



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 17, 2024 – 12:24 PM EST

PDB ID : 3SUA
Title : Crystal structure of the intracellular domain of Plexin-B1 in complex with Rac1
Authors : Bell, C.H.; Aricescu, A.R.; Jones, E.Y.; Siebold, C.
Deposited on : 2011-07-11
Resolution : 4.39 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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

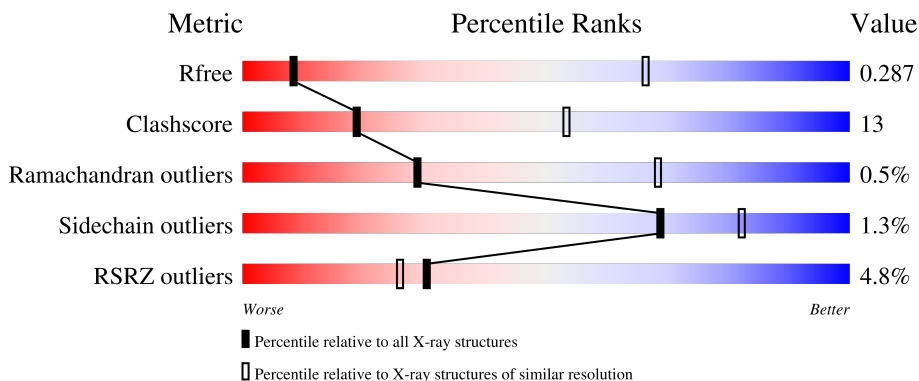
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.39 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.



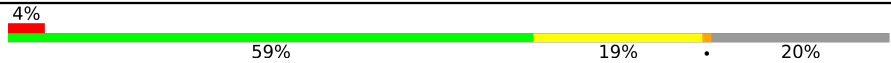
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1022 (4.92-3.80)
Clashscore	141614	1085 (4.92-3.80)
Ramachandran outliers	138981	1036 (4.92-3.80)
Sidechain outliers	138945	1019 (4.92-3.80)
RSRZ outliers	127900	1094 (5.06-3.70)

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	184	
1	B	184	
1	C	184	
2	D	633	
2	E	633	

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Mol	Chain	Length	Quality of chain
2	F	633	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into four segments: a small red segment at the beginning labeled '4%', followed by a large green segment labeled '59%', a yellow segment labeled '19%', and a grey segment at the end labeled '20%'. A small black dot is visible on the grey segment.</p>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16493 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 Ras-related C3 botulinum toxin substrate 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	178	1392	895	230	259	8	0	0	0
1	B	178	1392	895	230	259	8	0	0	0
1	C	178	1392	895	230	259	8	0	0	0

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	178	LYS	-	expression tag	UNP P63000
A	179	HIS	-	expression tag	UNP P63000
A	180	HIS	-	expression tag	UNP P63000
A	181	HIS	-	expression tag	UNP P63000
A	182	HIS	-	expression tag	UNP P63000
A	183	HIS	-	expression tag	UNP P63000
A	184	HIS	-	expression tag	UNP P63000
B	178	LYS	-	expression tag	UNP P63000
B	179	HIS	-	expression tag	UNP P63000
B	180	HIS	-	expression tag	UNP P63000
B	181	HIS	-	expression tag	UNP P63000
B	182	HIS	-	expression tag	UNP P63000
B	183	HIS	-	expression tag	UNP P63000
B	184	HIS	-	expression tag	UNP P63000
C	178	LYS	-	expression tag	UNP P63000
C	179	HIS	-	expression tag	UNP P63000
C	180	HIS	-	expression tag	UNP P63000
C	181	HIS	-	expression tag	UNP P63000
C	182	HIS	-	expression tag	UNP P63000
C	183	HIS	-	expression tag	UNP P63000
C	184	HIS	-	expression tag	UNP P63000

- Molecule 2 is a protein called Plexin-B1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	503	Total	C	N	O	S	0	0	0
			4061	2608	698	741	14			
2	E	505	Total	C	N	O	S	0	0	0
			4076	2619	700	743	14			
2	F	506	Total	C	N	O	S	0	0	0
			4081	2622	701	744	14			

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1503	MET	-	expression tag	UNP O43157
D	1504	GLY	-	expression tag	UNP O43157
D	1505	HIS	-	expression tag	UNP O43157
D	1506	HIS	-	expression tag	UNP O43157
D	1507	HIS	-	expression tag	UNP O43157
D	1508	HIS	-	expression tag	UNP O43157
D	1509	HIS	-	expression tag	UNP O43157
D	1510	HIS	-	expression tag	UNP O43157
D	1625	THR	SER	SEE REMARK 999	UNP O43157
E	1503	MET	-	expression tag	UNP O43157
E	1504	GLY	-	expression tag	UNP O43157
E	1505	HIS	-	expression tag	UNP O43157
E	1506	HIS	-	expression tag	UNP O43157
E	1507	HIS	-	expression tag	UNP O43157
E	1508	HIS	-	expression tag	UNP O43157
E	1509	HIS	-	expression tag	UNP O43157
E	1510	HIS	-	expression tag	UNP O43157
E	1625	THR	SER	SEE REMARK 999	UNP O43157
F	1503	MET	-	expression tag	UNP O43157
F	1504	GLY	-	expression tag	UNP O43157
F	1505	HIS	-	expression tag	UNP O43157
F	1506	HIS	-	expression tag	UNP O43157
F	1507	HIS	-	expression tag	UNP O43157
F	1508	HIS	-	expression tag	UNP O43157
F	1509	HIS	-	expression tag	UNP O43157
F	1510	HIS	-	expression tag	UNP O43157
F	1625	THR	SER	SEE REMARK 999	UNP O43157

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

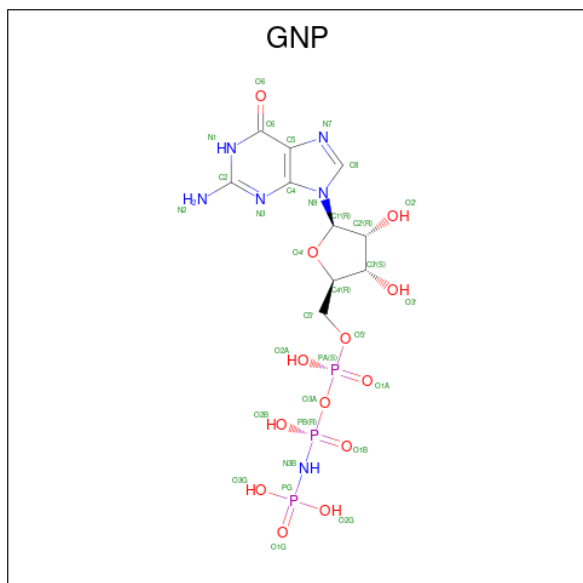
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		

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

- Molecule 4 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: C₁₀H₁₇N₆O₁₃P₃).

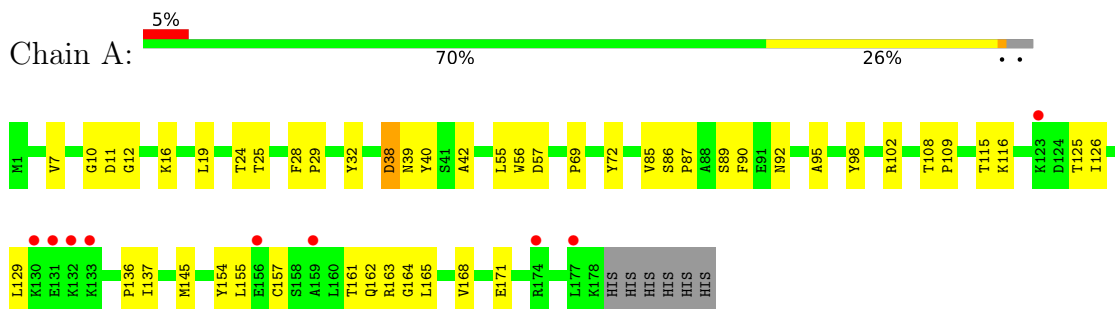


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O P 32 10 6 13 3	0	0
4	B	1	Total C N O P 32 10 6 13 3	0	0
4	C	1	Total C N O P 32 10 6 13 3	0	0

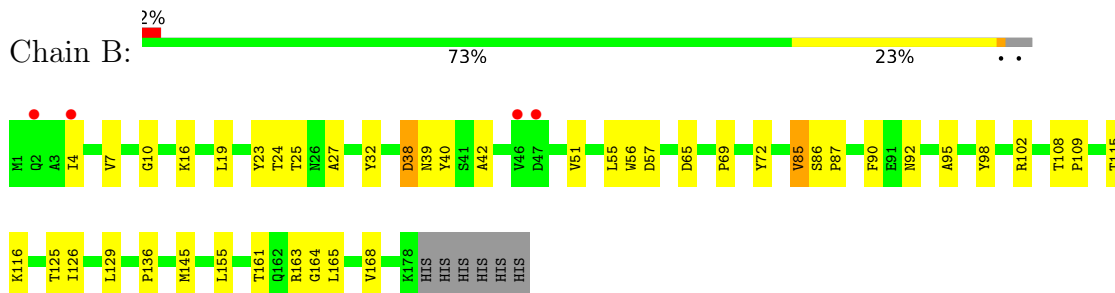
3 Residue-property plots [i](#)

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.

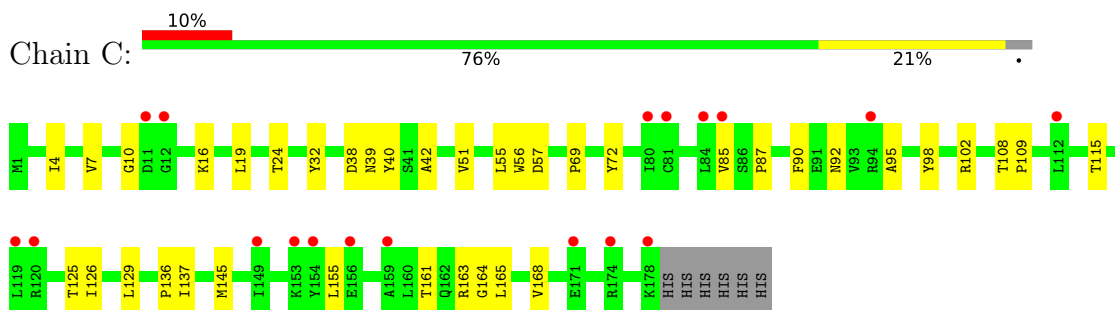
- Molecule 1: Ras-related C3 botulinum toxin substrate 1



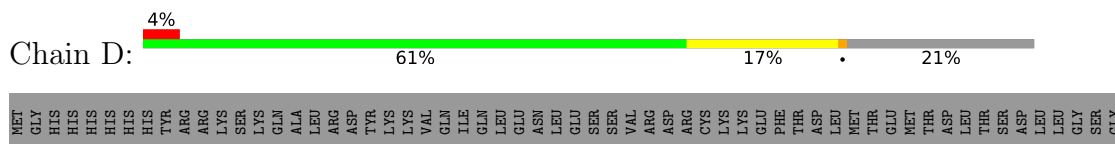
- Molecule 1: Ras-related C3 botulinum toxin substrate 1

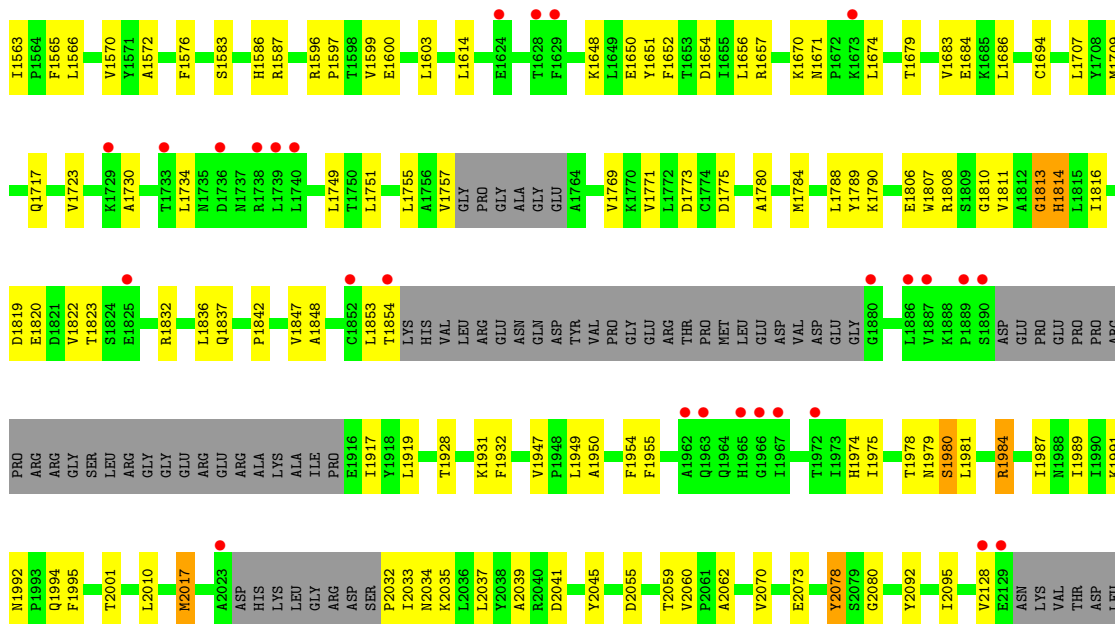


- Molecule 1: Ras-related C3 botulinum toxin substrate 1

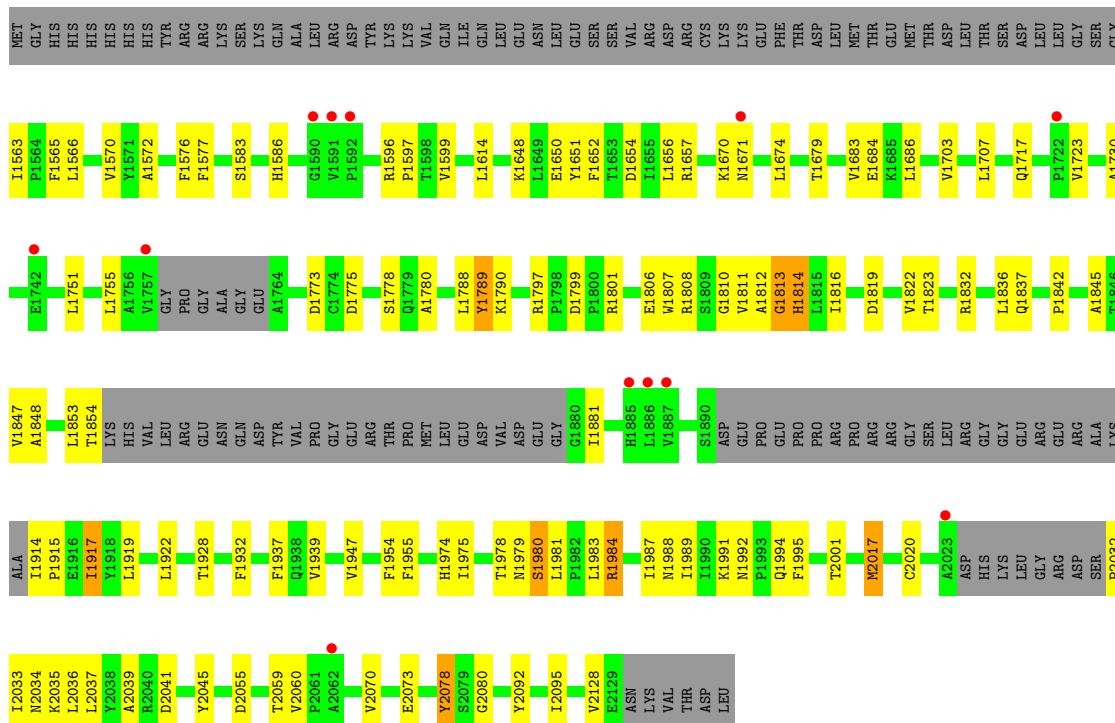


- Molecule 2: Plexin-B1



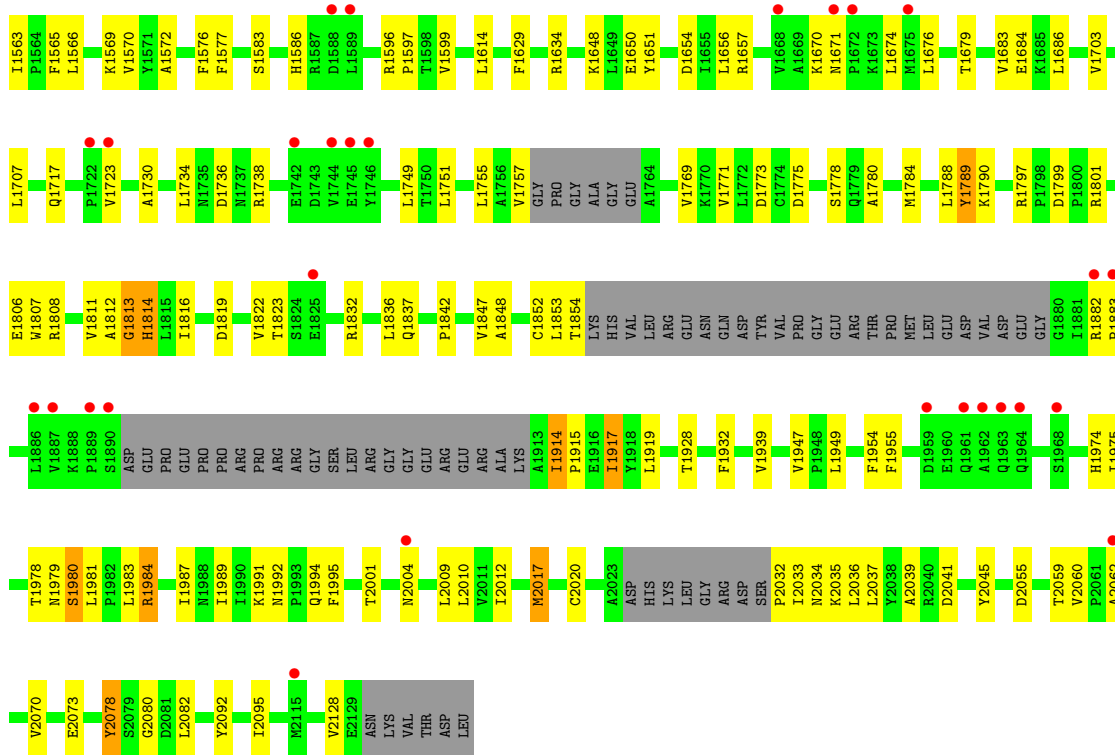


• Molecule 2: Plexin-B1



• Molecule 2: Plexin-B1





4 Data and refinement statistics

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	142.34Å 224.25Å 258.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.81 – 4.39 47.81 – 4.39	Depositor EDS
% Data completeness (in resolution range)	(Not available) (47.81-4.39) 95.6 (47.81-4.39)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.27 (at 4.45Å)	Xtrriage
Refinement program	BUSTER 2.9.2	Depositor
R, R_{free}	0.234 , 0.264 0.256 , 0.287	Depositor DCC
R_{free} test set	1318 reflections (5.16%)	wwPDB-VP
Wilson B-factor (Å ²)	186.5	Xtrriage
Anisotropy	0.516	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 205.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	16493	wwPDB-VP
Average B, all atoms (Å ²)	124.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.60% 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, GNP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.43	0/1422	0.74	2/1933 (0.1%)
1	B	0.45	0/1422	0.72	1/1933 (0.1%)
1	C	0.43	0/1422	0.71	0/1933
2	D	0.48	0/4145	0.75	5/5626 (0.1%)
2	E	0.46	0/4161	0.75	6/5649 (0.1%)
2	F	0.48	0/4166	0.75	6/5656 (0.1%)
All	All	0.47	0/16738	0.74	20/22730 (0.1%)

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1980	SER	N-CA-C	-8.45	88.18	111.00
2	F	1980	SER	N-CA-C	-7.89	89.71	111.00
2	E	1980	SER	N-CA-C	-7.71	90.20	111.00
2	F	1980	SER	CB-CA-C	7.57	124.49	110.10
2	D	1980	SER	CB-CA-C	7.27	123.91	110.10
2	F	1917	ILE	N-CA-C	7.27	130.63	111.00
2	E	1917	ILE	N-CA-C	7.08	130.12	111.00
2	E	1980	SER	CB-CA-C	6.86	123.13	110.10
1	A	162	GLN	CA-CB-CG	6.56	127.83	113.40
2	F	1577	PHE	N-CA-C	6.44	128.39	111.00
2	D	1814	HIS	N-CA-C	6.37	128.20	111.00
2	E	1814	HIS	N-CA-C	6.35	128.13	111.00
2	F	1814	HIS	N-CA-C	6.29	127.97	111.00
2	F	1789	TYR	CB-CA-C	-5.96	98.47	110.40
2	E	1789	TYR	CB-CA-C	-5.78	98.84	110.40
2	D	1789	TYR	CB-CA-C	-5.69	99.01	110.40
2	D	1917	ILE	N-CA-C	5.59	126.09	111.00
2	E	1577	PHE	N-CA-C	5.23	125.12	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	38	ASP	N-CA-C	5.17	124.96	111.00
1	B	38	ASP	N-CA-C	5.06	124.65	111.00

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	1392	0	1418	44	0
1	B	1392	0	1418	40	0
1	C	1392	0	1418	41	0
2	D	4061	0	4121	98	0
2	E	4076	0	4139	113	0
2	F	4081	0	4144	118	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	32	0	13	3	0
4	B	32	0	13	3	0
4	C	32	0	13	3	0
All	All	16493	0	16697	436	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 (436) 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:C:19:LEU:CD1	1:C:165:LEU:HD13	1.35	1.53
1:C:19:LEU:HD11	1:C:165:LEU:CD1	1.45	1.42
1:C:19:LEU:CD1	1:C:165:LEU:CD1	1.94	1.41
1:C:19:LEU:HD12	1:C:165:LEU:CD1	1.74	1.14
2:E:1922:LEU:CD1	2:E:2033:ILE:HD11	1.77	1.14
2:E:1922:LEU:HD13	2:E:2033:ILE:HD11	1.10	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:19:LEU:HD12	1:B:165:LEU:CD1	1.86	1.06
1:B:19:LEU:HD12	1:B:165:LEU:HD11	1.38	1.05
1:A:39:ASN:ND2	2:D:1813:GLY:O	1.90	1.04
2:D:1949:LEU:HD11	2:D:2062:ALA:HB1	1.41	1.02
2:F:1980:SER:O	2:F:1984:ARG:HB2	1.59	1.01
2:F:1949:LEU:HD11	2:F:2062:ALA:HB1	1.41	1.01
2:F:2078:TYR:CE2	2:F:2080:GLY:O	2.14	1.00
2:D:1980:SER:O	2:D:1984:ARG:HB2	1.62	0.99
2:E:1975:ILE:HA	2:E:1978:THR:HG22	1.43	0.99
2:F:1975:ILE:HA	2:F:1978:THR:HG22	1.45	0.99
2:E:1984:ARG:O	2:E:1988:ASN:ND2	1.97	0.97
1:C:19:LEU:CD1	1:C:165:LEU:HD11	1.90	0.96
2:D:1975:ILE:HA	2:D:1978:THR:HG22	1.46	0.95
2:E:1980:SER:O	2:E:1984:ARG:HB2	1.67	0.94
2:D:2078:TYR:CE2	2:D:2080:GLY:O	2.19	0.94
2:E:2078:TYR:CE2	2:E:2080:GLY:O	2.20	0.94
2:F:1566:LEU:HD22	2:F:1570:VAL:HG11	1.50	0.92
2:D:1566:LEU:HD22	2:D:1570:VAL:HG11	1.51	0.92
2:D:1853:LEU:HD12	2:D:1854:THR:N	1.85	0.92
2:F:1949:LEU:HD11	2:F:2062:ALA:CB	2.00	0.91
2:F:1814:HIS:O	2:F:1814:HIS:ND1	2.02	0.91
2:F:1980:SER:O	2:F:1984:ARG:CB	2.19	0.91
2:D:1980:SER:O	2:D:1984:ARG:CB	2.20	0.90
2:E:1778:SER:HB2	2:E:1819:ASP:OD2	1.71	0.90
2:D:1814:HIS:ND1	2:D:1814:HIS:O	2.04	0.90
2:D:1949:LEU:HD11	2:D:2062:ALA:CB	2.00	0.90
1:C:19:LEU:HD12	1:C:165:LEU:HD11	1.51	0.89
2:E:1814:HIS:O	2:E:1814:HIS:ND1	2.04	0.89
2:F:2033:ILE:HG13	2:F:2034:ASN:H	1.38	0.89
2:E:1853:LEU:HD12	2:E:1854:THR:N	1.89	0.88
2:D:2033:ILE:HG13	2:D:2034:ASN:H	1.39	0.88
2:E:1566:LEU:HD22	2:E:1570:VAL:HG11	1.53	0.88
2:D:1994:GLN:CD	2:D:2001:THR:HG22	1.95	0.87
1:C:19:LEU:HD12	1:C:165:LEU:HD13	1.36	0.87
2:D:1949:LEU:CD1	2:D:2062:ALA:CB	2.53	0.86
2:E:1994:GLN:CD	2:E:2001:THR:HG22	1.93	0.86
2:F:1853:LEU:HD12	2:F:1854:THR:N	1.89	0.86
2:E:1980:SER:O	2:E:1984:ARG:CB	2.24	0.85
2:F:1778:SER:HB2	2:F:1819:ASP:OD2	1.76	0.85
2:F:1816:ILE:CD1	2:F:1853:LEU:HD21	2.06	0.84
1:C:19:LEU:HD11	1:C:165:LEU:HD13	1.05	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:155:LEU:HD13	1:B:168:VAL:HA	1.60	0.83
1:B:19:LEU:CD1	1:B:165:LEU:CD1	2.56	0.82
2:E:1922:LEU:CD1	2:E:2033:ILE:CD1	2.56	0.82
1:C:155:LEU:HD13	1:C:168:VAL:HA	1.62	0.82
1:C:38:ASP:OD2	1:C:40:TYR:CZ	2.32	0.82
2:F:1949:LEU:CD1	2:F:2062:ALA:CB	2.57	0.81
1:C:19:LEU:HD11	1:C:165:LEU:HD12	1.58	0.80
2:E:1922:LEU:HD13	2:E:2033:ILE:CD1	2.02	0.80
2:E:1975:ILE:HA	2:E:1978:THR:CG2	2.12	0.79
1:A:155:LEU:CD2	1:A:168:VAL:HA	2.14	0.78
2:E:2033:ILE:HG23	2:E:2034:ASN:H	1.50	0.77
1:A:19:LEU:HG	1:A:165:LEU:CD1	2.16	0.76
2:D:1975:ILE:HA	2:D:1978:THR:CG2	2.16	0.76
2:F:2033:ILE:HG13	2:F:2034:ASN:N	2.01	0.76
2:D:1949:LEU:CD1	2:D:2062:ALA:HB1	2.15	0.75
2:D:2033:ILE:HG13	2:D:2034:ASN:N	2.02	0.74
4:B:200:GNP:H8	4:B:200:GNP:H5'2	1.70	0.73
1:C:38:ASP:OD1	1:C:39:ASN:N	2.21	0.73
2:F:1975:ILE:HA	2:F:1978:THR:CG2	2.17	0.73
2:F:1816:ILE:CD1	2:F:1853:LEU:CD2	2.67	0.72
4:A:200:GNP:H8	4:A:200:GNP:H5'2	1.71	0.72
1:A:11:ASP:OD1	1:A:12:GLY:N	2.23	0.72
2:D:1566:LEU:HD22	2:D:1570:VAL:CG1	2.18	0.72
4:C:200:GNP:H8	4:C:200:GNP:H5'2	1.71	0.72
2:F:1816:ILE:HD12	2:F:1853:LEU:HD21	1.72	0.72
1:A:19:LEU:HD11	1:A:157:CYS:SG	2.30	0.72
2:F:1563:ILE:HG21	2:F:1565:PHE:HE1	1.54	0.72
2:F:2032:PRO:HD2	2:F:2035:LYS:HB2	1.72	0.72
2:D:2032:PRO:HD2	2:D:2035:LYS:HB2	1.72	0.71
2:E:2032:PRO:HD2	2:E:2035:LYS:HB2	1.73	0.71
2:F:1563:ILE:HG22	2:F:1565:PHE:CE1	2.26	0.70
2:E:1563:ILE:HG22	2:E:1565:PHE:CE1	2.26	0.70
1:B:23:TYR:HB2	1:B:165:LEU:HD21	1.74	0.70
2:F:1566:LEU:HD22	2:F:1570:VAL:CG1	2.19	0.70
2:F:1949:LEU:CD1	2:F:2062:ALA:HB2	2.21	0.70
2:F:1563:ILE:CG2	2:F:1565:PHE:CE1	2.75	0.70
2:E:1994:GLN:CD	2:E:2001:THR:CG2	2.60	0.69
2:D:1949:LEU:CD1	2:D:2062:ALA:HB2	2.21	0.69
1:B:19:LEU:CD1	1:B:165:LEU:HD12	2.22	0.69
1:A:155:LEU:HD22	1:A:168:VAL:HA	1.73	0.69
2:F:1563:ILE:CG2	2:F:1565:PHE:HE1	2.05	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1656:LEU:HD21	2:F:1686:LEU:HB3	1.75	0.68
1:B:32:TYR:HE1	4:B:200:GNP:HNB3	1.41	0.68
2:D:1679:THR:O	2:D:1679:THR:HG22	1.93	0.68
2:D:1994:GLN:CD	2:D:2001:THR:CG2	2.62	0.68
2:E:1566:LEU:HD22	2:E:1570:VAL:CG1	2.24	0.67
2:E:1563:ILE:HG21	2:E:1565:PHE:HE1	1.58	0.67
1:A:32:TYR:HE1	4:A:200:GNP:HNB3	1.43	0.67
2:E:2033:ILE:HG23	2:E:2034:ASN:N	2.10	0.67
2:D:1709:MET:HB3	2:D:1932:PHE:CE1	2.31	0.66
2:E:1563:ILE:CG2	2:E:1565:PHE:HE1	2.07	0.66
2:E:1563:ILE:CG2	2:E:1565:PHE:CE1	2.77	0.66
1:C:32:TYR:HE1	4:C:200:GNP:HNB3	1.42	0.66
1:A:19:LEU:HG	1:A:165:LEU:HD13	1.76	0.66
2:E:1679:THR:HG22	2:E:1679:THR:O	1.96	0.66
1:B:155:LEU:CD1	1:B:168:VAL:HA	2.27	0.65
2:D:1563:ILE:HD12	2:D:1565:PHE:HE1	1.61	0.65
2:E:1994:GLN:NE2	2:E:2001:THR:HG22	2.11	0.64
1:A:126:ILE:HA	1:A:129:LEU:HD12	1.79	0.64
1:C:126:ILE:HA	1:C:129:LEU:HD12	1.80	0.64
1:C:155:LEU:CD1	1:C:168:VAL:HA	2.27	0.64
2:D:1563:ILE:HD12	2:D:1565:PHE:CE1	2.32	0.64
2:D:1980:SER:O	2:D:1984:ARG:HB3	1.98	0.63
2:E:1755:LEU:HB2	2:E:1788:LEU:HD22	1.80	0.63
2:F:1755:LEU:HB2	2:F:1788:LEU:HD22	1.79	0.63
2:D:1994:GLN:NE2	2:D:2001:THR:HG22	2.13	0.62
2:D:1751:LEU:HD12	2:D:1751:LEU:O	2.00	0.62
2:F:1949:LEU:CD1	2:F:2062:ALA:HB1	2.20	0.61
2:D:1819:ASP:OD1	2:D:1820:GLU:N	2.32	0.61
2:D:1755:LEU:HB2	2:D:1788:LEU:HD22	1.83	0.61
2:F:1563:ILE:HG22	2:F:1565:PHE:CD1	2.35	0.61
2:E:1707:LEU:HD21	2:E:1989:ILE:HG22	1.82	0.60
2:F:1980:SER:O	2:F:1984:ARG:HB3	2.00	0.60
1:C:39:ASN:ND2	2:F:1814:HIS:HB3	2.17	0.60
2:E:1751:LEU:HD12	2:E:1751:LEU:O	2.00	0.60
1:A:19:LEU:HG	1:A:165:LEU:HD11	1.84	0.60
1:A:24:THR:HG22	1:A:42:ALA:HB2	1.85	0.59
2:E:2033:ILE:CG2	2:E:2034:ASN:H	2.14	0.59
1:B:126:ILE:HA	1:B:129:LEU:HD12	1.84	0.59
2:E:1563:ILE:HG22	2:E:1565:PHE:CD1	2.37	0.59
2:F:1807:TRP:CZ2	2:F:1842:PRO:HD3	2.37	0.59
2:F:2033:ILE:CG1	2:F:2034:ASN:H	2.13	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:PRO:HA	1:A:72:TYR:CD2	2.38	0.58
1:B:69:PRO:HA	1:B:72:TYR:CD2	2.38	0.58
2:F:1679:THR:HG22	2:F:1679:THR:O	2.03	0.58
2:F:2078:TYR:HE2	2:F:2080:GLY:O	1.84	0.58
1:B:39:ASN:ND2	2:E:1814:HIS:HB3	2.17	0.58
2:F:1814:HIS:O	2:F:1814:HIS:CG	2.54	0.58
2:D:1947:VAL:HG23	2:D:2055:ASP:OD2	2.03	0.58
1:A:155:LEU:HD23	1:A:168:VAL:HA	1.86	0.58
2:D:1652:PHE:O	2:D:1656:LEU:HD13	2.04	0.58
2:D:1807:TRP:CZ2	2:D:1842:PRO:HD3	2.39	0.58
2:D:1814:HIS:O	2:D:1814:HIS:CG	2.56	0.58
1:C:69:PRO:HA	1:C:72:TYR:CD2	2.38	0.58
2:E:1914:ILE:HB	2:E:1915:PRO:HD2	1.85	0.58
2:E:1980:SER:O	2:E:1984:ARG:HB3	2.00	0.58
2:F:1978:THR:OG1	2:F:2020:CYS:HB3	2.04	0.58
2:E:1814:HIS:O	2:E:1814:HIS:CG	2.56	0.58
1:C:38:ASP:OD2	1:C:40:TYR:OH	2.22	0.57
2:E:2033:ILE:HG12	2:E:2037:LEU:HD12	1.85	0.57
1:B:27:ALA:HB1	2:F:1917:ILE:HG12	1.86	0.57
1:A:161:THR:HB	1:A:163:ARG:HG3	1.86	0.57
2:D:1717:GLN:HG2	2:D:1928:THR:HG21	1.86	0.57
2:D:1807:TRP:HZ2	2:D:1842:PRO:HD3	1.68	0.57
2:E:1807:TRP:CZ2	2:E:1842:PRO:HD3	2.40	0.57
2:F:2059:THR:HG22	2:F:2060:VAL:N	2.20	0.57
2:F:1807:TRP:HZ2	2:F:1842:PRO:HD3	1.68	0.57
1:C:24:THR:HG22	1:C:42:ALA:HB2	1.86	0.56
2:D:1992:ASN:HD21	2:D:1994:GLN:HB2	1.70	0.56
1:C:161:THR:HB	1:C:163:ARG:HG3	1.85	0.56
2:E:1807:TRP:HZ2	2:E:1842:PRO:HD3	1.71	0.56
2:E:2059:THR:HG22	2:E:2060:VAL:N	2.19	0.56
2:F:1684:GLU:HB3	2:F:1984:ARG:HH22	1.71	0.56
2:F:1717:GLN:HG2	2:F:1928:THR:HG21	1.87	0.56
1:B:27:ALA:HB1	2:F:1917:ILE:CG1	2.35	0.56
2:E:1947:VAL:HG23	2:E:2055:ASP:OD2	2.06	0.56
1:A:29:PRO:HA	2:E:1917:ILE:CG2	2.36	0.56
2:D:1707:LEU:HD21	2:D:1989:ILE:HG22	1.87	0.56
1:A:38:ASP:OD1	2:D:1810:GLY:HA3	2.06	0.56
2:F:1914:ILE:HG13	2:F:1915:PRO:HD2	1.87	0.56
2:D:1808:ARG:HH12	2:D:1848:ALA:HB2	1.71	0.56
1:B:161:THR:HB	1:B:163:ARG:HG3	1.87	0.55
2:F:1751:LEU:HD12	2:F:1751:LEU:O	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1947:VAL:HG23	2:F:2055:ASP:OD2	2.06	0.55
1:C:40:TYR:HB2	1:C:55:LEU:HB2	1.88	0.55
2:E:1778:SER:N	2:E:1819:ASP:OD1	2.40	0.55
1:B:24:THR:HG22	1:B:42:ALA:HB2	1.88	0.55
2:D:2059:THR:HG22	2:D:2060:VAL:N	2.20	0.55
2:D:2078:TYR:HE2	2:D:2080:GLY:O	1.85	0.54
1:C:19:LEU:HD22	1:C:115:THR:HG22	1.88	0.54
2:F:1707:LEU:HD21	2:F:1989:ILE:CG2	2.38	0.54
2:D:2033:ILE:CG1	2:D:2034:ASN:H	2.14	0.54
1:A:40:TYR:HB2	1:A:55:LEU:HB2	1.89	0.54
1:B:40:TYR:HB2	1:B:55:LEU:HB2	1.90	0.54
1:C:39:ASN:HB2	2:F:1812:ALA:HB3	1.90	0.53
2:F:1983:LEU:HD21	2:F:2017:MET:HA	1.90	0.53
2:E:1654:ASP:HB2	2:E:1657:ARG:HH21	1.73	0.53
1:B:19:LEU:HD11	1:B:165:LEU:HG	1.89	0.53
2:F:1780:ALA:HB2	2:F:1836:LEU:HD11	1.91	0.53
2:E:1652:PHE:O	2:E:1656:LEU:HD13	2.09	0.53
2:E:1707:LEU:HD21	2:E:1989:ILE:CG2	2.39	0.52
1:A:154:TYR:C	1:A:155:LEU:HD12	2.29	0.52
2:D:1709:MET:HB3	2:D:1932:PHE:CD1	2.44	0.52
2:F:1778:SER:N	2:F:1819:ASP:OD1	2.43	0.52
1:A:129:LEU:HD13	1:A:136:PRO:HD3	1.92	0.52
2:D:1919:LEU:HD21	2:F:1811:VAL:CG1	2.40	0.52
2:F:1975:ILE:HG23	2:F:1979:ASN:ND2	2.25	0.52
2:F:1992:ASN:HD21	2:F:1994:GLN:HB2	1.74	0.52
1:B:129:LEU:HD13	1:B:136:PRO:HD3	1.92	0.52
2:D:1671:ASN:HB3	2:D:1674:LEU:HD12	1.92	0.51
2:E:2059:THR:CG2	2:E:2060:VAL:N	2.73	0.51
1:A:90:PHE:CE2	1:A:145:MET:HE3	2.45	0.51
2:E:1780:ALA:HB2	2:E:1836:LEU:HD11	1.92	0.51
1:C:129:LEU:HD13	1:C:136:PRO:HD3	1.92	0.51
2:D:1563:ILE:O	2:D:1563:ILE:HG13	2.11	0.51
2:E:1808:ARG:HH12	2:E:1848:ALA:HB2	1.76	0.51
2:E:1974:HIS:O	2:E:1978:THR:HG22	2.10	0.51
2:E:1992:ASN:HD21	2:E:1994:GLN:HB2	1.75	0.51
1:B:38:ASP:OD1	2:E:1810:GLY:HA3	2.10	0.51
1:C:85:VAL:HG11	1:C:125:THR:HG21	1.93	0.51
2:E:1717:GLN:HG2	2:E:1928:THR:HG21	1.93	0.51
2:D:1780:ALA:HB2	2:D:1836:LEU:HD11	1.91	0.51
2:E:2078:TYR:HE2	2:E:2080:GLY:O	1.86	0.51
2:F:1654:ASP:HB2	2:F:1657:ARG:HH21	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:38:ASP:OD2	1:C:40:TYR:CE2	2.63	0.50
2:D:1654:ASP:HB2	2:D:1657:ARG:HH21	1.75	0.50
1:B:115:THR:HG22	1:B:116:LYS:N	2.26	0.50
1:A:115:THR:HG22	1:A:116:LYS:N	2.27	0.50
2:D:1974:HIS:O	2:D:1978:THR:HG22	2.12	0.50
2:F:1583:SER:HB3	2:F:1586:HIS:HD2	1.76	0.50
2:F:1671:ASN:HB3	2:F:1674:LEU:HD12	1.94	0.50
2:F:1987:ILE:HD11	2:F:2017:MET:HB2	1.94	0.50
2:D:2059:THR:CG2	2:D:2060:VAL:N	2.75	0.49
2:F:1648:LYS:HB3	2:F:1651:TYR:HB3	1.94	0.49
2:F:2059:THR:CG2	2:F:2060:VAL:N	2.74	0.49
2:F:2078:TYR:CZ	2:F:2080:GLY:O	2.63	0.49
1:A:85:VAL:HG11	1:A:125:THR:HG21	1.93	0.49
2:E:1671:ASN:HB3	2:E:1674:LEU:HD12	1.93	0.49
2:F:2092:TYR:HA	2:F:2095:ILE:HD12	1.94	0.49
2:D:1955:PHE:CZ	2:D:1981:LEU:HB3	2.48	0.49
1:B:85:VAL:HG11	1:B:125:THR:HG21	1.93	0.49
2:E:2092:TYR:HA	2:E:2095:ILE:HD12	1.94	0.49
2:E:1773:ASP:HB2	2:E:1837:GLN:HB2	1.95	0.49
2:F:1656:LEU:HD21	2:F:1686:LEU:CB	2.40	0.49
2:F:1954:PHE:CE2	2:F:1980:SER:HB3	2.48	0.49
1:C:40:TYR:HE1	1:C:57:ASP:HB2	1.78	0.48
1:A:19:LEU:CD1	1:A:157:CYS:SG	3.01	0.48
1:C:39:ASN:HD21	2:F:1814:HIS:HB3	1.78	0.48
1:B:40:TYR:HE1	1:B:57:ASP:HB2	1.78	0.48
2:D:1707:LEU:HD21	2:D:1989:ILE:CG2	2.43	0.48
2:D:1975:ILE:HG23	2:D:1979:ASN:ND2	2.27	0.48
2:F:1734:LEU:O	2:F:2033:ILE:HD12	2.14	0.48
2:F:1808:ARG:HH12	2:F:1848:ALA:HB2	1.78	0.48
2:D:1773:ASP:HB2	2:D:1837:GLN:HB2	1.95	0.48
2:E:1975:ILE:HG23	2:E:1979:ASN:ND2	2.29	0.48
2:E:1648:LYS:HB3	2:E:1651:TYR:HB3	1.96	0.48
1:B:10:GLY:N	1:B:16:LYS:HD3	2.29	0.48
1:A:29:PRO:HA	2:E:1917:ILE:HG23	1.96	0.48
2:E:1994:GLN:OE1	2:E:2001:THR:CG2	2.62	0.48
2:D:1987:ILE:O	2:D:1991:LYS:HB2	2.14	0.48
2:D:1583:SER:HB3	2:D:1586:HIS:HD2	1.78	0.47
1:A:11:ASP:OD2	1:A:89:SER:HA	2.13	0.47
2:D:1648:LYS:HB3	2:D:1651:TYR:HB3	1.95	0.47
2:D:1734:LEU:O	2:D:2033:ILE:HD12	2.14	0.47
2:D:1947:VAL:HG23	2:D:2055:ASP:CG	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:2092:TYR:HA	2:D:2095:ILE:HD12	1.95	0.47
2:E:1987:ILE:O	2:E:1991:LYS:HB2	2.15	0.47
1:A:40:TYR:HE1	1:A:57:ASP:HB2	1.79	0.47
2:E:1978:THR:OG1	2:E:2020:CYS:HB3	2.14	0.47
2:E:2033:ILE:CG2	2:E:2034:ASN:N	2.76	0.47
2:D:1822:VAL:HG13	2:D:1823:THR:HG23	1.98	0.46
2:E:2059:THR:CG2	2:E:2060:VAL:H	2.29	0.46
2:E:1583:SER:HB3	2:E:1586:HIS:HD2	1.79	0.46
2:E:1811:VAL:HG13	2:F:1919:LEU:HD21	1.97	0.46
2:E:1955:PHE:CZ	2:E:1981:LEU:HB3	2.50	0.46
1:A:10:GLY:N	1:A:16:LYS:HD3	2.29	0.46
2:F:2070:VAL:O	2:F:2073:GLU:HG2	2.15	0.46
2:F:1987:ILE:O	2:F:1991:LYS:HB2	2.15	0.46
1:C:10:GLY:N	1:C:16:LYS:HD3	2.30	0.46
2:E:1983:LEU:HD21	2:E:2017:MET:HA	1.97	0.46
1:A:28:PHE:O	2:E:1917:ILE:HG22	2.16	0.46
2:E:2055:ASP:OD1	2:E:2059:THR:OG1	2.22	0.46
2:F:1955:PHE:CZ	2:F:1981:LEU:HB3	2.50	0.46
2:F:1773:ASP:HB2	2:F:1837:GLN:HB2	1.97	0.46
2:D:1991:LYS:HE2	2:D:2010:LEU:CD1	2.46	0.46
2:D:1994:GLN:OE1	2:D:2001:THR:CG2	2.64	0.46
2:D:2070:VAL:O	2:D:2073:GLU:HG2	2.16	0.46
2:F:1974:HIS:O	2:F:1978:THR:HG22	2.15	0.46
2:F:1992:ASN:HB3	2:F:1995:PHE:CE1	2.50	0.46
2:D:2059:THR:CG2	2:D:2060:VAL:H	2.30	0.45
2:F:1563:ILE:HG21	2:F:1565:PHE:CE1	2.41	0.45
1:B:115:THR:CG2	1:B:116:LYS:N	2.79	0.45
2:D:1751:LEU:HD22	2:D:1847:VAL:HG21	1.98	0.45
2:E:2070:VAL:O	2:E:2073:GLU:HG2	2.16	0.45
2:F:1634:ARG:HD2	2:F:1679:THR:O	2.17	0.45
2:E:1808:ARG:HG2	2:E:1813:GLY:HA3	1.99	0.45
2:F:2059:THR:CG2	2:F:2060:VAL:H	2.29	0.45
2:E:1983:LEU:HD22	2:E:2017:MET:HG2	1.99	0.45
2:E:1987:ILE:HD11	2:E:2017:MET:HB2	1.99	0.45
2:F:1806:GLU:HB2	2:F:1816:ILE:HG22	1.99	0.45
2:F:1983:LEU:HD22	2:F:2017:MET:HG2	1.97	0.45
2:D:1955:PHE:HZ	2:D:1981:LEU:HB3	1.81	0.45
2:E:1684:GLU:HB3	2:E:1984:ARG:HH22	1.81	0.45
2:E:1707:LEU:CD2	2:E:1989:ILE:HG22	2.46	0.45
2:E:1992:ASN:HB3	2:E:1995:PHE:CE1	2.52	0.45
1:C:7:VAL:HA	1:C:56:TRP:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:161:THR:CB	1:C:163:ARG:HG3	2.47	0.44
2:F:1751:LEU:HD22	2:F:1847:VAL:HG21	1.98	0.44
2:D:1808:ARG:HG2	2:D:1813:GLY:HA3	1.98	0.44
2:E:1614:LEU:HD12	2:E:1614:LEU:H	1.82	0.44
2:F:1717:GLN:CG	2:F:1928:THR:HG21	2.46	0.44
2:E:1922:LEU:HD11	2:E:2033:ILE:CD1	2.41	0.44
2:E:1811:VAL:CG1	2:F:1919:LEU:HD21	2.47	0.44
2:D:1987:ILE:HD11	2:D:2017:MET:HB2	1.99	0.44
1:B:19:LEU:CD1	1:B:165:LEU:HG	2.48	0.44
1:C:39:ASN:ND2	2:F:1813:GLY:O	2.51	0.44
2:E:1751:LEU:HD22	2:E:1847:VAL:HG21	1.99	0.44
1:C:69:PRO:HA	1:C:72:TYR:CE2	2.53	0.44
1:C:90:PHE:CE2	1:C:145:MET:HE3	2.53	0.44
2:E:1806:GLU:HB2	2:E:1816:ILE:HG22	2.00	0.44
2:D:1650:GLU:CD	2:D:1650:GLU:H	2.22	0.43
2:E:1775:ASP:O	2:E:1836:LEU:HD12	2.18	0.43
2:E:1816:ILE:HD12	2:E:1816:ILE:O	2.18	0.43
2:F:1650:GLU:CD	2:F:1650:GLU:H	2.21	0.43
1:A:164:GLY:O	1:A:168:VAL:HG23	2.18	0.43
2:D:1679:THR:O	2:D:1679:THR:CG2	2.63	0.43
2:F:1947:VAL:HG23	2:F:2055:ASP:CG	2.37	0.43
1:A:7:VAL:HA	1:A:56:TRP:HB2	2.01	0.43
2:D:1775:ASP:O	2:D:1836:LEU:HD12	2.17	0.43
2:E:1954:PHE:CE2	2:E:1980:SER:HB3	2.53	0.43
2:E:2033:ILE:O	2:E:2037:LEU:HB2	2.19	0.43
2:E:1914:ILE:CB	2:E:1915:PRO:HD2	2.49	0.43
2:F:1822:VAL:HG13	2:F:1823:THR:HG23	2.00	0.43
1:A:115:THR:CG2	1:A:116:LYS:N	2.81	0.43
2:D:1931:LYS:HG3	2:D:1932:PHE:CD2	2.53	0.43
2:F:1816:ILE:HD11	2:F:1853:LEU:HD21	1.94	0.43
1:B:90:PHE:CE2	1:B:145:MET:CE	3.02	0.43
2:D:1811:VAL:HG13	2:E:1919:LEU:HD21	2.00	0.43
2:E:1822:VAL:HG13	2:E:1823:THR:HG23	2.00	0.43
1:A:155:LEU:HD21	1:A:171:GLU:HG3	2.00	0.43
1:B:98:TYR:CE1	1:B:102:ARG:HG3	2.54	0.43
1:B:108:THR:HA	1:B:109:PRO:HD3	1.98	0.43
1:C:98:TYR:CE1	1:C:102:ARG:HG3	2.54	0.43
2:D:1654:ASP:HA	2:D:1657:ARG:HE	1.84	0.43
2:E:1955:PHE:HZ	2:E:1981:LEU:HB3	1.83	0.43
2:F:1614:LEU:H	2:F:1614:LEU:HD12	1.83	0.43
2:D:1992:ASN:HB3	2:D:1995:PHE:CE1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1679:THR:O	2:E:1679:THR:CG2	2.66	0.43
2:D:1614:LEU:HD12	2:D:1614:LEU:H	1.84	0.43
2:E:1947:VAL:HG23	2:E:2055:ASP:CG	2.38	0.43
2:F:1994:GLN:HG3	2:F:2001:THR:HG21	2.00	0.43
1:A:29:PRO:HA	2:E:1917:ILE:HG22	2.01	0.43
1:A:69:PRO:HA	1:A:72:TYR:CE2	2.54	0.42
2:D:1683:VAL:HA	2:D:1686:LEU:HD12	2.01	0.42
2:F:1596:ARG:HB3	2:F:1597:PRO:HD3	2.01	0.42
2:E:2041:ASP:HB3	2:E:2045:TYR:CE1	2.54	0.42
2:F:1707:LEU:CD2	2:F:1989:ILE:CG2	2.97	0.42
1:B:39:ASN:HD21	2:E:1814:HIS:HB3	1.81	0.42
2:F:1569:LYS:HG3	2:F:2082:LEU:HD23	2.01	0.42
2:F:1676:LEU:HA	2:F:1684:GLU:OE2	2.19	0.42
4:A:200:GNP:H5'2	4:A:200:GNP:C8	2.47	0.42
1:B:69:PRO:HA	1:B:72:TYR:CE2	2.55	0.42
2:E:1572:ALA:HB1	2:E:1576:PHE:CE1	2.55	0.42
1:A:25:THR:HG22	2:E:2036:LEU:HB2	2.01	0.42
1:B:86:SER:HA	1:B:87:PRO:HD3	1.89	0.42
4:B:200:GNP:H5'2	4:B:200:GNP:C8	2.46	0.42
2:D:2033:ILE:O	2:D:2037:LEU:HB2	2.19	0.42
2:E:1650:GLU:H	2:E:1650:GLU:CD	2.22	0.42
2:F:1654:ASP:HA	2:F:1657:ARG:HE	1.85	0.42
2:F:1703:VAL:HG22	2:F:1939:VAL:HG12	2.02	0.42
1:B:7:VAL:HA	1:B:56:TRP:HB2	2.01	0.42
1:C:92:ASN:HA	1:C:95:ALA:HB3	2.01	0.42
2:D:1806:GLU:HB2	2:D:1816:ILE:HG22	2.00	0.42
2:F:1775:ASP:O	2:F:1836:LEU:HD12	2.19	0.42
1:C:90:PHE:CE2	1:C:145:MET:CE	3.02	0.42
2:D:1919:LEU:HD21	2:F:1811:VAL:HG13	2.00	0.42
2:D:1694:CYS:HB3	2:D:1950:ALA:HB2	2.01	0.42
2:E:1654:ASP:HA	2:E:1657:ARG:HE	1.85	0.42
2:F:2033:ILE:O	2:F:2037:LEU:HB2	2.19	0.42
2:F:2041:ASP:HB3	2:F:2045:TYR:CE1	2.54	0.42
1:A:98:TYR:CE1	1:A:102:ARG:HG3	2.54	0.42
2:D:1954:PHE:CE2	2:D:1980:SER:HB3	2.54	0.42
2:D:2041:ASP:HB3	2:D:2045:TYR:CE1	2.55	0.42
2:E:1703:VAL:HG22	2:E:1939:VAL:HG12	2.01	0.42
2:E:1789:TYR:O	2:E:1797:ARG:NH2	2.53	0.42
2:F:1994:GLN:CD	2:F:2001:THR:OG1	2.58	0.42
2:D:1749:LEU:HB2	2:D:1771:VAL:HG23	2.02	0.42
2:E:1751:LEU:HD13	2:E:1847:VAL:CG2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1755:LEU:HG	2:F:1757:VAL:HG23	2.02	0.42
1:A:86:SER:HA	1:A:87:PRO:HD3	1.88	0.41
2:D:1599:VAL:HG22	2:D:2128:VAL:HA	2.02	0.41
2:F:1991:LYS:HE2	2:F:2010:LEU:CD1	2.50	0.41
1:B:164:GLY:O	1:B:168:VAL:HG23	2.20	0.41
2:D:1816:ILE:O	2:D:1816:ILE:HD12	2.20	0.41
2:D:1572:ALA:HB1	2:D:1576:PHE:CE1	2.55	0.41
2:F:1955:PHE:HZ	2:F:1981:LEU:HB3	1.84	0.41
2:F:2009:LEU:HA	2:F:2012:ILE:HD12	2.02	0.41
2:F:1751:LEU:HD13	2:F:1847:VAL:HG23	2.03	0.41
1:A:155:LEU:HB3	1:A:168:VAL:HG22	2.02	0.41
1:B:90:PHE:CE2	1:B:145:MET:HE3	2.55	0.41
1:B:92:ASN:HA	1:B:95:ALA:HB3	2.03	0.41
2:F:1599:VAL:HG22	2:F:2128:VAL:HA	2.02	0.41
2:D:1707:LEU:CD2	2:D:1989:ILE:HG22	2.50	0.41
2:F:1789:TYR:O	2:F:1797:ARG:NH2	2.54	0.41
1:A:87:PRO:HA	1:A:137:ILE:HD11	2.03	0.41
2:D:1717:GLN:CG	2:D:1928:THR:HG21	2.49	0.41
2:E:1723:VAL:HG22	2:E:1730:ALA:HB2	2.02	0.41
2:E:1799:ASP:OD2	2:E:1801:ARG:HB2	2.21	0.41
2:F:1723:VAL:HG22	2:F:1730:ALA:HB2	2.02	0.41
2:D:1596:ARG:HB3	2:D:1597:PRO:HD3	2.02	0.41
2:D:1723:VAL:HG22	2:D:1730:ALA:HB2	2.02	0.41
2:D:1853:LEU:HD12	2:D:1853:LEU:C	2.41	0.41
2:E:1599:VAL:HG22	2:E:2128:VAL:HA	2.02	0.41
2:E:1683:VAL:HA	2:E:1686:LEU:HD12	2.01	0.41
1:A:92:ASN:HA	1:A:95:ALA:HB3	2.03	0.41
1:A:161:THR:CB	1:A:163:ARG:HG3	2.49	0.41
1:C:87:PRO:HA	1:C:137:ILE:HD11	2.03	0.41
2:D:1769:VAL:HG21	2:D:1784:MET:HA	2.02	0.41
2:E:1751:LEU:HD13	2:E:1847:VAL:HG23	2.03	0.41
2:E:1937:PHE:N	2:E:1937:PHE:CD1	2.88	0.41
2:F:1749:LEU:HB2	2:F:1771:VAL:HG23	2.02	0.41
2:F:1769:VAL:HG21	2:F:1784:MET:HA	2.03	0.41
1:A:90:PHE:CE2	1:A:145:MET:CE	3.04	0.41
1:A:154:TYR:O	1:A:155:LEU:HD12	2.20	0.41
2:E:1717:GLN:CG	2:E:1928:THR:HG21	2.51	0.41
2:E:1842:PRO:HD2	2:E:1845:ALA:HB2	2.03	0.41
2:F:1808:ARG:HG2	2:F:1813:GLY:HA3	2.02	0.41
1:B:4:ILE:HD12	1:B:51:VAL:HG11	2.04	0.40
2:E:1596:ARG:HB3	2:E:1597:PRO:HD3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25:THR:HG22	2:F:2036:LEU:HB2	2.02	0.40
1:C:108:THR:HA	1:C:109:PRO:HD3	1.98	0.40
2:D:1600:GLU:HA	2:D:1603:LEU:HD12	2.04	0.40
2:D:1811:VAL:CG1	2:E:1919:LEU:HD21	2.51	0.40
2:F:1683:VAL:HA	2:F:1686:LEU:HD12	2.02	0.40
2:F:1738:ARG:HD2	2:F:2004:ASN:HA	2.03	0.40
1:B:19:LEU:CD1	1:B:165:LEU:CG	3.00	0.40
1:B:161:THR:CB	1:B:163:ARG:HG3	2.49	0.40
1:C:4:ILE:HD12	1:C:51:VAL:HG11	2.03	0.40
1:C:164:GLY:O	1:C:168:VAL:HG23	2.21	0.40
4:C:200:GNP:H5'2	4:C:200:GNP:C8	2.47	0.40
2:D:1684:GLU:HB3	2:D:1984:ARG:HH22	1.85	0.40
2:D:1755:LEU:HG	2:D:1757:VAL:HG23	2.04	0.40
2:F:1572:ALA:HB1	2:F:1576:PHE:CE1	2.57	0.40
2:F:1882:ARG:HA	2:F:1883:PRO:HD3	1.98	0.40
1:B:39:ASN:HB2	2:E:1812:ALA:HB3	2.04	0.40
2:F:1751:LEU:HD13	2:F:1847:VAL:CG2	2.51	0.40
1:A:108:THR:HA	1:A:109:PRO:HD3	1.99	0.40
2:F:1629:PHE:CE2	2:F:1634:ARG:HG2	2.56	0.40
2:F:1799:ASP:OD2	2:F:1801:ARG:HB2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	176/184 (96%)	162 (92%)	14 (8%)	0	100 100
1	B	176/184 (96%)	163 (93%)	13 (7%)	0	100 100
1	C	176/184 (96%)	161 (92%)	15 (8%)	0	100 100
2	D	493/633 (78%)	430 (87%)	59 (12%)	4 (1%)	19 60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	495/633 (78%)	431 (87%)	61 (12%)	3 (1%)	25	65
2	F	496/633 (78%)	430 (87%)	63 (13%)	3 (1%)	25	65
All	All	2012/2451 (82%)	1777 (88%)	225 (11%)	10 (0%)	29	68

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	2039	ALA
2	E	1670	LYS
2	E	2039	ALA
2	F	2039	ALA
2	D	1670	LYS
2	D	1587	ARG
2	F	1670	LYS
2	D	1813	GLY
2	E	1813	GLY
2	F	1813	GLY

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	154/160 (96%)	154 (100%)	0	100	100
1	B	154/160 (96%)	152 (99%)	2 (1%)	69	82
1	C	154/160 (96%)	154 (100%)	0	100	100
2	D	448/563 (80%)	443 (99%)	5 (1%)	73	85
2	E	450/563 (80%)	443 (98%)	7 (2%)	62	79
2	F	450/563 (80%)	441 (98%)	9 (2%)	55	74
All	All	1810/2169 (83%)	1787 (99%)	23 (1%)	69	82

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	65	ASP
1	B	85	VAL
2	D	1790	LYS
2	D	1832	ARG
2	D	1984	ARG
2	D	2017	MET
2	D	2078	TYR
2	E	1790	LYS
2	E	1832	ARG
2	E	1881	ILE
2	E	1932	PHE
2	E	1984	ARG
2	E	2017	MET
2	E	2078	TYR
2	F	1736	ASP
2	F	1790	LYS
2	F	1832	ARG
2	F	1852	CYS
2	F	1914	ILE
2	F	1932	PHE
2	F	1984	ARG
2	F	2017	MET
2	F	2078	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	39	ASN
1	C	39	ASN
2	D	1611	ASN
2	D	1671	ASN
2	D	1930	GLN
2	D	1961	GLN
2	D	1964	GLN
2	D	1992	ASN
2	D	2000	GLN
2	D	2068	ASN
2	D	2089	HIS
2	E	1611	ASN
2	E	1671	ASN
2	E	1930	GLN
2	E	1961	GLN
2	E	1992	ASN

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Mol	Chain	Res	Type
2	E	2000	GLN
2	E	2089	HIS
2	F	1611	ASN
2	F	1671	ASN
2	F	1930	GLN
2	F	1961	GLN
2	F	1979	ASN
2	F	1992	ASN
2	F	2000	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 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	GNP	A	200	3	29,34,34	1.62	5 (17%)	33,54,54	2.36	13 (39%)
4	GNP	B	200	3	29,34,34	1.72	6 (20%)	33,54,54	2.39	11 (33%)
4	GNP	C	200	3	29,34,34	1.52	6 (20%)	33,54,54	2.42	13 (39%)

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	GNP	A	200	3	-	6/14/38/38	0/3/3/3
4	GNP	B	200	3	-	6/14/38/38	0/3/3/3
4	GNP	C	200	3	-	6/14/38/38	0/3/3/3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	200	GNP	O4'-C1'	4.03	1.46	1.41
4	A	200	GNP	O4'-C1'	4.02	1.46	1.41
4	C	200	GNP	O4'-C1'	3.53	1.46	1.41
4	B	200	GNP	C2'-C1'	3.34	1.58	1.53
4	A	200	GNP	C2'-C1'	3.02	1.58	1.53
4	B	200	GNP	C6-N1	2.67	1.37	1.33
4	B	200	GNP	C5-C6	2.54	1.45	1.41
4	B	200	GNP	PB-N3B	2.49	1.69	1.63
4	C	200	GNP	C6-N1	2.45	1.37	1.33
4	A	200	GNP	PB-N3B	2.43	1.69	1.63
4	A	200	GNP	C5-C6	2.35	1.45	1.41
4	C	200	GNP	C2'-C1'	2.35	1.57	1.53
4	C	200	GNP	C2-N2	2.33	1.38	1.33
4	C	200	GNP	C5-C6	2.31	1.45	1.41
4	A	200	GNP	C6-N1	2.27	1.37	1.33
4	B	200	GNP	C4-N3	2.17	1.39	1.35
4	C	200	GNP	PB-N3B	2.07	1.68	1.63

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	200	GNP	C2-N3-C4	6.46	122.74	115.36
4	A	200	GNP	C2-N3-C4	6.14	122.37	115.36
4	B	200	GNP	PB-O3A-PA	-6.00	111.50	132.62
4	C	200	GNP	PB-O3A-PA	-5.95	111.68	132.62
4	B	200	GNP	C2-N3-C4	5.81	121.99	115.36
4	A	200	GNP	PB-O3A-PA	-5.80	112.18	132.62
4	C	200	GNP	N3-C2-N1	-4.88	120.71	127.22
4	B	200	GNP	C4-C5-C6	-4.71	116.30	120.80
4	B	200	GNP	N3-C2-N1	-4.56	121.13	127.22
4	A	200	GNP	N3-C2-N1	-4.43	121.31	127.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	200	GNP	C4-C5-C6	-4.34	116.65	120.80
4	B	200	GNP	O2B-PB-O1B	-3.76	102.04	109.92
4	C	200	GNP	C4-C5-C6	-3.72	117.25	120.80
4	C	200	GNP	O2B-PB-O1B	-3.62	102.33	109.92
4	A	200	GNP	O2B-PB-O1B	-3.59	102.39	109.92
4	B	200	GNP	O2B-PB-O3A	3.20	115.34	104.64
4	C	200	GNP	O2B-PB-O3A	3.04	114.78	104.64
4	A	200	GNP	O2B-PB-O3A	3.02	114.73	104.64
4	B	200	GNP	C2-N1-C6	2.65	120.14	115.93
4	C	200	GNP	C2-N1-C6	2.64	120.12	115.93
4	C	200	GNP	O1B-PB-N3B	2.55	115.53	111.77
4	A	200	GNP	C2-N1-C6	2.47	119.86	115.93
4	C	200	GNP	C3'-C2'-C1'	2.47	104.70	100.98
4	B	200	GNP	O1B-PB-N3B	2.44	115.36	111.77
4	B	200	GNP	O2G-PG-O1G	-2.34	107.56	113.45
4	A	200	GNP	C3'-C2'-C1'	2.28	104.42	100.98
4	C	200	GNP	C5-C6-N1	-2.28	120.31	123.43
4	A	200	GNP	O1B-PB-N3B	2.27	115.12	111.77
4	A	200	GNP	O2G-PG-O3G	2.25	113.63	107.64
4	C	200	GNP	O2G-PG-O3G	2.21	113.53	107.64
4	B	200	GNP	C3'-C2'-C1'	2.19	104.28	100.98
4	C	200	GNP	O2G-PG-O1G	-2.18	107.98	113.45
4	A	200	GNP	O2G-PG-O1G	-2.13	108.11	113.45
4	B	200	GNP	O2G-PG-O3G	2.08	113.17	107.64
4	A	200	GNP	C5-C6-N1	-2.02	120.67	123.43
4	A	200	GNP	O3G-PG-O1G	-2.02	108.39	113.45
4	C	200	GNP	C4-C5-N7	-2.01	107.30	109.40

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	200	GNP	PB-N3B-PG-O1G
4	A	200	GNP	PG-N3B-PB-O1B
4	A	200	GNP	PG-N3B-PB-O3A
4	A	200	GNP	C5'-O5'-PA-O3A
4	A	200	GNP	C5'-O5'-PA-O1A
4	B	200	GNP	PB-N3B-PG-O1G
4	B	200	GNP	PG-N3B-PB-O1B
4	B	200	GNP	PG-N3B-PB-O3A
4	B	200	GNP	C5'-O5'-PA-O3A
4	B	200	GNP	C5'-O5'-PA-O1A

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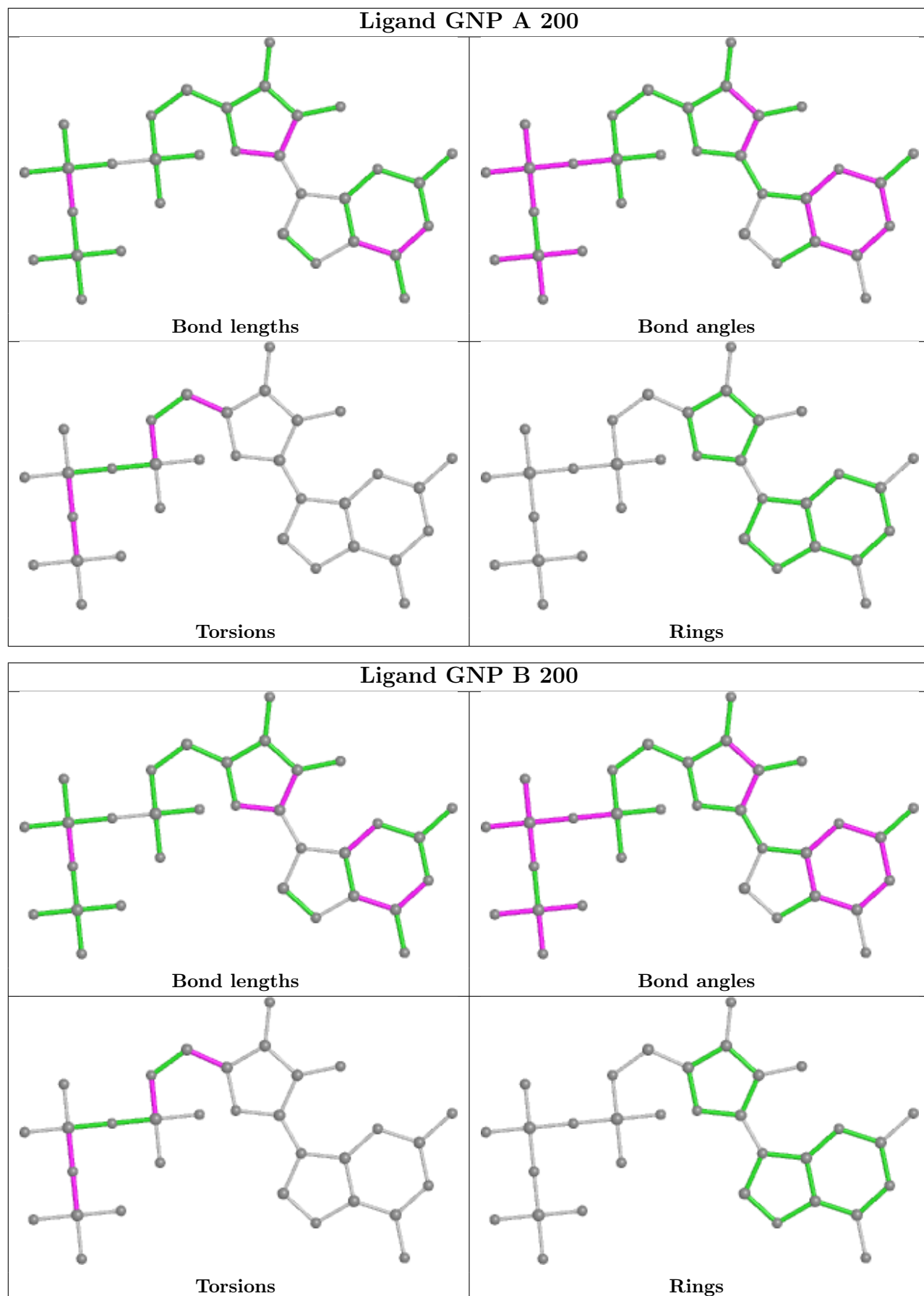
Mol	Chain	Res	Type	Atoms
4	C	200	GNP	PB-N3B-PG-O1G
4	C	200	GNP	PG-N3B-PB-O1B
4	C	200	GNP	PG-N3B-PB-O3A
4	C	200	GNP	C5'-O5'-PA-O3A
4	C	200	GNP	C5'-O5'-PA-O1A
4	A	200	GNP	O4'-C4'-C5'-O5'
4	B	200	GNP	O4'-C4'-C5'-O5'
4	C	200	GNP	O4'-C4'-C5'-O5'

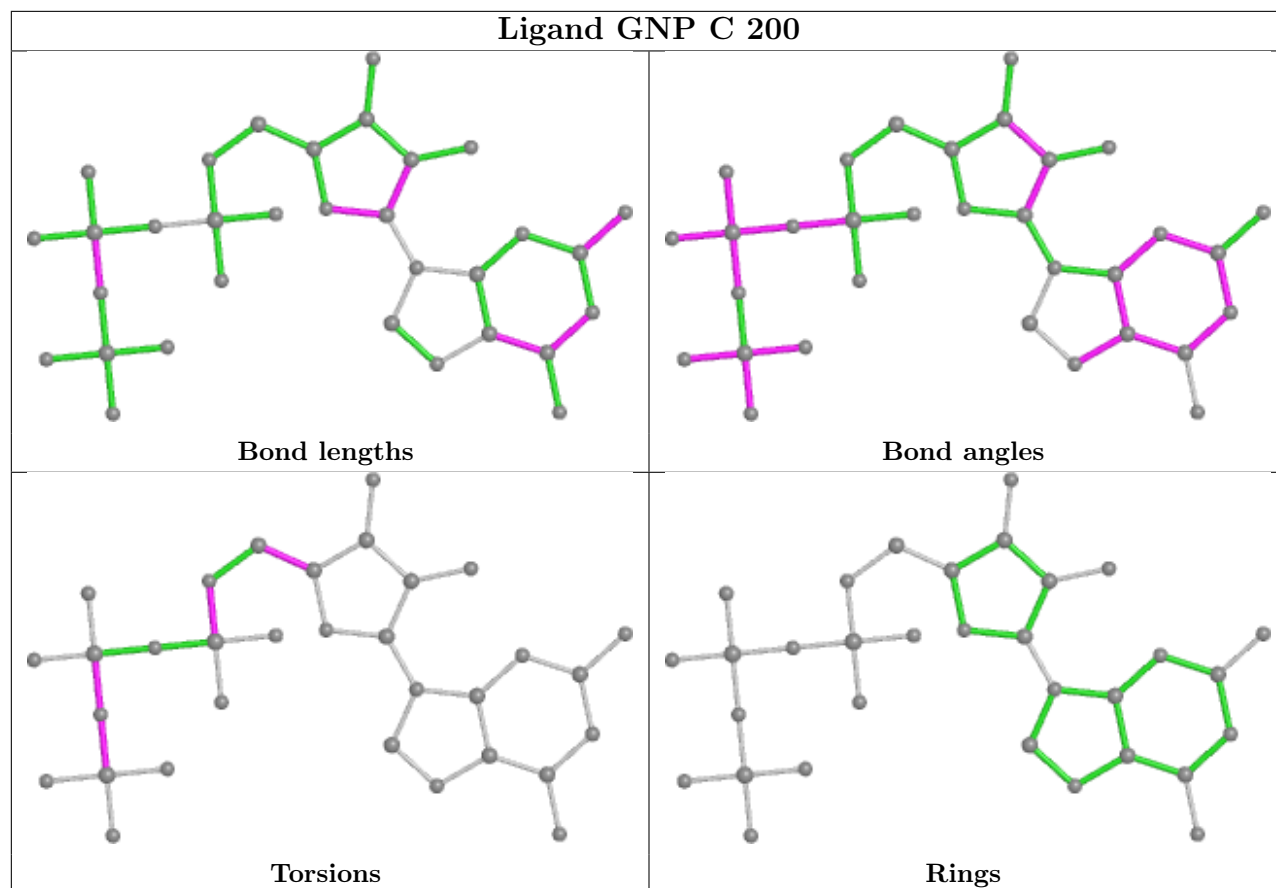
There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	200	GNP	3	0
4	B	200	GNP	3	0
4	C	200	GNP	3	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	178/184 (96%)	0.23	9 (5%) 28 24	41, 112, 244, 271	0
1	B	178/184 (96%)	0.25	4 (2%) 62 52	20, 92, 190, 252	0
1	C	178/184 (96%)	0.59	18 (10%) 7 7	46, 138, 250, 281	0
2	D	503/633 (79%)	0.17	27 (5%) 25 22	21, 90, 253, 287	0
2	E	505/633 (79%)	0.12	12 (2%) 59 49	21, 120, 266, 296	0
2	F	506/633 (79%)	0.18	28 (5%) 25 22	20, 101, 257, 281	0
All	All	2048/2451 (83%)	0.21	98 (4%) 30 26	20, 107, 255, 296	0

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	1722	PRO	5.3
2	E	1591	VAL	4.5
2	F	1961	GLN	4.3
2	F	1882	ARG	4.3
2	D	1733	THR	4.2
2	F	1890	SER	4.2
2	D	1967	ILE	4.1
2	D	2023	ALA	3.8
1	C	11	ASP	3.5
2	D	1889	PRO	3.4
2	F	1883	PRO	3.4
2	D	1825	GLU	3.3
2	D	1624	GLU	3.3
1	C	80	ILE	3.3
1	C	85	VAL	3.3
1	B	2	GLN	3.2
2	F	1825	GLU	3.2
2	D	1890	SER	3.2
2	D	1962	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
2	E	1671	ASN	3.2
2	F	1588	ASP	3.2
2	E	1590	GLY	3.1
1	C	178	LYS	3.1
1	C	159	ALA	3.1
2	D	1738	ARG	3.0
1	C	154	TYR	3.0
2	F	1671	ASN	3.0
2	F	2115	MET	3.0
2	F	1742	GLU	3.0
2	E	1885	HIS	2.9
1	C	171	GLU	2.9
2	E	2023	ALA	2.9
2	F	1745	GLU	2.9
2	D	1854	THR	2.9
2	F	1959	ASP	2.9
2	D	1880	GLY	2.8
1	A	177	LEU	2.8
2	F	1668	VAL	2.8
1	C	112	LEU	2.8
2	F	1886	LEU	2.8
1	A	132	LYS	2.8
2	F	1887	VAL	2.6
1	B	47	ASP	2.6
2	F	1589	LEU	2.6
2	F	1672	PRO	2.6
2	D	1740	LEU	2.6
1	B	46	VAL	2.5
1	C	119	LEU	2.5
2	E	1742	GLU	2.5
2	F	1746	TYR	2.5
2	D	2128	VAL	2.5
2	D	1729	LYS	2.5
2	F	1968	SER	2.5
2	F	1889	PRO	2.5
2	D	1972	THR	2.5
1	C	12	GLY	2.5
2	E	2062	ALA	2.4
1	C	120	ARG	2.4
2	D	1966	GLY	2.4
1	A	159	ALA	2.4
2	D	1886	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
2	D	1673	LYS	2.3
2	F	1963	GLN	2.3
2	D	1629	PHE	2.3
2	D	1965	HIS	2.3
1	A	130	LYS	2.3
2	D	2129	GLU	2.3
1	C	149	ILE	2.3
2	E	1757	VAL	2.3
1	C	174	ARG	2.3
2	F	1723	VAL	2.3
2	F	2004	ASN	2.2
2	D	1628	THR	2.2
2	F	1744	VAL	2.2
1	C	156	GLU	2.2
1	A	133	LYS	2.2
2	D	1887	VAL	2.2
1	A	156	GLU	2.1
1	B	4	ILE	2.1
2	E	1887	VAL	2.1
2	F	1675	MET	2.1
2	F	1964	GLN	2.1
2	D	1739	LEU	2.1
2	D	1963	GLN	2.1
2	E	1886	LEU	2.1
1	C	153	LYS	2.1
2	F	2062	ALA	2.1
1	A	174	ARG	2.1
2	E	1722	PRO	2.1
1	A	131	GLU	2.1
2	F	1962	ALA	2.1
1	C	94	ARG	2.1
2	D	1852	CYS	2.1
2	E	1592	PRO	2.0
1	C	84	LEU	2.0
1	C	81	CYS	2.0
1	A	123	LYS	2.0
2	D	1736	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates [i](#)

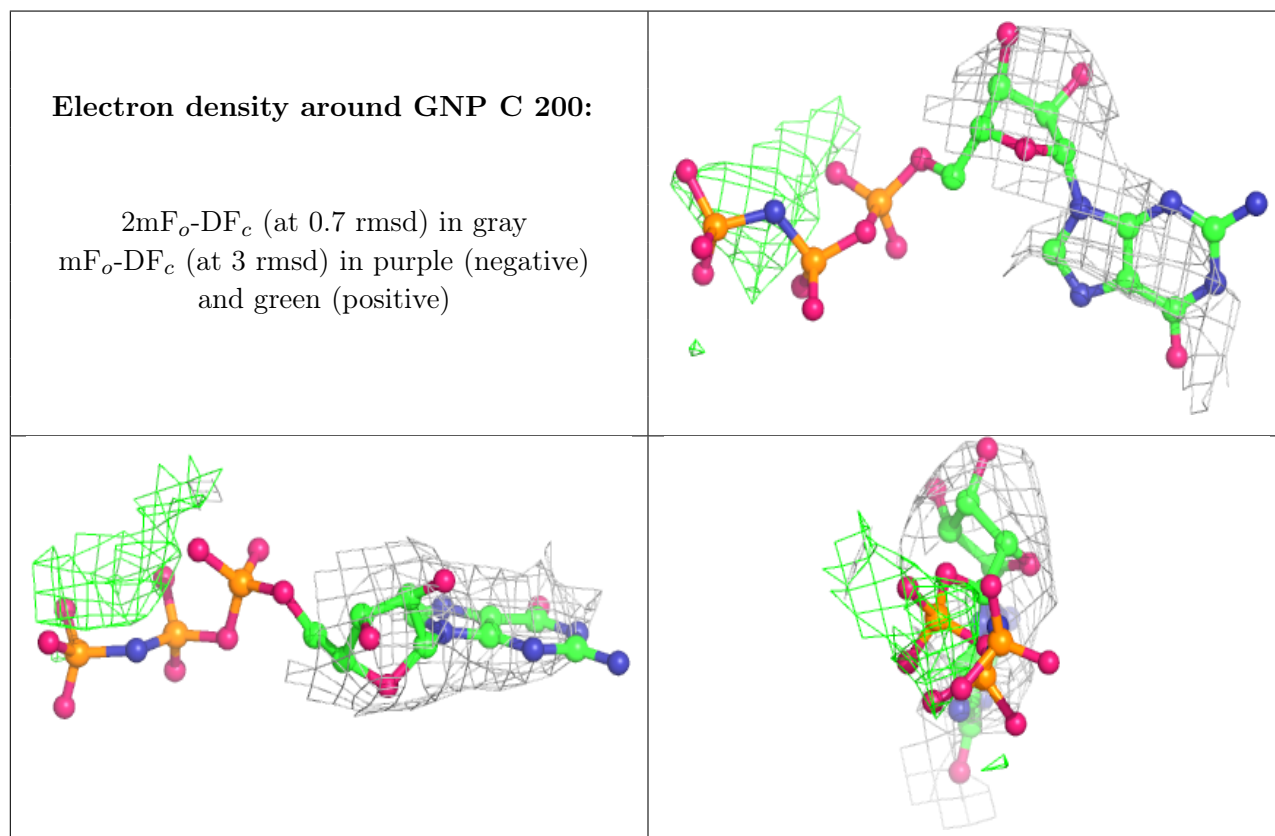
There are no monosaccharides in this entry.

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.

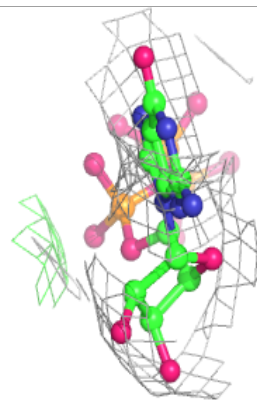
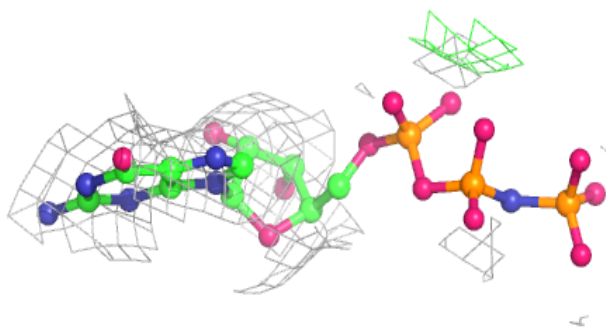
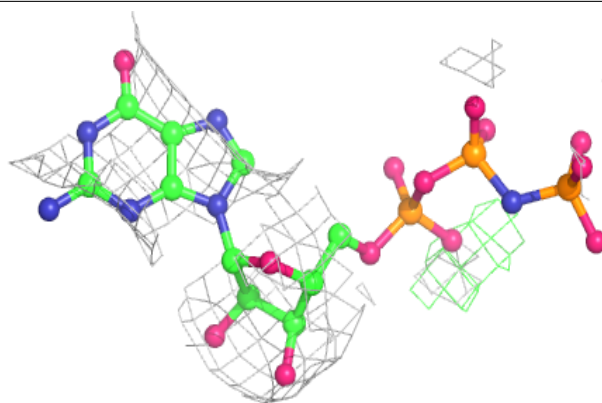
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	GNP	C	200	32/32	0.87	0.29	99,127,142,151	0
4	GNP	A	200	32/32	0.88	0.26	69,89,107,121	0
4	GNP	B	200	32/32	0.90	0.27	47,62,77,79	0
3	MG	B	201	1/1	0.94	0.16	19,19,19,19	0
3	MG	A	201	1/1	0.97	0.09	38,38,38,38	0
3	MG	C	201	1/1	0.98	0.16	57,57,57,57	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

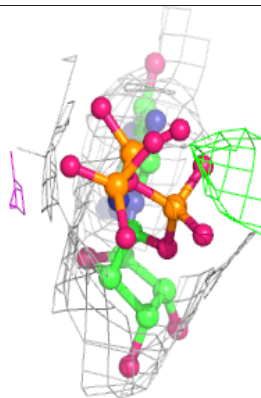
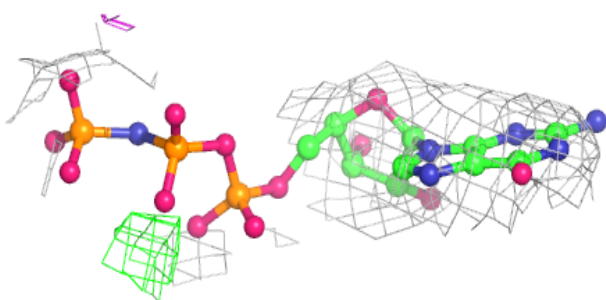
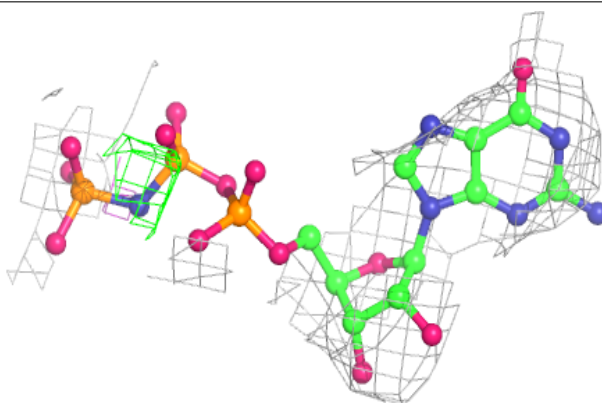


Electron density around GNP A 200:

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

**Electron density around GNP B 200:**

$2mF_o-DF_c$ (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.