Full wwPDB X-ray Structure Validation Report (i)

Oct 22, 2023 – 05:45 PM EDT

PDB ID	:	3DEJ
Title	:	Crystal Structures of Caspase-3 with Bound Isoquinoline-1,3,4-trione Derivative Inhibitors
Authors	:	Wu, J.; Du, J.; Li, J.; Ding, J.
Deposited on	:	2008-06-10
Resolution	:	2.60 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 (i) 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 (i)) were used in the production of this report:

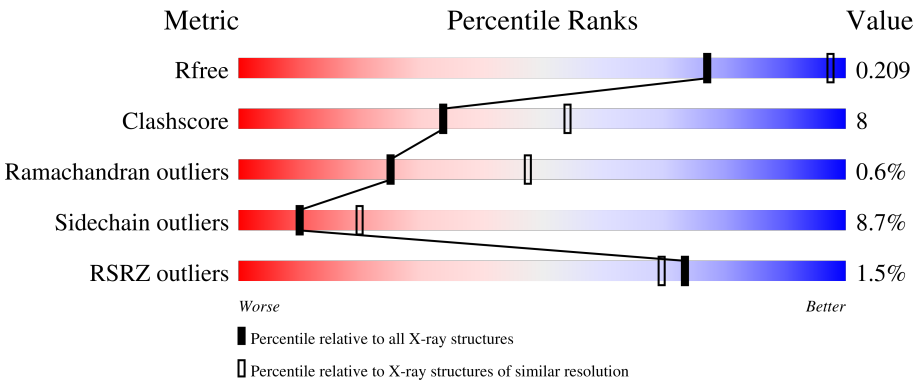
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 <=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	249	70% 20% • 6%
1	B	249	% 71% 21% • 6%
1	C	249	3% 67% 23% • 6%
1	D	249	2% 63% 27% • 8%

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
2	RXC	C	300	-	-	X	X

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7701 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.

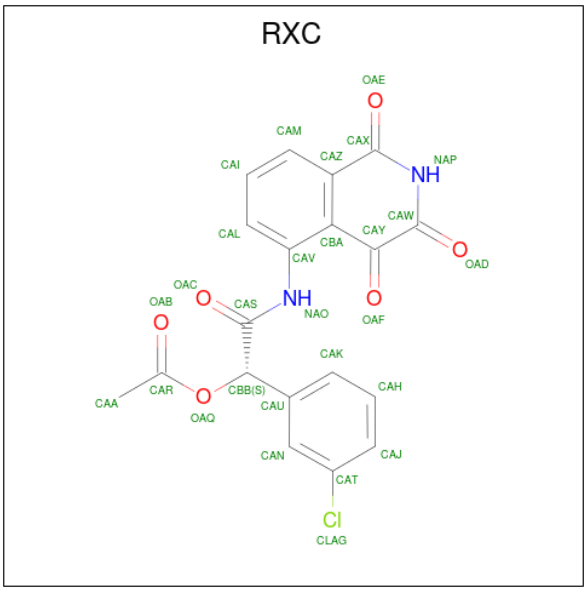
- Molecule 1 is a protein called Caspase-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	233	1890	1196	324	356	14	0	0	0
1	B	235	1908	1206	328	360	14	0	0	0
1	C	233	1890	1196	324	356	14	0	0	0
1	D	229	1861	1181	320	346	14	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	190	ASP	GLU	SEE REMARK 999	UNP P42574
B	190	ASP	GLU	SEE REMARK 999	UNP P42574
C	190	ASP	GLU	SEE REMARK 999	UNP P42574
D	190	ASP	GLU	SEE REMARK 999	UNP P42574

- Molecule 2 is (1S)-1-(3-chlorophenyl)-2-oxo-2-[(1,3,4-trioxo-1,2,3,4-tetrahydroisoquinolin-5-yl)amino]ethyl acetate (three-letter code: RXC) (formula: $C_{19}H_{13}ClN_2O_6$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Cl	N	O		
2	C	1	28	19	1	2	6	0	0

- Molecule 3 is water.

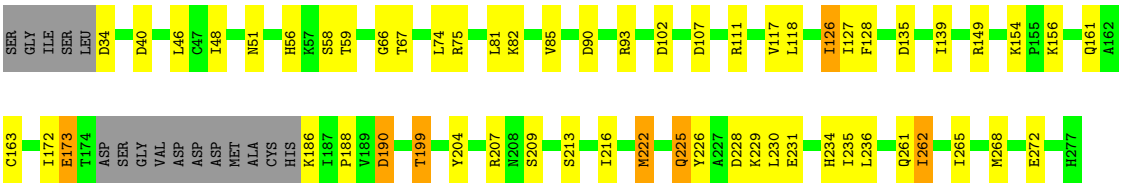
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	53	53	53	0	0
			Total	O		
3	B	40	40	40	0	0
			Total	O		
3	C	22	22	22	0	0
			Total	O		
3	D	9	9	9	0	0

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.

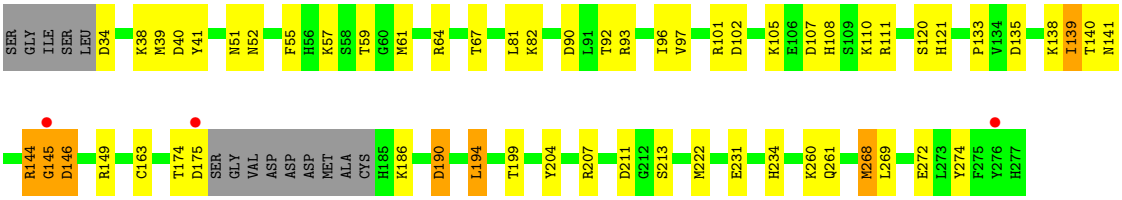
- Molecule 1: Caspase-3

Chain A:



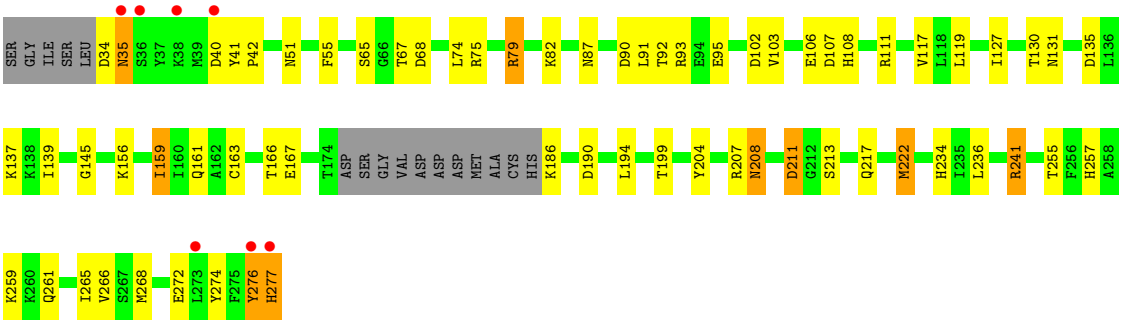
- Molecule 1: Caspase-3

Chain B:



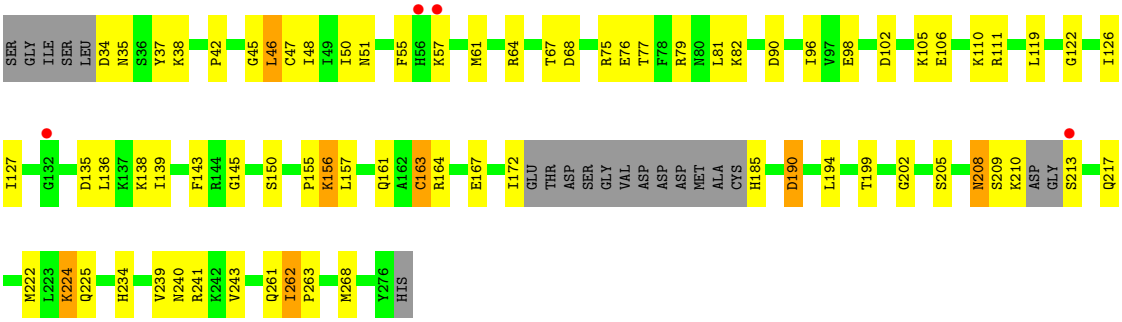
- Molecule 1: Caspase-3

Chain C:



- Molecule 1: Caspase-3

Chain D:


SER
GLY
ILE
SER
LEU
D34
N35
S36
Y37
K38
P42
G45
L46
C47
I48
I49
I50
N51
F55
H56
K57
M61
R64
T67
D68
R75
E76
T77
F78
R79
N80
L81
K82
D90
I96
V97
E98
D102
K105
E106
K110
R111
L119
G122
I126
I127
G132
D135
L136
K137
K138
I139
F143
R144
G145
S150
P155
K156
L157
Q161
A162
C163
R164
E167
I172
GLU
THR
ASP
SER
GLY
VAL
ASP
ASP
ASP
MET
ALA
CYS
H185
D190
L194
T199
G202
S205
N208
S209
K210
ASP
GLY
S213
Q217
M222
L223
K224
Q225
H234
V239
N240
R241
K242
V243
Q261
I262
P263
M268
Y276
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	65.43Å 96.67Å 180.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.45 – 2.60 46.45 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.2 (46.45-2.60) 99.2 (46.45-2.60)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.49 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.214 , 0.274 0.217 , 0.209	Depositor DCC
R_{free} test set	1783 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	52.4	Xtriage
Anisotropy	0.193	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 42.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7701	wwPDB-VP
Average B, all atoms (Å^2)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.29% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: OCS, RXC

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	0.57	0/1919	0.81	8/2576 (0.3%)
1	B	0.53	0/1938	0.81	8/2602 (0.3%)
1	C	0.49	0/1919	0.78	9/2576 (0.3%)
1	D	0.43	0/1889	0.73	5/2535 (0.2%)
All	All	0.51	0/7665	0.78	30/10289 (0.3%)

There are no bond length outliers.

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	190	ASP	CB-CG-OD2	8.71	126.14	118.30
1	A	190	ASP	CB-CG-OD2	7.31	124.88	118.30
1	D	102	ASP	CB-CG-OD2	6.72	124.35	118.30
1	D	190	ASP	CB-CG-OD2	6.69	124.32	118.30
1	B	135	ASP	CB-CG-OD2	6.68	124.31	118.30
1	A	102	ASP	CB-CG-OD2	6.67	124.30	118.30
1	A	135	ASP	CB-CG-OD2	6.32	123.99	118.30
1	C	102	ASP	CB-CG-OD2	6.13	123.82	118.30
1	B	34	ASP	CB-CG-OD2	5.96	123.66	118.30
1	C	135	ASP	CB-CG-OD2	5.90	123.61	118.30
1	D	68	ASP	CB-CG-OD2	5.69	123.42	118.30
1	C	211	ASP	CB-CG-OD2	5.63	123.37	118.30
1	B	40	ASP	CB-CG-OD2	5.59	123.33	118.30
1	A	40	ASP	CB-CG-OD2	5.58	123.32	118.30
1	A	228	ASP	CB-CG-OD2	5.55	123.30	118.30
1	C	190	ASP	CB-CG-OD2	5.54	123.29	118.30
1	C	90	ASP	CB-CG-OD2	5.54	123.29	118.30
1	C	68	ASP	CB-CG-OD2	5.50	123.25	118.30
1	B	146	ASP	CB-CG-OD2	5.47	123.22	118.30
1	D	135	ASP	CB-CG-OD2	5.45	123.20	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	90	ASP	CB-CG-OD2	5.44	123.20	118.30
1	C	34	ASP	CB-CG-OD2	5.44	123.20	118.30
1	D	34	ASP	CB-CG-OD2	5.42	123.17	118.30
1	A	34	ASP	CB-CG-OD2	5.40	123.16	118.30
1	C	107	ASP	CB-CG-OD2	5.30	123.07	118.30
1	A	107	ASP	CB-CG-OD2	5.25	123.02	118.30
1	B	102	ASP	CB-CG-OD2	5.18	122.97	118.30
1	B	107	ASP	CB-CG-OD2	5.18	122.96	118.30
1	C	40	ASP	CB-CG-OD2	5.16	122.94	118.30
1	A	90	ASP	CB-CG-OD2	5.05	122.85	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1890	0	1859	39	0
1	B	1908	0	1870	31	0
1	C	1890	0	1858	35	0
1	D	1861	0	1838	30	0
2	C	28	0	13	9	0
3	A	53	0	0	2	0
3	B	40	0	0	0	0
3	C	22	0	0	0	0
3	D	9	0	0	0	0
All	All	7701	0	7438	127	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 8.

All (127) 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:255:THR:CG2	2:C:300:RXC:HAH	1.76	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:255:THR:HG23	2:C:300:RXC:CAH	1.81	1.10
1:C:166:THR:O	2:C:300:RXC:HAL	1.59	1.00
1:C:255:THR:HG23	2:C:300:RXC:HAH	0.91	0.88
1:D:262:ILE:HD13	1:D:263:PRO:HD2	1.56	0.86
1:D:208:ASN:HD22	1:D:209:SER:N	1.83	0.76
1:A:199:THR:HG21	1:A:204:TYR:O	1.86	0.75
1:A:46:LEU:HD11	1:A:111:ARG:CZ	2.16	0.75
1:B:108:HIS:HA	1:B:111:ARG:HD2	1.70	0.72
1:C:208:ASN:ND2	1:C:211:ASP:H	1.89	0.70
1:A:234:HIS:CE1	1:B:234:HIS:CE1	2.81	0.69
1:C:208:ASN:HD22	1:C:211:ASP:H	1.39	0.69
1:B:199:THR:HG22	1:B:261:GLN:HG3	1.73	0.69
1:C:255:THR:CG2	2:C:300:RXC:CAH	2.56	0.68
1:B:199:THR:HG21	1:B:204:TYR:O	1.96	0.65
1:C:199:THR:HG21	1:C:204:TYR:O	1.96	0.65
1:D:42:PRO:HG2	1:D:110:LYS:HD2	1.77	0.65
1:A:225:GLN:O	1:A:225:GLN:HG3	1.95	0.65
1:D:262:ILE:HD13	1:D:263:PRO:CD	2.28	0.63
1:D:37:TYR:CD1	1:D:155:PRO:HD3	2.35	0.62
1:D:122:GLY:O	1:D:163:OCS:HB3	2.00	0.61
1:C:166:THR:O	2:C:300:RXC:OAC	2.19	0.61
1:D:46:LEU:HD13	1:D:48:ILE:HD13	1.82	0.61
1:D:157:LEU:HD23	1:D:194:LEU:HB3	1.81	0.61
1:A:74:LEU:HD13	1:A:117:VAL:HG11	1.81	0.60
1:C:74:LEU:HD13	1:C:117:VAL:HG11	1.81	0.60
1:D:157:LEU:CD2	1:D:194:LEU:HB3	2.33	0.59
1:D:167:GLU:HB2	1:D:202:GLY:O	2.02	0.59
1:D:45:GLY:HA2	1:D:111:ARG:HB3	1.85	0.59
1:D:50:ILE:HD13	1:D:96:ILE:HG12	1.84	0.59
1:A:222:MET:HA	1:A:222:MET:HE2	1.85	0.59
1:A:46:LEU:HD23	1:A:48:ILE:HD11	1.84	0.58
1:D:45:GLY:HA2	1:D:111:ARG:HD3	1.84	0.58
1:A:231:GLU:HG3	1:A:272:GLU:HB3	1.86	0.58
1:D:199:THR:HG23	1:D:261:GLN:HG3	1.86	0.57
1:A:222:MET:HA	1:A:222:MET:CE	2.34	0.57
1:D:208:ASN:HD22	1:D:209:SER:H	1.52	0.57
1:B:93:ARG:HH21	1:B:133:PRO:HD2	1.68	0.56
1:C:35:ASN:HA	1:D:241:ARG:HH12	1.68	0.56
1:C:241:ARG:HH12	1:D:35:ASN:HA	1.72	0.55
1:C:222:MET:HA	1:C:222:MET:CE	2.36	0.55
1:A:199:THR:HG22	1:A:261:GLN:HG3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:ILE:HD11	3:A:280:HOH:O	2.07	0.55
1:B:207:ARG:HA	1:B:213:SER:HA	1.88	0.55
1:A:262:ILE:HD12	1:B:268:MET:HB3	1.90	0.54
1:B:38:LYS:HD3	1:B:41:TYR:CE1	2.43	0.54
1:A:225:GLN:HG2	1:A:226:TYR:CE2	2.43	0.54
1:D:143:PHE:O	1:D:156:LYS:HE2	2.07	0.54
1:C:91:LEU:O	1:C:130:THR:HG23	2.08	0.53
1:A:207:ARG:HG2	1:A:213:SER:HB3	1.89	0.53
1:B:194:LEU:HD12	1:B:269:LEU:HD11	1.90	0.53
1:B:92:THR:O	1:B:96:ILE:HG12	2.09	0.53
1:D:45:GLY:HA2	1:D:111:ARG:CD	2.39	0.52
1:B:55:PHE:HE1	1:B:64:ARG:HG3	1.75	0.52
1:C:75:ARG:O	1:C:79:ARG:HB2	2.10	0.52
1:B:97:VAL:HG21	1:B:138:LYS:HE3	1.92	0.52
1:C:236:LEU:HB3	1:C:265:ILE:HD12	1.93	0.51
2:C:300:RXC:OAF	2:C:300:RXC:NAO	2.30	0.51
1:A:161:GLN:HB2	1:A:216:ILE:HD11	1.92	0.51
1:B:141:ASN:HA	1:B:144:ARG:HG3	1.92	0.51
1:C:119:LEU:HD23	1:C:161:GLN:HB3	1.92	0.51
1:B:144:ARG:O	1:B:146:ASP:N	2.45	0.50
1:A:75:ARG:HG3	1:A:85:VAL:HG11	1.94	0.50
1:C:108:HIS:HA	1:C:111:ARG:HD2	1.93	0.50
1:A:56:HIS:HB3	3:A:302:HOH:O	2.11	0.49
1:B:101:ARG:O	1:B:105:LYS:HG3	2.12	0.49
1:C:194:LEU:HD12	1:C:266:VAL:O	2.12	0.49
1:B:120:SER:OG	1:B:121:HIS:N	2.46	0.49
1:C:222:MET:HA	1:C:222:MET:HE2	1.95	0.48
1:C:213:SER:O	1:C:217:GLN:HB2	2.13	0.48
1:D:240:ASN:HA	1:D:263:PRO:HG2	1.96	0.48
1:B:97:VAL:CG2	1:B:138:LYS:HE3	2.44	0.47
1:A:126:ILE:HD11	1:A:128:PHE:CE2	2.49	0.47
1:A:118:LEU:HD13	1:A:127:ILE:HD13	1.96	0.47
1:C:51:ASN:ND2	1:C:67:THR:OG1	2.48	0.47
1:B:39:MET:HG3	1:B:274:TYR:O	2.15	0.47
1:C:103:VAL:O	1:C:106:GLU:HB2	2.14	0.46
1:D:51:ASN:HD21	1:D:67:THR:CG2	2.28	0.46
1:C:272:GLU:HB3	1:C:274:TYR:CE2	2.50	0.46
1:C:276:TYR:CG	1:C:277:HIS:N	2.83	0.46
2:C:300:RXC:HAL	2:C:300:RXC:OAC	2.15	0.46
1:C:117:VAL:HG22	1:C:159:ILE:HG13	1.96	0.46
1:A:173:GLU:OE1	1:B:149:ARG:NH2	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:LEU:O	1:A:82:LYS:HB2	2.14	0.46
1:B:52:ASN:HB2	1:B:120:SER:HB2	1.98	0.46
1:A:172:ILE:HG12	1:B:145:GLY:O	2.15	0.45
1:A:186:LYS:N	1:B:175:ASP:HA	2.31	0.45
1:D:164:ARG:HD3	1:D:199:THR:O	2.16	0.45
1:D:75:ARG:O	1:D:79:ARG:HB2	2.17	0.45
1:C:55:PHE:CD2	1:C:130:THR:HA	2.52	0.44
1:B:231:GLU:HG3	1:B:272:GLU:HG2	1.99	0.44
1:A:161:GLN:HG2	1:A:216:ILE:HD12	1.99	0.44
1:D:119:LEU:HD23	1:D:161:GLN:HB3	1.98	0.44
1:A:207:ARG:HA	1:A:213:SER:HA	1.98	0.44
1:A:66:GLY:HA3	1:A:209:SER:O	2.19	0.43
1:A:154:LYS:O	1:A:156:LYS:HD3	2.19	0.43
1:C:166:THR:HB	2:C:300:RXC:CAL	2.48	0.43
1:D:208:ASN:ND2	1:D:209:SER:N	2.57	0.43
1:A:186:LYS:O	1:B:260:LYS:HE2	2.19	0.43
1:C:207:ARG:HA	1:C:213:SER:HA	1.99	0.43
1:A:230:LEU:HB2	1:A:235:ILE:CD1	2.48	0.43
1:A:161:GLN:CB	1:A:216:ILE:HD11	2.48	0.43
1:B:139:ILE:HG13	1:B:140:THR:N	2.33	0.43
1:A:46:LEU:CD1	1:A:111:ARG:CZ	2.92	0.42
1:A:51:ASN:HD21	1:A:67:THR:CG2	2.32	0.42
1:A:236:LEU:HD13	1:A:265:ILE:HD12	2.01	0.42
1:B:51:ASN:HD21	1:B:67:THR:CG2	2.32	0.42
1:D:239:VAL:O	1:D:243:VAL:HG23	2.18	0.42
1:A:188:PRO:HG3	1:B:260:LYS:HB3	2.01	0.42
1:B:81:LEU:O	1:B:82:LYS:HB2	2.19	0.42
1:A:226:TYR:HB2	1:A:235:ILE:HD12	2.02	0.42
1:C:92:THR:HB	1:C:131:ASN:OD1	2.20	0.42
1:B:93:ARG:NH2	1:B:133:PRO:HD2	2.35	0.42
1:D:55:PHE:HE1	1:D:64:ARG:HG3	1.85	0.42
1:A:46:LEU:HB3	1:A:48:ILE:HD12	2.01	0.41
1:A:51:ASN:HD21	1:A:67:THR:HG23	1.85	0.41
1:D:224:LYS:HG3	1:D:225:GLN:N	2.36	0.41
1:C:199:THR:HG22	1:C:261:GLN:HG3	2.03	0.41
1:D:81:LEU:O	1:D:82:LYS:HB2	2.20	0.41
1:C:41:TYR:HB3	1:C:42:PRO:HD2	2.02	0.41
1:C:234:HIS:CE1	1:D:234:HIS:CE1	3.09	0.41
1:A:74:LEU:CD1	1:A:117:VAL:HG11	2.50	0.40
1:C:92:THR:HG23	1:C:95:GLU:OE1	2.21	0.40
1:B:51:ASN:HD21	1:B:67:THR:HG23	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:THR:HB	1:B:61:MET:HG3	2.03	0.40
1:A:161:GLN:HB2	1:A:216:ILE:CD1	2.51	0.40
1:C:257:HIS:O	1:C:259:LYS:HE2	2.22	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	228/249 (92%)	223 (98%)	5 (2%)	0	100	100
1	B	230/249 (92%)	221 (96%)	7 (3%)	2 (1%)	17	35
1	C	228/249 (92%)	220 (96%)	7 (3%)	1 (0%)	34	57
1	D	222/249 (89%)	209 (94%)	11 (5%)	2 (1%)	17	35
All	All	908/996 (91%)	873 (96%)	30 (3%)	5 (1%)	25	47

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	145	GLY
1	B	145	GLY
1	D	145	GLY
1	B	174	THR
1	D	106	GLU

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	208/221 (94%)	194 (93%)	14 (7%)	16	33
1	B	210/221 (95%)	200 (95%)	10 (5%)	25	49
1	C	208/221 (94%)	189 (91%)	19 (9%)	9	18
1	D	205/221 (93%)	176 (86%)	29 (14%)	3	6
All	All	831/884 (94%)	759 (91%)	72 (9%)	10	20

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	SER
1	A	59	THR
1	A	93	ARG
1	A	126	ILE
1	A	139	ILE
1	A	149	ARG
1	A	173	GLU
1	A	190	ASP
1	A	199	THR
1	A	222	MET
1	A	225	GLN
1	A	229	LYS
1	A	262	ILE
1	A	268	MET
1	B	57	LYS
1	B	110	LYS
1	B	139	ILE
1	B	144	ARG
1	B	186	LYS
1	B	190	ASP
1	B	194	LEU
1	B	211	ASP
1	B	222	MET
1	B	268	MET
1	C	35	ASN
1	C	65	SER
1	C	79	ARG
1	C	82	LYS
1	C	87	ASN
1	C	93	ARG

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Mol	Chain	Res	Type
1	C	127	ILE
1	C	137	LYS
1	C	139	ILE
1	C	156	LYS
1	C	159	ILE
1	C	167	GLU
1	C	186	LYS
1	C	208	ASN
1	C	222	MET
1	C	241	ARG
1	C	268	MET
1	C	276	TYR
1	C	277	HIS
1	D	38	LYS
1	D	46	LEU
1	D	47	CYS
1	D	57	LYS
1	D	61	MET
1	D	76	GLU
1	D	77	THR
1	D	90	ASP
1	D	98	GLU
1	D	105	LYS
1	D	126	ILE
1	D	127	ILE
1	D	136	LEU
1	D	138	LYS
1	D	139	ILE
1	D	150	SER
1	D	156	LYS
1	D	172	ILE
1	D	185	HIS
1	D	190	ASP
1	D	205	SER
1	D	208	ASN
1	D	210	LYS
1	D	213	SER
1	D	217	GLN
1	D	222	MET
1	D	224	LYS
1	D	262	ILE
1	D	268	MET

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	35	ASN
1	A	51	ASN
1	A	161	GLN
1	A	217	GLN
1	A	234	HIS
1	B	51	ASN
1	B	161	GLN
1	B	217	GLN
1	C	51	ASN
1	C	208	ASN
1	C	217	GLN
1	C	225	GLN
1	D	35	ASN
1	D	51	ASN
1	D	208	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\#\|Z\| > 2$
1	OCS	A	163	1	7,8,9	1.51	2 (28%)	6,11,13	3.08	2 (33%)
1	OCS	B	163	1	7,8,9	1.34	1 (14%)	6,11,13	2.65	2 (33%)
1	OCS	C	163	1	7,8,9	1.03	0	6,11,13	4.93	2 (33%)
1	OCS	D	163	1	7,8,9	1.28	1 (14%)	6,11,13	2.37	3 (50%)

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
1	OCS	A	163	1	-	2/4/7/9	-
1	OCS	B	163	1	-	4/4/7/9	-
1	OCS	C	163	1	-	4/4/7/9	-
1	OCS	D	163	1	-	0/4/7/9	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	163	OCS	CB-SG	-2.43	1.68	1.77
1	D	163	OCS	CB-SG	-2.37	1.68	1.77
1	B	163	OCS	CB-SG	-2.25	1.69	1.77
1	A	163	OCS	OD3-SG	2.21	1.51	1.45

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	163	OCS	OD3-SG-CB	11.45	120.55	106.94
1	A	163	OCS	OD3-SG-CB	6.77	114.98	106.94
1	B	163	OCS	OD3-SG-CB	4.30	112.05	106.94
1	B	163	OCS	OD2-SG-CB	4.17	112.39	105.74
1	D	163	OCS	OD3-SG-CB	3.69	111.32	106.94
1	D	163	OCS	OD1-SG-CB	3.56	111.17	106.94
1	C	163	OCS	OD3-SG-OD1	-2.78	104.34	113.95
1	D	163	OCS	OD3-SG-OD1	-2.07	106.80	113.95
1	A	163	OCS	OD2-SG-CB	2.04	108.98	105.74

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	163	OCS	CA-CB-SG-OD1
1	B	163	OCS	N-CA-CB-SG
1	B	163	OCS	CA-CB-SG-OD1
1	B	163	OCS	CA-CB-SG-OD2
1	B	163	OCS	CA-CB-SG-OD3
1	C	163	OCS	N-CA-CB-SG
1	C	163	OCS	CA-CB-SG-OD1
1	A	163	OCS	CA-CB-SG-OD3

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Mol	Chain	Res	Type	Atoms
1	C	163	OCS	CA-CB-SG-OD3
1	C	163	OCS	CA-CB-SG-OD2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	163	OCS	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand is modelled in this entry.

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	$\#\|Z\| > 2$
2	RXC	C	300	-	30,30,30	3.37	8 (26%)	42,43,43	1.89	10 (23%)

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
2	RXC	C	300	-	-	5/16/32/32	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	300	RXC	CAW-CAY	-15.02	1.39	1.54
2	C	300	RXC	OAQ-CAR	4.96	1.46	1.35
2	C	300	RXC	CAZ-CAX	-4.73	1.39	1.47
2	C	300	RXC	CAT-CLAG	3.63	1.82	1.74
2	C	300	RXC	OAF-CAY	3.06	1.29	1.23
2	C	300	RXC	OAE-CAX	2.54	1.28	1.23
2	C	300	RXC	CBB-CAS	-2.54	1.50	1.53
2	C	300	RXC	CBA-CAY	-2.02	1.41	1.46

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	300	RXC	OAQ-CAR-CAA	4.53	119.43	111.09
2	C	300	RXC	CBB-OAQ-CAR	-3.90	110.12	115.69
2	C	300	RXC	CAZ-CAX-NAP	3.89	118.79	114.86
2	C	300	RXC	CAU-CBB-CAS	3.67	117.56	110.38
2	C	300	RXC	OAQ-CAR-OAB	-3.22	116.56	122.96
2	C	300	RXC	OAE-CAX-CAZ	-2.59	118.81	123.30
2	C	300	RXC	CAV-CBA-CAY	-2.41	117.78	121.14
2	C	300	RXC	CAH-CAK-CAU	-2.36	117.72	120.65
2	C	300	RXC	OAC-CAS-CBB	-2.26	117.47	120.23
2	C	300	RXC	CBA-CAV-NAO	-2.06	115.75	118.52

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	300	RXC	NAO-CAS-CBB-CAU
2	C	300	RXC	OAC-CAS-CBB-CAU
2	C	300	RXC	CAA-CAR-OAQ-CBB
2	C	300	RXC	OAB-CAR-OAQ-CBB
2	C	300	RXC	CAU-CBB-OAQ-CAR

There are no ring outliers.

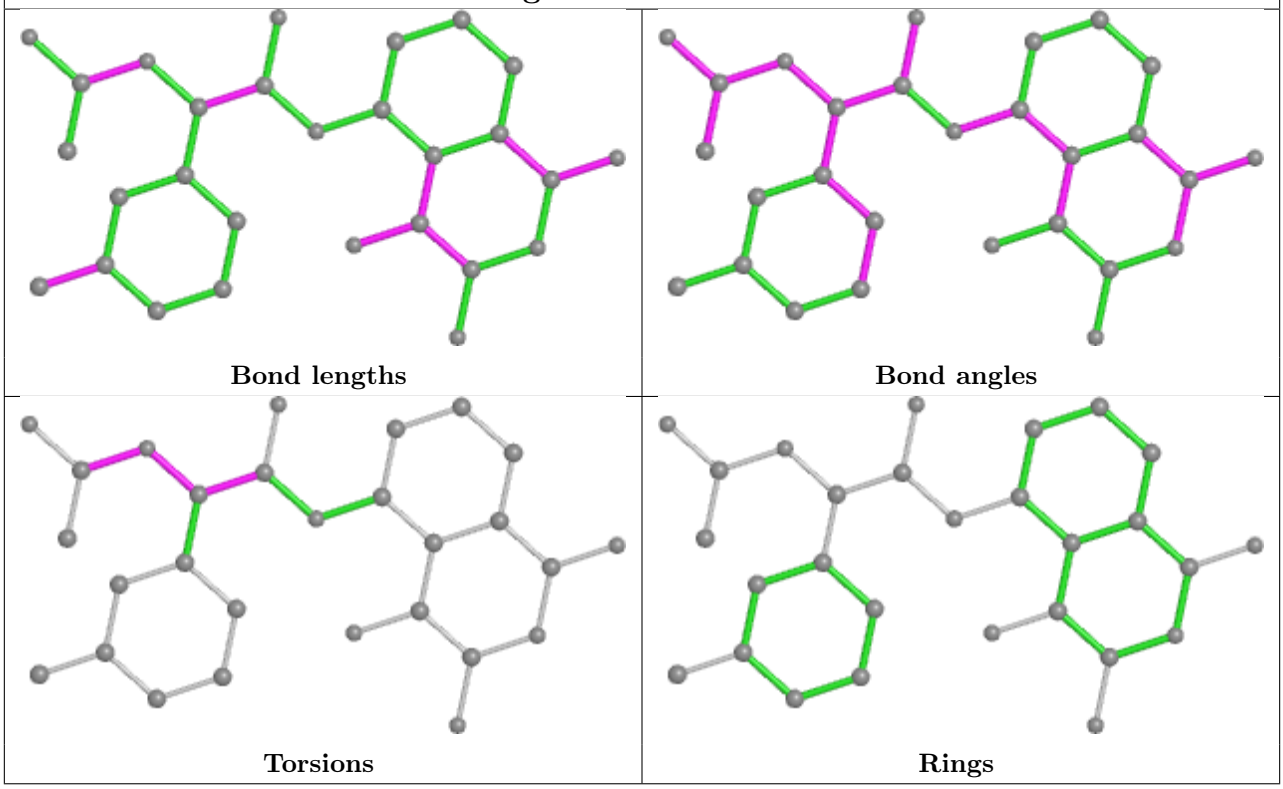
1 monomer is involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	300	RXC	9	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 then 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 RXC C 300



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	232/249 (93%)	-0.29	0	100	100	28, 48, 79, 112	0
1	B	234/249 (93%)	-0.19	3 (1%)	77	73	29, 48, 77, 113	0
1	C	232/249 (93%)	0.08	7 (3%)	50	43	34, 60, 96, 138	0
1	D	228/249 (91%)	0.31	4 (1%)	68	64	47, 81, 109, 124	0
All	All	926/996 (92%)	-0.02	14 (1%)	73	70	28, 57, 100, 138	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	132	GLY	4.2
1	C	276	TYR	3.7
1	C	36	SER	3.7
1	C	277	HIS	3.6
1	B	145	GLY	2.5
1	D	213	SER	2.5
1	C	38	LYS	2.4
1	C	273	LEU	2.4
1	D	57	LYS	2.3
1	C	40	ASP	2.1
1	B	276	TYR	2.1
1	C	35	ASN	2.1
1	B	175	ASP	2.0
1	D	56	HIS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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
1	OCS	C	163	9/10	0.91	0.20	42,44,58,59	0
1	OCS	B	163	9/10	0.92	0.17	45,48,59,59	0
1	OCS	A	163	9/10	0.92	0.19	39,42,54,54	0
1	OCS	D	163	9/10	0.92	0.20	75,77,81,81	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

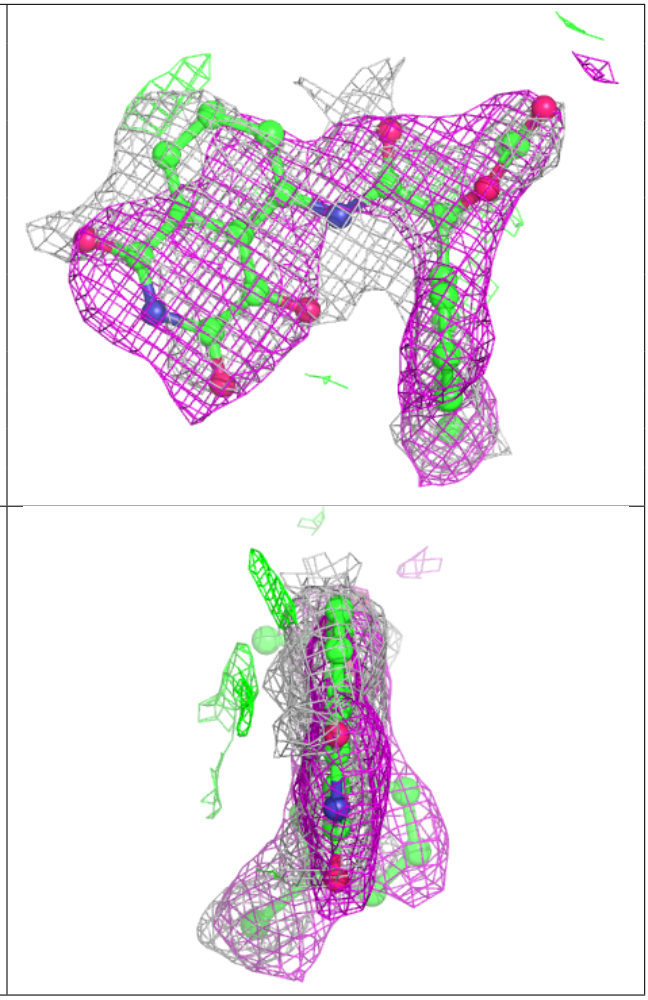
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	RXC	C	300	28/28	0.78	0.47	45,48,50,55	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 RXC C 300:

$2mF_o$-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.