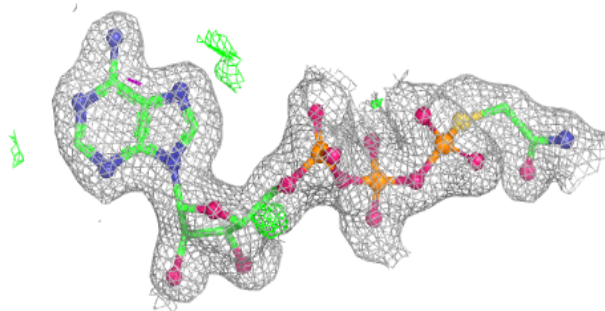
Electron density around 112 E 1101:

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

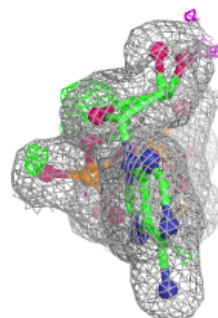
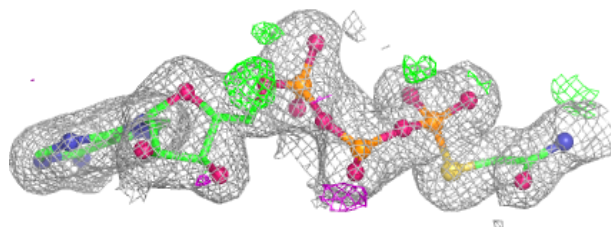
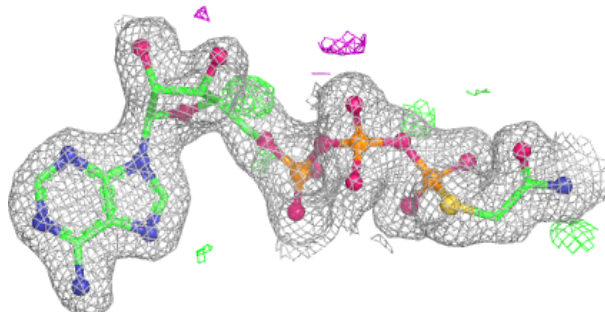


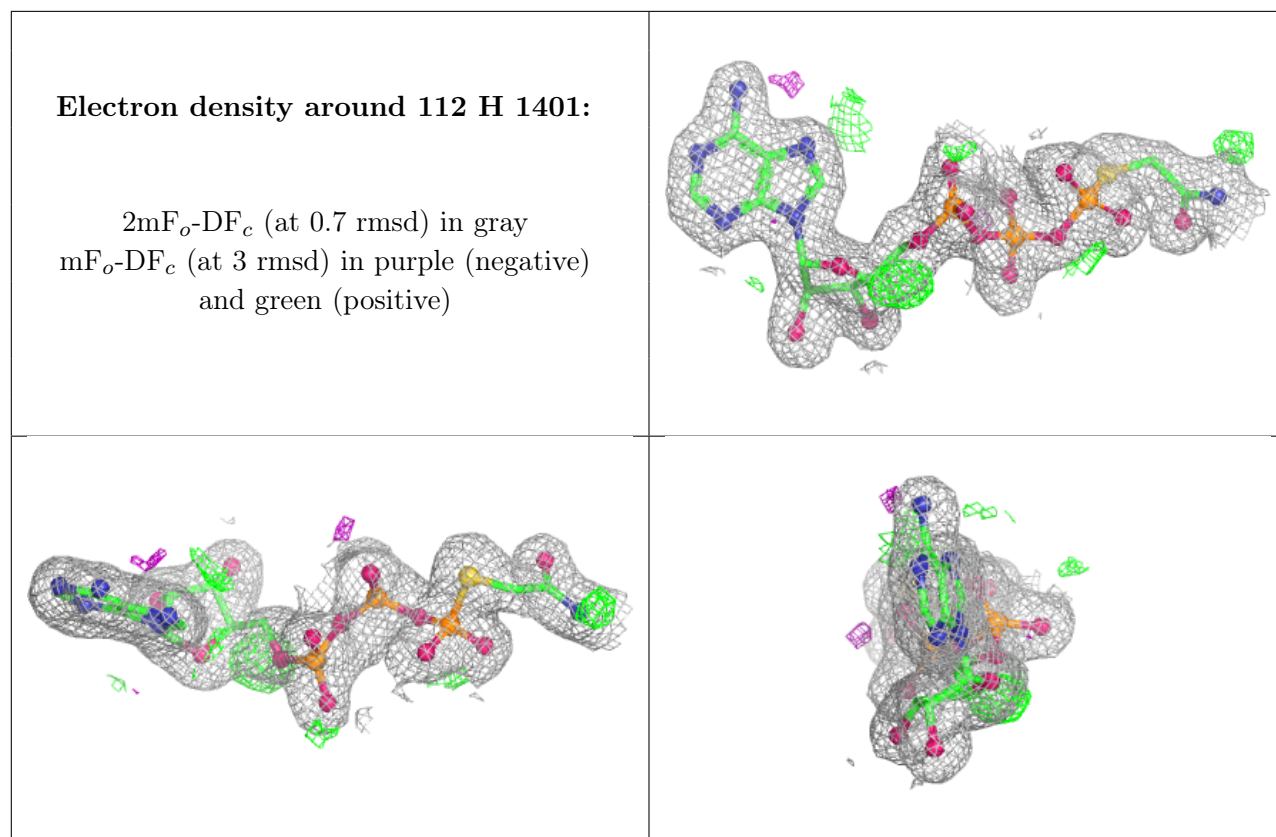
Electron density around 112 F 1201:

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

**Electron density around 112 G 1301:**

$2mF_o-DF_c$ (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.