Full wwPDB X-ray Structure Validation Report (i)

Feb 18, 2024 – 08:51 PM EST

PDB ID	:	4IG3
Title	:	HIV-1 reverse transcriptase with bound fragment near Knuckles site
Authors	:	Bauman, J.D.; Patel, D.; Arnold, E.
Deposited on	:	2012-12-15
Resolution	:	1.95 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:

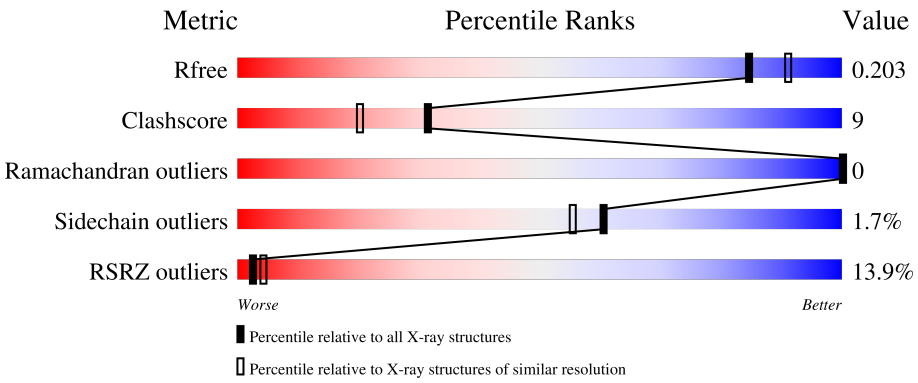
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 1.95 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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	557	11% 87% 12% •
2	B	429	17% 83% 14% •

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
4	DMS	A	602	-	-	X	-
4	DMS	A	605	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 9006 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 Reverse transcriptase/ribonuclease H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	556	4521	2926	751	836	8	0	1	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	expression tag	UNP P03366
A	0	VAL	-	expression tag	UNP P03366
A	172	ALA	LYS	engineered mutation	UNP P03366
A	173	ALA	LYS	engineered mutation	UNP P03366
A	280	SER	CYS	engineered mutation	UNP P03366

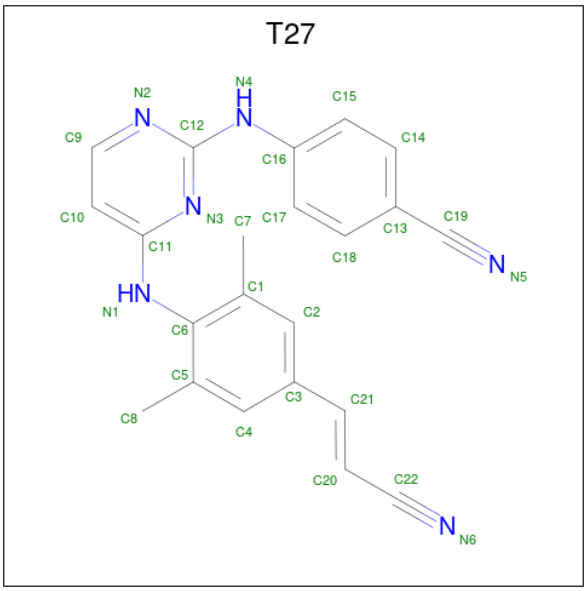
- Molecule 2 is a protein called P51 RT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	416	3458	2254	571	626	7	0	3	0

There are 2 discrepancies between the modelled and reference sequences:

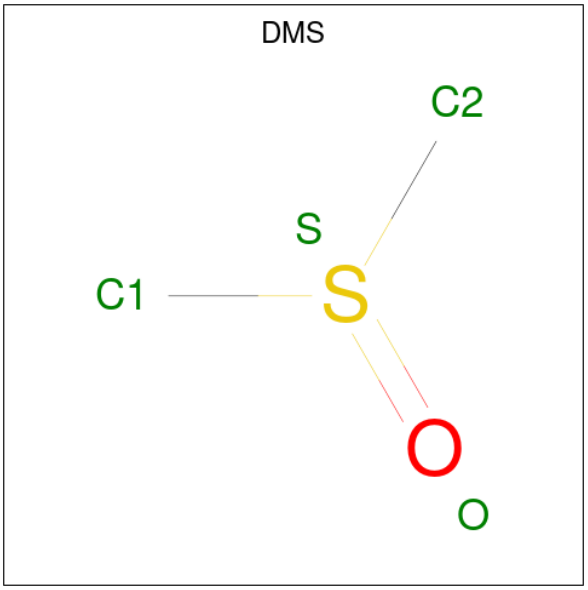
Chain	Residue	Modelled	Actual	Comment	Reference
B	0	GLY	-	expression tag	UNP P03366
B	280	SER	CYS	engineered mutation	UNP P03366

- Molecule 3 is 4-{[4-({4-[(E)-2-cyanoethenyl]-2,6-dimethylphenyl}amino)pyrimidin-2-yl]amino}benzonitrile (three-letter code: T27) (formula: $C_{22}H_{18}N_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	N		
3	A	1	28	22	6	0	0

- Molecule 4 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
4	A	1	4	2	1	1	0	0
			Total	C	O	S		
4	A	1	4	2	1	1	0	0
			Total	C	O	S		
4	A	1	4	2	1	1	0	0

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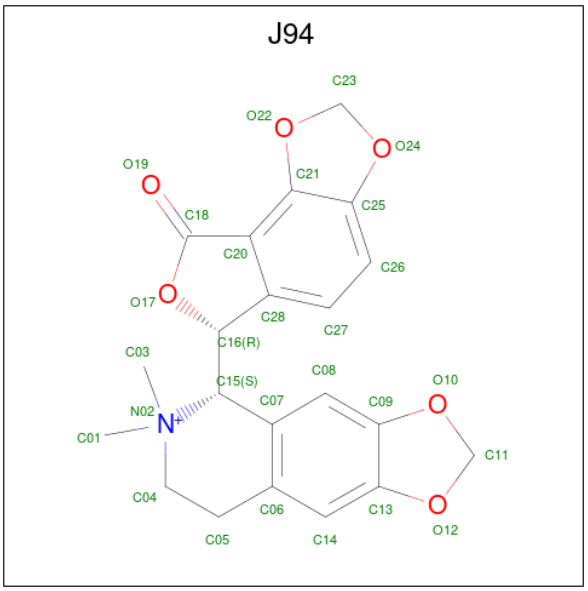
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
4	A	1	4	2	1	1	0	0
			Total	C	O	S		
4	A	1	4	2	1	1	0	0
			Total	C	O	S		
4	A	1	4	2	1	1	0	0
			Total	C	O	S		
4	A	1	4	2	1	1	0	0
			Total	C	O	S		
4	B	1	4	2	1	1	0	0
			Total	C	O	S		
4	B	1	4	2	1	1	0	0
			Total	C	O	S		
4	B	1	4	2	1	1	0	0
			Total	C	O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

- Molecule 5 is (5S)-6,6-dimethyl-5-[(6R)-8-oxo-6,8-dihydrofuro[3,4-e][1,3]benzodioxol-6-yl]-5,6,7,8-tetrahydro[1,3]dioxolo[4,5-g]isoquinolin-6-ium (three-letter code: J94) (formula: $C_{21}H_{20}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	A	1	28	21	1	6	0	0

- Molecule 6 is water.

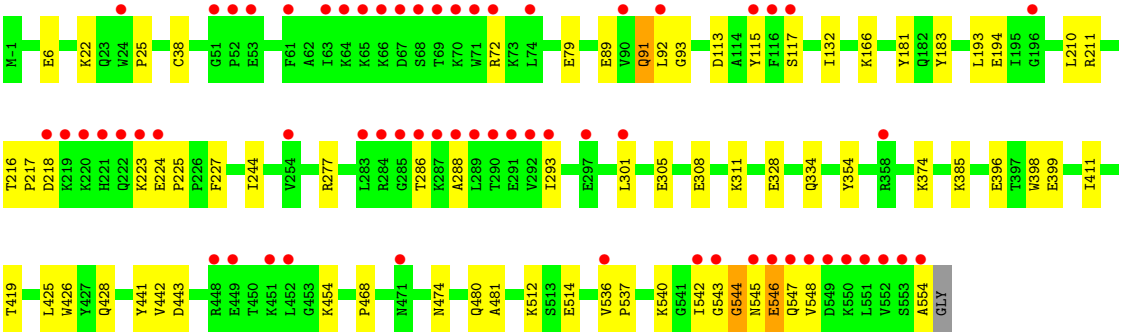
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	569	569	569	0	0
			Total	O		
6	B	342	342	342	0	0

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.

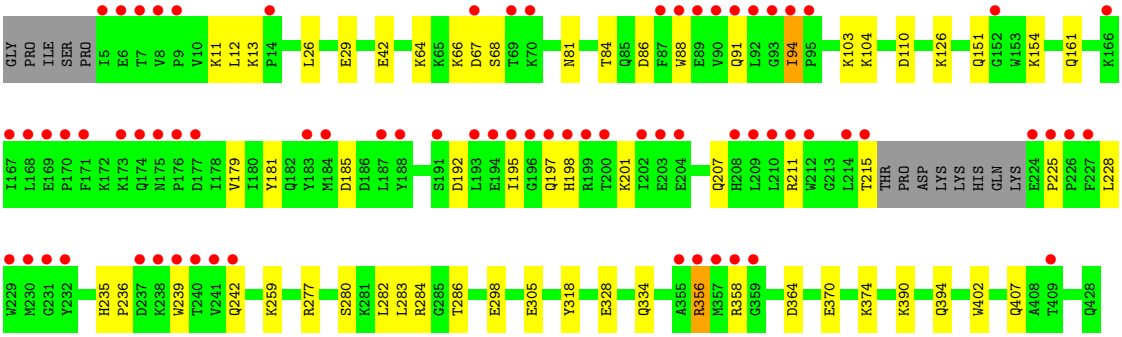
• Molecule 1: Reverse transcriptase/ribonuclease H

Chain A:



• Molecule 2: P51 RT

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	161.76Å 73.07Å 109.03Å 90.00° 100.03° 90.00°	Depositor
Resolution (Å)	33.21 – 1.95 33.21 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.1 (33.21-1.95) 90.6 (33.21-1.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.31 (at 1.89Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1233)	Depositor
R, R_{free}	0.178 , 0.203 0.178 , 0.203	Depositor DCC
R_{free} test set	1926 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å^2)	26.5	Xtriage
Anisotropy	0.158	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 49.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	9006	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.33% 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: T27, J94, DMS

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	0.47	0/4643	0.68	2/6311 (0.0%)
2	B	0.47	0/3565	0.70	1/4844 (0.0%)
All	All	0.47	0/8208	0.69	3/11155 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	544	GLY	N-CA-C	-6.76	96.19	113.10
1	A	210	LEU	CA-CB-CG	5.45	127.84	115.30
2	B	364	ASP	CB-CA-C	-5.06	100.27	110.40

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	4521	0	4576	86	0
2	B	3458	0	3483	69	0
3	A	28	0	18	1	0
4	A	28	0	42	17	0
4	B	32	0	48	11	0
5	A	28	0	20	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	569	0	0	38	1
6	B	342	0	0	16	1
All	All	9006	0	8187	146	1

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 9.

All (146) 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:A:426:TRP:H	4:A:602:DMS:H23	1.11	1.14
2:B:26:LEU:H	4:B:503:DMS:H13	1.15	1.04
1:A:428:GLN:H	4:A:603:DMS:H22	1.32	0.93
2:B:68:SER:O	6:B:893:HOH:O	1.85	0.91
1:A:480:GLN:NE2	6:A:1257:HOH:O	2.11	0.84
2:B:334:GLN:OE1	6:B:882:HOH:O	1.96	0.83
2:B:94:ILE:O	6:B:894:HOH:O	1.97	0.83
1:A:328:GLU:OE2	6:A:1127:HOH:O	1.97	0.81
1:A:72:ARG:NH2	6:A:1227:HOH:O	2.15	0.80
2:B:91:GLN:HE22	2:B:94:ILE:HG23	1.45	0.80
1:A:468:PRO:O	6:A:993:HOH:O	2.00	0.78
1:A:224:GLU:OE1	6:A:890:HOH:O	2.05	0.75
1:A:547:GLN:NE2	6:A:1035:HOH:O	2.18	0.75
1:A:308:GLU:OE1	6:A:1155:HOH:O	2.05	0.75
2:B:390:LYS:NZ	6:B:858:HOH:O	2.18	0.74
1:A:426:TRP:H	4:A:602:DMS:C2	1.97	0.74
1:A:89:GLU:OE1	6:A:1225:HOH:O	2.06	0.74
1:A:546:GLU:OE2	2:B:284:ARG:HG2	1.89	0.72
1:A:244:ILE:H	4:A:607:DMS:H21	1.55	0.72
2:B:402:TRP:HE1	4:B:506:DMS:C2	2.02	0.71
1:A:512:LYS:NZ	4:A:605:DMS:S	2.63	0.71
2:B:358:ARG:NH1	2:B:370[B]:GLU:OE2	2.24	0.70
4:B:507:DMS:S	6:B:922:HOH:O	2.50	0.69
2:B:318:TYR:HB3	4:B:507:DMS:H12	1.74	0.69
1:A:334:GLN:H	4:A:605:DMS:C1	2.06	0.69
2:B:11:LYS:HD2	2:B:12:LEU:H	1.58	0.69
2:B:103:LYS:NZ	6:B:912:HOH:O	2.07	0.69
2:B:42:GLU:OE1	6:B:854:HOH:O	2.10	0.68
2:B:29:GLU:OE2	6:B:855:HOH:O	2.12	0.67
1:A:546:GLU:O	6:A:1163:HOH:O	2.13	0.67
1:A:288:ALA:N	6:A:1252:HOH:O	2.07	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:514:GLU:OE1	6:A:992:HOH:O	2.13	0.66
1:A:244:ILE:H	4:A:607:DMS:C2	2.07	0.66
2:B:26:LEU:N	4:B:503:DMS:H13	2.00	0.66
1:A:543:GLY:N	2:B:283:LEU:O	2.29	0.65
1:A:443:ASP:OD1	6:A:780:HOH:O	2.15	0.64
2:B:207:GLN:O	2:B:211:ARG:HG3	1.98	0.64
1:A:79:GLU:OE1	6:A:1247:HOH:O	2.15	0.63
1:A:443:ASP:HB2	1:A:548:VAL:HG23	1.81	0.62
1:A:543:GLY:HA3	2:B:284:ARG:C	2.19	0.62
2:B:64:LYS:O	2:B:407:GLN:NE2	2.25	0.61
1:A:426:TRP:N	4:A:602:DMS:H23	1.97	0.61
2:B:225:PRO:HG3	2:B:228:LEU:HD22	1.82	0.60
2:B:305:GLU:OE1	6:B:744:HOH:O	2.17	0.59
1:A:72:ARG:NH2	6:A:1048:HOH:O	2.04	0.59
1:A:72:ARG:NH1	6:A:1065:HOH:O	2.13	0.58
1:A:536:VAL:HB	1:A:542:ILE:HD13	1.85	0.58
1:A:334:GLN:H	4:A:605:DMS:H13	1.68	0.58
1:A:115:TYR:CE1	6:A:1112:HOH:O	2.52	0.57
1:A:540:LYS:O	2:B:280:SER:HB3	2.04	0.57
2:B:94:ILE:HB	6:B:894:HOH:O	2.05	0.57
2:B:370[B]:GLU:OE2	6:B:815:HOH:O	2.17	0.57
4:A:607:DMS:H21	6:A:913:HOH:O	2.04	0.56
2:B:402:TRP:HE1	4:B:506:DMS:H22	1.68	0.56
1:A:543:GLY:HA3	2:B:284:ARG:HA	1.88	0.56
1:A:428:GLN:N	4:A:603:DMS:H22	2.13	0.56
1:A:91:GLN:NE2	6:A:1225:HOH:O	2.37	0.56
2:B:26:LEU:O	4:B:503:DMS:H23	2.07	0.55
2:B:402:TRP:HE1	4:B:506:DMS:H21	1.70	0.55
2:B:104:LYS:HE3	2:B:192:ASP:HB3	1.89	0.54
1:A:543:GLY:HA3	2:B:284:ARG:O	2.07	0.54
1:A:545:ASN:HB2	6:A:1147:HOH:O	2.08	0.54
2:B:235:HIS:NE2	6:B:940:HOH:O	2.33	0.54
1:A:286:THR:HG22	6:A:1252:HOH:O	2.07	0.54
2:B:81:ASN:O	2:B:154:LYS:HE2	2.08	0.54
2:B:225:PRO:HB2	2:B:228:LEU:HD13	1.90	0.53
1:A:426:TRP:HD1	4:A:602:DMS:H21	1.72	0.53
2:B:318:TYR:HB3	4:B:507:DMS:C1	2.38	0.53
2:B:126:LYS:HD2	4:B:502:DMS:H21	1.91	0.52
1:A:542:ILE:HB	6:A:754:HOH:O	2.09	0.52
1:A:542:ILE:HG12	2:B:283:LEU:HD12	1.91	0.52
2:B:181:TYR:OH	6:B:904:HOH:O	2.16	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:THR:HB	6:A:943:HOH:O	2.10	0.52
1:A:223:LYS:NZ	6:A:1000:HOH:O	2.44	0.51
1:A:441:TYR:O	1:A:548:VAL:HG11	2.11	0.51
1:A:396:GLU:HG3	6:A:964:HOH:O	2.11	0.50
1:A:545:ASN:CB	6:A:1147:HOH:O	2.59	0.50
1:A:72:ARG:NH1	6:A:1205:HOH:O	2.44	0.50
1:A:545:ASN:ND2	6:A:1147:HOH:O	1.97	0.50
1:A:543:GLY:HA3	2:B:284:ARG:CA	2.41	0.50
1:A:543:GLY:CA	2:B:284:ARG:HA	2.43	0.48
1:A:193:LEU:O	6:A:911:HOH:O	2.20	0.48
1:A:542:ILE:HG23	2:B:283:LEU:HB3	1.95	0.48
2:B:197:GLN:O	2:B:201:LYS:HG2	2.13	0.48
1:A:224:GLU:HG3	1:A:225:PRO:HD2	1.95	0.48
2:B:370[B]:GLU:CD	6:B:815:HOH:O	2.50	0.48
2:B:298:GLU:OE1	2:B:298:GLU:N	2.45	0.48
2:B:94:ILE:HG23	2:B:161:GLN:HE22	1.79	0.47
1:A:474:ASN:H	4:A:606:DMS:C2	2.27	0.47
2:B:86:ASP:HB3	2:B:88:TRP:CE2	2.49	0.47
1:A:25:PRO:HA	6:A:1157:HOH:O	2.15	0.47
1:A:334:GLN:H	4:A:605:DMS:H11	1.76	0.47
1:A:543:GLY:CA	2:B:283:LEU:O	2.63	0.47
1:A:544:GLY:HA2	2:B:286:THR:HG22	1.97	0.47
6:A:1104:HOH:O	2:B:394:GLN:HG3	2.15	0.47
2:B:235:HIS:H	4:B:504:DMS:H23	1.80	0.47
1:A:544:GLY:O	1:A:548:VAL:HG22	2.15	0.47
1:A:537:PRO:O	1:A:542:ILE:HD12	2.16	0.46
3:A:601:T27:H15	3:A:601:T27:N3	2.31	0.46
2:B:277:ARG:NH1	6:B:878:HOH:O	2.14	0.46
1:A:223:LYS:HG2	1:A:227:PHE:HE1	1.80	0.46
2:B:11:LYS:HD2	2:B:12:LEU:N	2.30	0.46
2:B:66:LYS:O	2:B:67:ASP:HB2	2.16	0.46
1:A:181:TYR:CE2	1:A:183:TYR:HB2	2.51	0.45
2:B:86:ASP:HB3	2:B:88:TRP:CZ2	2.52	0.45
1:A:25:PRO:O	6:A:1204:HOH:O	2.20	0.45
2:B:225:PRO:CG	2:B:228:LEU:HD22	2.47	0.45
1:A:293:ILE:O	6:A:1160:HOH:O	2.21	0.45
2:B:356:ARG:H	2:B:356:ARG:CD	2.30	0.45
2:B:110:ASP:O	2:B:228:LEU:HD12	2.17	0.45
2:B:370[B]:GLU:OE2	2:B:374:LYS:HE2	2.18	0.44
1:A:398:TRP:CZ2	1:A:411:ILE:HG12	2.52	0.44
1:A:6:GLU:OE2	5:A:609:J94:H14	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:543:GLY:O	1:A:545:ASN:N	2.49	0.44
1:A:385:LYS:HD2	6:A:1183:HOH:O	2.17	0.43
1:A:542:ILE:O	1:A:545:ASN:HB3	2.19	0.43
5:A:609:J94:H14	5:A:609:J94:H4	1.81	0.43
1:A:22:LYS:NZ	6:A:1263:HOH:O	2.51	0.43
1:A:543:GLY:H	2:B:283:LEU:C	2.21	0.43
2:B:13:LYS:HE3	2:B:84:THR:O	2.18	0.43
1:A:277:ARG:NH2	4:A:608:DMS:O	2.50	0.43
1:A:543:GLY:C	1:A:545:ASN:N	2.72	0.43
2:B:11:LYS:CD	2:B:12:LEU:H	2.29	0.43
2:B:103:LYS:HE3	2:B:179:VAL:CG2	2.49	0.43
1:A:223:LYS:NZ	6:A:825:HOH:O	2.50	0.43
2:B:66:LYS:HZ1	2:B:358:ARG:NH1	2.17	0.42
2:B:195:ILE:HA	2:B:198:HIS:HB3	2.02	0.42
2:B:236:PRO:HA	2:B:239:TRP:CG	2.55	0.42
4:A:605:DMS:H13	6:A:1062:HOH:O	2.19	0.42
1:A:354:TYR:HD1	1:A:374:LYS:HD2	1.84	0.42
1:A:442:VAL:HB	1:A:481:ALA:HB1	2.01	0.42
1:A:92:LEU:HD12	1:A:93:GLY:N	2.34	0.42
2:B:236:PRO:HA	2:B:239:TRP:CD2	2.55	0.42
1:A:540:LYS:O	2:B:280:SER:CB	2.68	0.41
1:A:288:ALA:HB3	6:A:1252:HOH:O	2.19	0.41
1:A:454:LYS:NZ	1:A:554:ALA:HB3	2.34	0.41
2:B:151:GLN:HB3	2:B:185:ASP:OD2	2.20	0.41
2:B:328:GLU:OE1	6:B:771:HOH:O	2.22	0.41
1:A:301:LEU:O	1:A:305:GLU:HG3	2.21	0.41
1:A:425:LEU:HA	4:A:602:DMS:H22	2.03	0.41
1:A:38:CYS:SG	1:A:132:ILE:HD11	2.61	0.41
1:A:166:LYS:HD2	1:A:166:LYS:HA	1.88	0.41
1:A:545:ASN:HA	1:A:548:VAL:HG22	2.02	0.40
2:B:358:ARG:NH2	2:B:370[B]:GLU:OE1	2.53	0.40
1:A:328:GLU:CG	6:A:1127:HOH:O	2.70	0.40
1:A:216:THR:HA	1:A:217:PRO:HD3	1.90	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1056:HOH:O	6:B:858:HOH:O[4_546]	1.77	0.43

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	555/557 (100%)	542 (98%)	13 (2%)	0	100	100
2	B	415/429 (97%)	401 (97%)	14 (3%)	0	100	100
All	All	970/986 (98%)	943 (97%)	27 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	496/495 (100%)	487 (98%)	9 (2%)	59	53
2	B	380/390 (97%)	374 (98%)	6 (2%)	62	58
All	All	876/885 (99%)	861 (98%)	15 (2%)	60	55

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	91	GLN
1	A	113	ASP
1	A	117	SER
1	A	194	GLU
1	A	211	ARG
1	A	218	ASP
1	A	311	LYS
1	A	399	GLU

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Mol	Chain	Res	Type
1	A	546	GLU
2	B	94	ILE
2	B	215	THR
2	B	242	GLN
2	B	259	LYS
2	B	282	LEU
2	B	356	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	334	GLN
2	B	91	GLN
2	B	161	GLN
2	B	418	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)

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)

17 ligands 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	$\#\|Z\| > 2$
4	DMS	B	508	-	3,3,3	0.62	0	3,3,3	0.76	0
4	DMS	B	503	-	3,3,3	0.75	0	3,3,3	1.14	0
4	DMS	B	507	-	3,3,3	0.59	0	3,3,3	0.85	0
4	DMS	B	506	-	3,3,3	0.59	0	3,3,3	0.83	0
5	J94	A	609	-	33,33,33	2.26	14 (42%)	48,52,52	1.41	5 (10%)
4	DMS	A	605	-	3,3,3	0.54	0	3,3,3	0.51	0
3	T27	A	601	-	30,30,30	1.23	3 (10%)	39,40,40	1.92	7 (17%)
4	DMS	A	602	-	3,3,3	0.47	0	3,3,3	0.49	0
4	DMS	A	608	-	3,3,3	0.66	0	3,3,3	0.83	0
4	DMS	B	502	-	3,3,3	0.53	0	3,3,3	0.49	0
4	DMS	A	607	-	3,3,3	0.56	0	3,3,3	0.49	0
4	DMS	B	505	-	3,3,3	0.88	0	3,3,3	1.34	1 (33%)
4	DMS	A	606	-	3,3,3	0.71	0	3,3,3	0.84	0
4	DMS	B	501	-	3,3,3	0.63	0	3,3,3	0.43	0
4	DMS	B	504	-	3,3,3	0.66	0	3,3,3	0.57	0
4	DMS	A	604	-	3,3,3	0.64	0	3,3,3	0.89	0
4	DMS	A	603	-	3,3,3	0.56	0	3,3,3	0.73	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	J94	A	609	-	-	0/4/44/44	0/6/6/6
3	T27	A	601	-	-	0/13/14/14	0/3/3/3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	609	J94	C15-C16	-4.86	1.46	1.54
5	A	609	J94	C20-C28	-4.36	1.34	1.39
5	A	609	J94	O17-C16	-3.80	1.41	1.46
5	A	609	J94	C27-C28	3.78	1.44	1.39
3	A	601	T27	C12-N4	3.76	1.44	1.36
5	A	609	J94	C05-C06	-3.58	1.45	1.51
5	A	609	J94	C14-C13	3.39	1.45	1.38
5	A	609	J94	O17-C18	3.17	1.40	1.36
3	A	601	T27	C11-N1	3.11	1.44	1.38
5	A	609	J94	C08-C07	2.98	1.44	1.39
5	A	609	J94	C06-C07	-2.70	1.35	1.40
5	A	609	J94	C03-N02	-2.28	1.43	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	609	J94	C07-C15	2.16	1.55	1.52
5	A	609	J94	C14-C06	2.10	1.43	1.39
5	A	609	J94	O22-C23	-2.07	1.39	1.43
3	A	601	T27	C13-C19	2.05	1.49	1.44
5	A	609	J94	C20-C21	2.03	1.45	1.40

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	601	T27	C9-N2-C12	5.48	120.31	115.45
3	A	601	T27	C9-C10-C11	5.24	120.19	116.76
3	A	601	T27	C10-C9-N2	-4.89	117.89	123.96
5	A	609	J94	O17-C18-O19	4.05	124.65	121.19
5	A	609	J94	O17-C16-C15	3.55	113.26	108.61
5	A	609	J94	O22-C21-C20	3.39	132.20	128.43
3	A	601	T27	N2-C12-N3	-3.31	123.41	126.55
3	A	601	T27	C6-N1-C11	-2.77	119.17	124.18
5	A	609	J94	O12-C13-C14	2.48	131.17	127.85
3	A	601	T27	C10-C11-N3	-2.38	119.14	123.16
3	A	601	T27	C4-C5-C6	2.26	120.87	118.23
5	A	609	J94	O24-C25-C26	2.18	131.78	127.81
4	B	505	DMS	C2-S-C1	2.07	109.11	98.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

13 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	503	DMS	3	0
4	B	507	DMS	3	0
4	B	506	DMS	3	0
5	A	609	J94	2	0
4	A	605	DMS	5	0
3	A	601	T27	1	0
4	A	602	DMS	5	0
4	A	608	DMS	1	0
4	B	502	DMS	1	0
4	A	607	DMS	3	0
4	A	606	DMS	1	0
4	B	504	DMS	1	0

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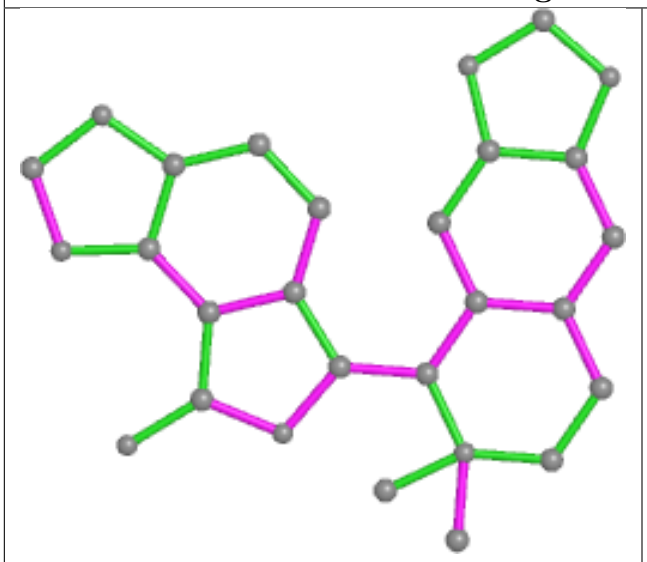
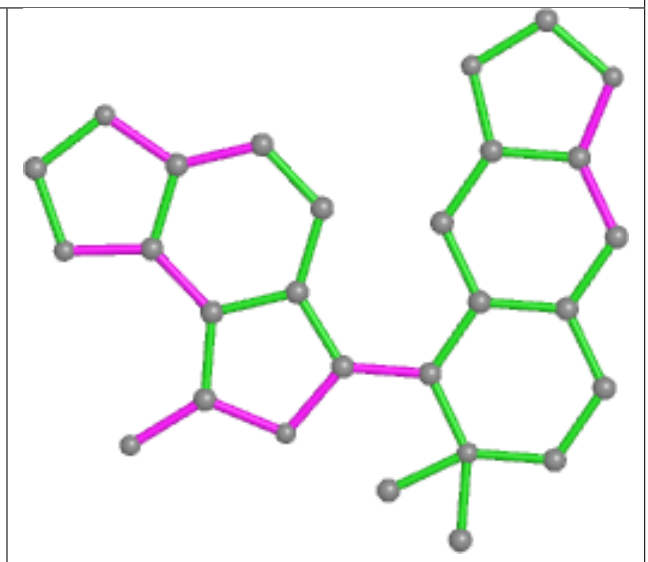
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	603	DMS	2	0

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.

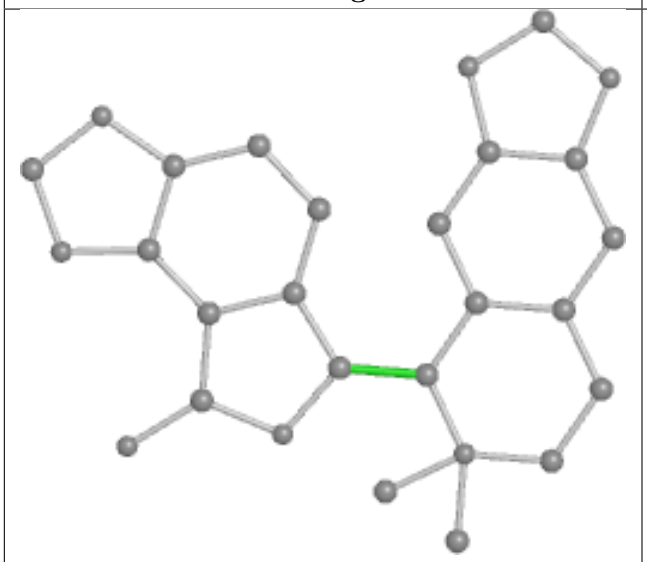
Ligand J94 A 609



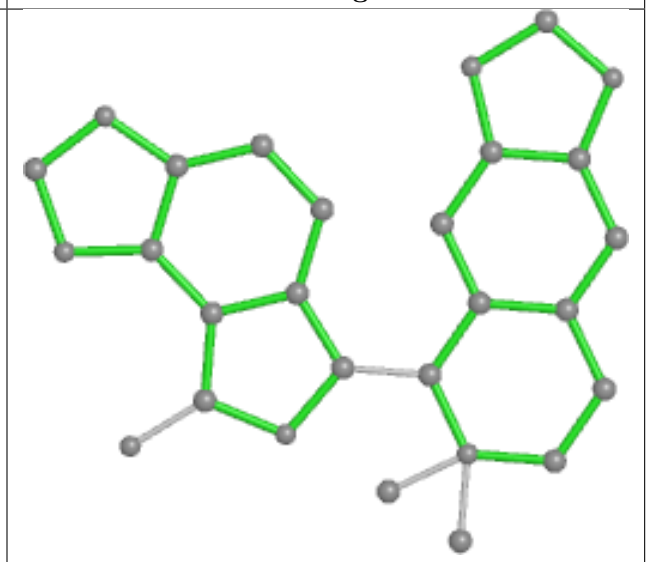
Bond lengths



Bond angles

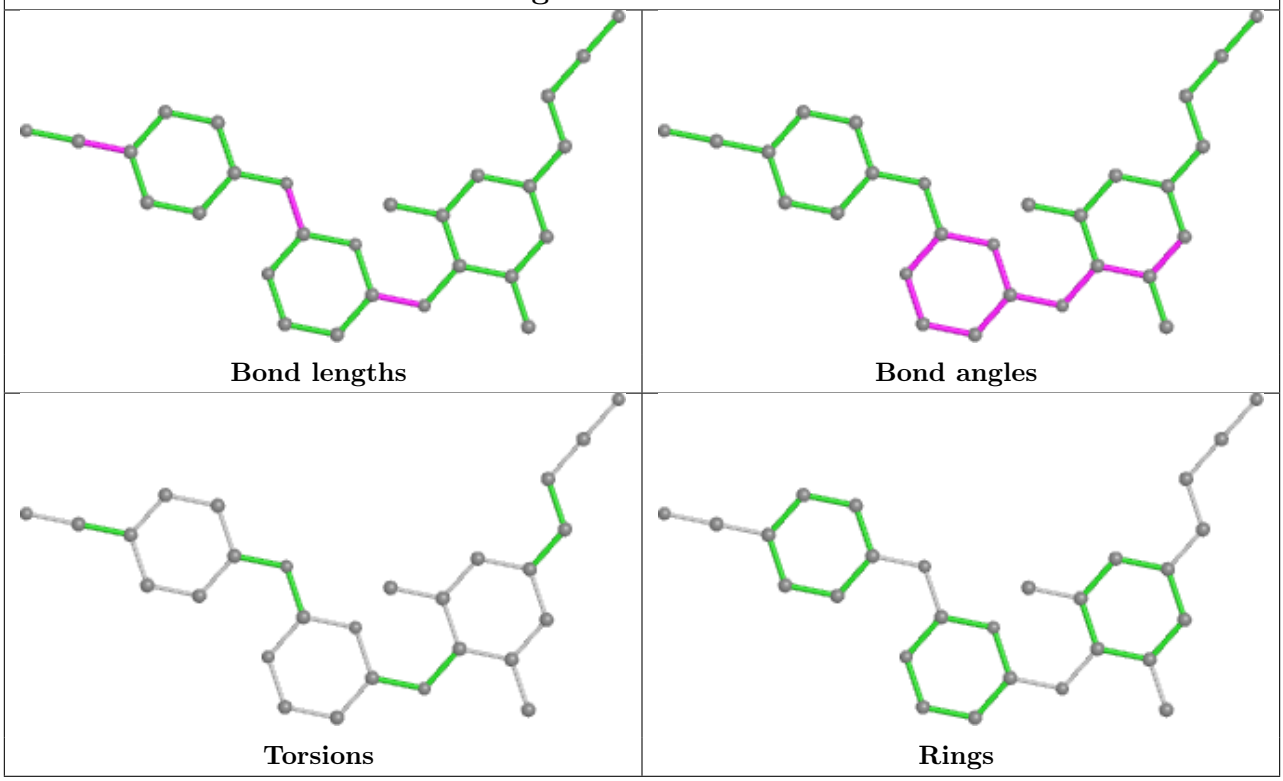


Torsions



Rings

Ligand T27 A 601



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	556/557 (99%)	0.42	62 (11%)	5	8	14, 33, 83, 121	0
2	B	416/429 (96%)	0.78	73 (17%)	1	1	16, 36, 96, 142	0
All	All	972/986 (98%)	0.57	135 (13%)	2	4	14, 34, 90, 142	0

All (135) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	92	LEU	17.0
2	B	90	VAL	14.9
1	A	285	GLY	9.4
2	B	93	GLY	9.4
1	A	67	ASP	9.2
2	B	88	TRP	9.2
1	A	69	THR	8.6
1	A	286	THR	8.6
1	A	553	SER	8.5
2	B	5	ILE	8.4
1	A	68	SER	7.4
1	A	289	LEU	7.3
2	B	95	PRO	7.1
1	A	66	LYS	6.8
2	B	214	LEU	6.7
1	A	222	GLN	6.5
1	A	219	LYS	6.3
2	B	356	ARG	6.3
1	A	92	LEU	6.2
1	A	287	LYS	6.1
1	A	542	ILE	6.0
2	B	89	GLU	6.0
1	A	288	ALA	6.0
2	B	229	TRP	5.9

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Mol	Chain	Res	Type	RSRZ
1	A	220	LYS	5.9
1	A	116	PHE	5.9
2	B	200	THR	5.9
2	B	215	THR	5.9
1	A	51	GLY	5.8
1	A	65	LYS	5.7
2	B	197	GLN	5.7
2	B	357	MET	5.6
2	B	240	THR	5.6
1	A	64	LYS	5.5
1	A	543	GLY	5.5
1	A	221	HIS	5.4
1	A	546	GLU	5.4
2	B	358	ARG	5.3
2	B	212	TRP	5.2
2	B	7	THR	5.0
1	A	548	VAL	4.9
1	A	552	VAL	4.9
2	B	94	ILE	4.7
1	A	63	ILE	4.7
2	B	196	GLY	4.7
2	B	239	TRP	4.6
1	A	72	ARG	4.6
1	A	115	TYR	4.6
2	B	226	PRO	4.6
1	A	218	ASP	4.5
2	B	210	LEU	4.5
2	B	211	ARG	4.5
2	B	67	ASP	4.4
1	A	70	LYS	4.4
2	B	237	ASP	4.4
2	B	359	GLY	4.3
1	A	290	THR	4.3
1	A	24	TRP	4.3
2	B	238	LYS	4.3
2	B	193	LEU	4.2
2	B	168	LEU	4.2
2	B	170	PRO	4.2
1	A	554	ALA	4.0
2	B	202	ILE	3.9
2	B	225	PRO	3.8
1	A	223	LYS	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	254	VAL	3.8
2	B	176	PRO	3.7
2	B	188	TYR	3.7
2	B	209	LEU	3.5
1	A	293	ILE	3.5
1	A	358	ARG	3.5
1	A	71	TRP	3.5
2	B	187	LEU	3.4
2	B	91	GLN	3.4
2	B	6	GLU	3.4
1	A	547	GLN	3.3
1	A	549	ASP	3.3
1	A	90	VAL	3.3
2	B	199	ARG	3.3
2	B	198	HIS	3.3
1	A	550	LYS	3.2
1	A	284	ARG	3.2
2	B	167	ILE	3.2
2	B	171	PHE	3.2
2	B	173	LYS	3.2
2	B	231	GLY	3.2
1	A	452	LEU	3.1
2	B	194	GLU	3.1
1	A	52	PRO	3.1
2	B	8	VAL	3.1
1	A	551	LEU	3.1
1	A	545	ASN	3.1
2	B	9	PRO	3.0
1	A	448	ARG	3.0
1	A	61	PHE	3.0
2	B	174	GLN	3.0
1	A	449	GLU	3.0
2	B	166	LYS	2.9
1	A	53	GLU	2.9
1	A	224	GLU	2.9
1	A	283	LEU	2.9
2	B	184	MET	2.8
2	B	227	PHE	2.8
2	B	183	TYR	2.8
2	B	208	HIS	2.8
2	B	241	VAL	2.7
1	A	471	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	292	VAL	2.6
1	A	117	SER	2.6
2	B	242	GLN	2.6
1	A	291	GLU	2.6
1	A	196	GLY	2.6
1	A	301	LEU	2.6
2	B	14	PRO	2.6
2	B	177	ASP	2.6
1	A	297	GLU	2.6
2	B	69	THR	2.5
1	A	74	LEU	2.5
2	B	355	ALA	2.5
2	B	87	PHE	2.5
2	B	191	SER	2.5
1	A	451	LYS	2.4
2	B	195	ILE	2.3
2	B	230	MET	2.2
2	B	203	GLU	2.2
2	B	169	GLU	2.2
2	B	175	ASN	2.2
2	B	232	TYR	2.2
2	B	70	LYS	2.1
1	A	536	VAL	2.1
2	B	204	GLU	2.1
2	B	409	THR	2.1
2	B	152	GLY	2.1
2	B	224	GLU	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

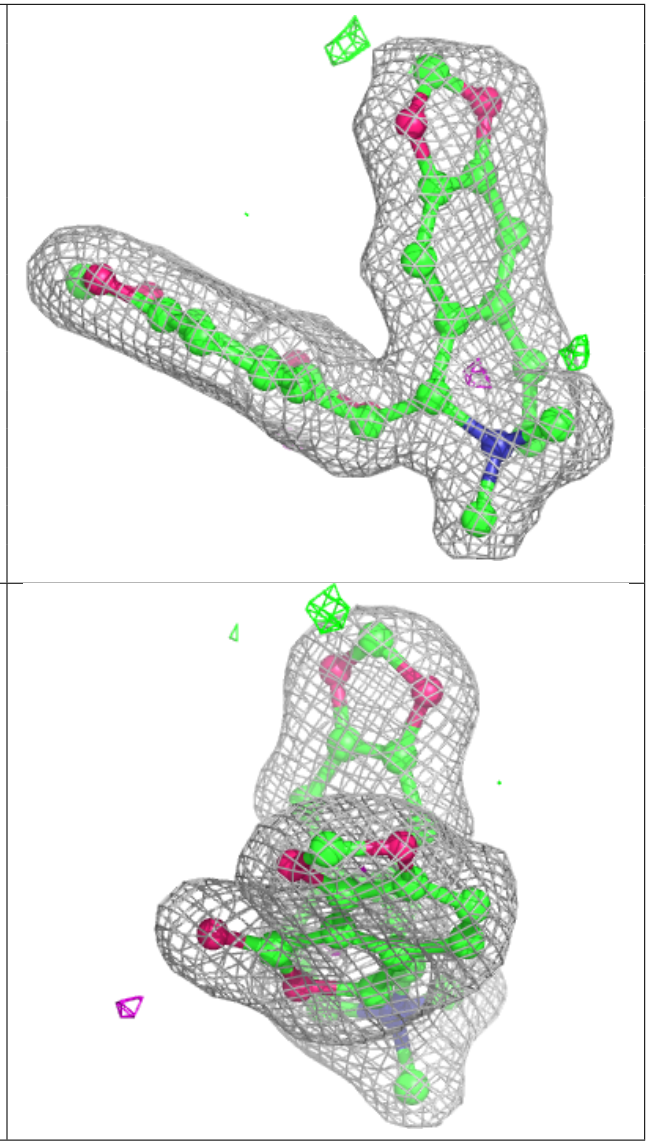
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	DMS	B	503	4/4	0.69	0.21	16,21,56,75	0
4	DMS	A	606	4/4	0.74	0.24	53,56,64,80	0
4	DMS	B	505	4/4	0.89	0.18	22,29,61,61	0
4	DMS	A	607	4/4	0.91	0.14	33,48,63,71	0
4	DMS	B	508	4/4	0.91	0.18	39,63,77,78	0
4	DMS	B	504	4/4	0.92	0.26	37,61,187,187	0
4	DMS	A	608	4/4	0.92	0.12	57,71,75,81	0
4	DMS	A	605	4/4	0.92	0.12	27,48,57,76	0
5	J94	A	609	28/28	0.93	0.09	22,30,36,38	0
4	DMS	A	602	4/4	0.94	0.12	15,31,39,52	0
3	T27	A	601	28/28	0.94	0.12	16,22,25,30	0
4	DMS	B	507	4/4	0.96	0.15	62,68,71,95	0
4	DMS	B	506	4/4	0.97	0.11	21,35,44,45	0
4	DMS	A	603	4/4	0.97	0.11	25,30,32,38	0
4	DMS	B	501	4/4	0.97	0.11	36,39,43,48	0
4	DMS	B	502	4/4	0.97	0.09	27,29,38,44	0
4	DMS	A	604	4/4	0.98	0.13	46,58,60,77	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.

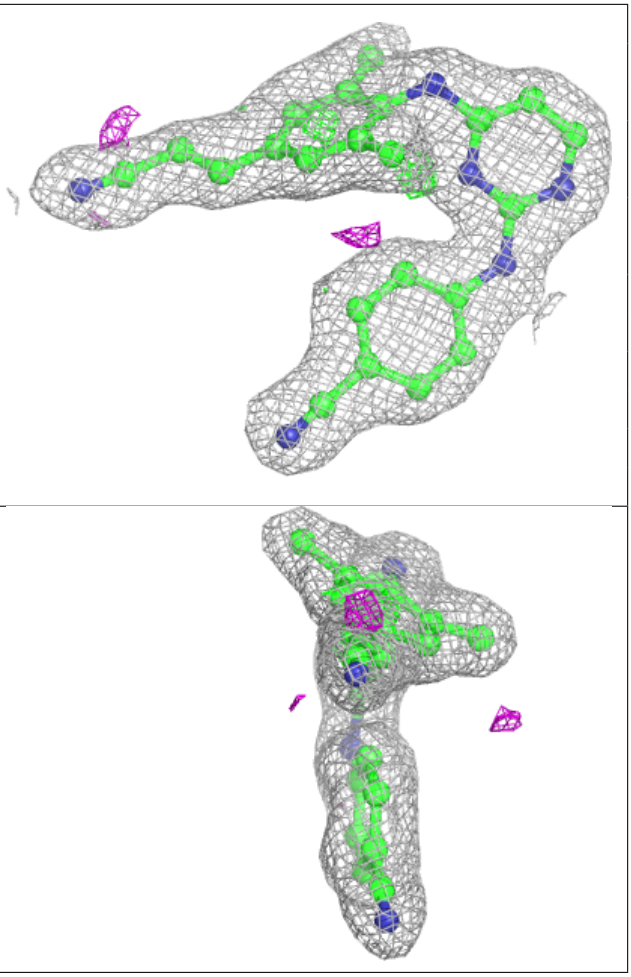
Electron density around J94 A 609:

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



Electron density around T27 A 601:

$2mF_o$-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.