Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2023 – 11:26 AM EDT

PDB ID	:	7RWI
Title	:	Mycobacterium tuberculosis RNA polymerase sigma L holoenzyme open promoter complex containing TNP-2198
Authors	:	Molodtsov, V.; Ebright, R.H.
Deposited on	:	2021-08-19
Resolution	:	3.70 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:

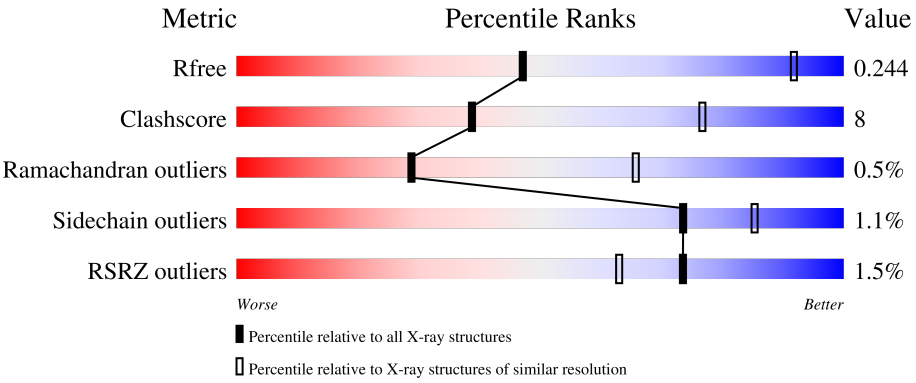
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 3.70 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	1049 (3.88-3.52)
Clashscore	141614	1027 (3.86-3.54)
Ramachandran outliers	138981	1069 (3.88-3.52)
Sidechain outliers	138945	1065 (3.88-3.52)
RSRZ outliers	127900	1578 (3.90-3.50)

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	347	50% 15% 35%
1	B	347	51% 15% 33%
2	C	1178	79% 15%
3	D	1316	81% 14%
4	E	110	59% 15% 26%

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Mol	Chain	Length	Quality of chain
5	F	177	6% 82% 16%
6	G	23	9% 26% 39% 35%
7	H	27	4% 52% 37% 11%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 24903 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 DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	225	Total	C	N	O	S	0	0	0
			1716	1080	296	338	2			
1	B	232	Total	C	N	O	S	0	0	0
			1732	1093	296	341	2			

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1126	Total	C	N	O	S	0	0	0
			8724	5459	1531	1695	39			

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1264	Total	C	N	O	S	0	0	0
			9884	6189	1790	1865	40			

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	E	81	Total	C	N	O	0	0	0
			630	403	106	121			

- Molecule 5 is a protein called RNA polymerase sigma factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	174	Total	C	N	O	S	0	0	0
			1352	840	256	254	2			

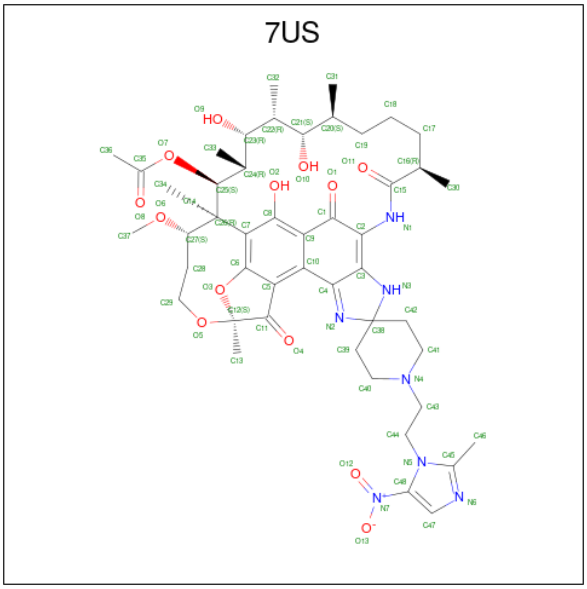
- Molecule 6 is a DNA chain called T DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	G	15	Total	C	N	O	P	0	0	0
			306	146	58	88	14			

- Molecule 7 is a DNA chain called NT DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	24	Total	C	N	O	P	0	0	0
			491	234	90	144	23			

- Molecule 8 is (3aM,9S,10bP,14S,15R,16S,17R,18R,19R,20S,21S,25R)-6,18,20-trihydroxy-14-methoxy-7,9,15,17,19,21,25-heptamethyl-1'-[2-(2-methyl-5-nitro-1H-imidazol-1-yl)ethyl]-5,10,26-trioxo-3,5,9,10-tetrahydrospiro[9,4-(epoxypentadecanoimino)furo[2',3':7,8]naphtho[1,2-d]imidazole-2,4'-piperidin]-16-yl acetate (three-letter code: 7US) (formula: $C_{48}H_{67}N_7O_{13}$).



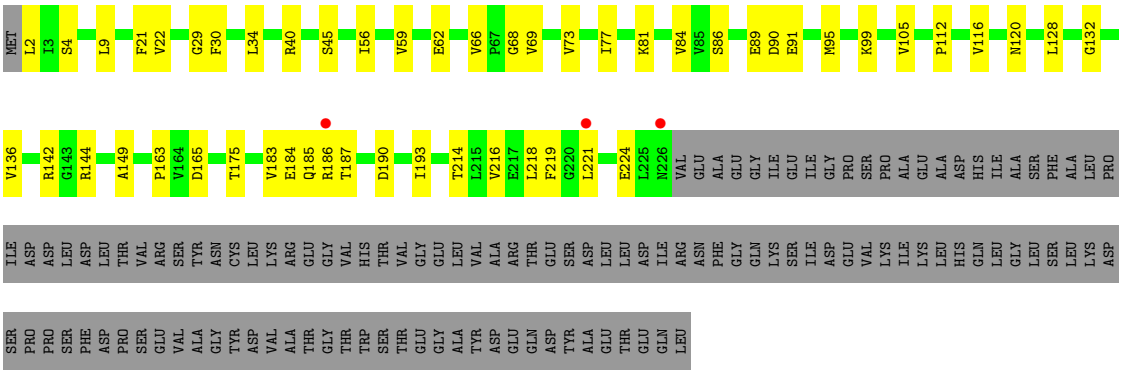
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	C	1	Total	C	N	O	38	0
			68	48	7	13		

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.

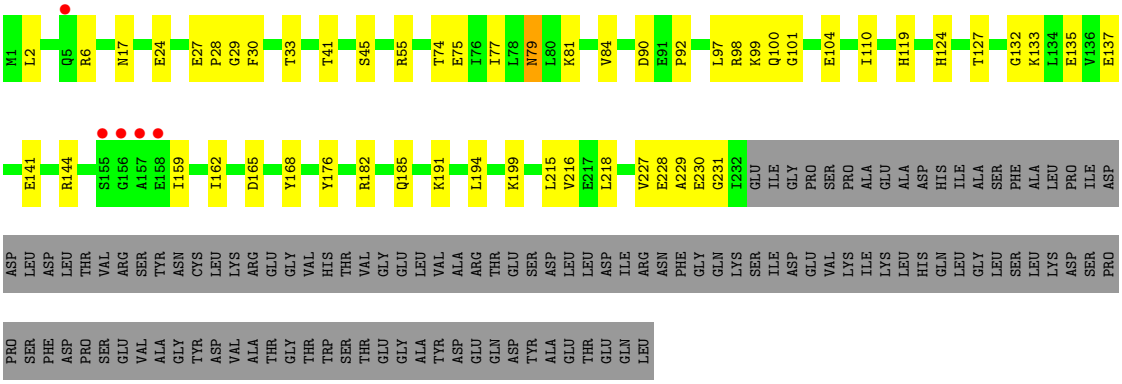
• Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain A:



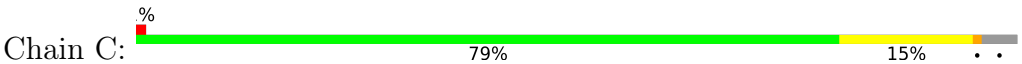
• Molecule 1: DNA-directed RNA polymerase subunit alpha

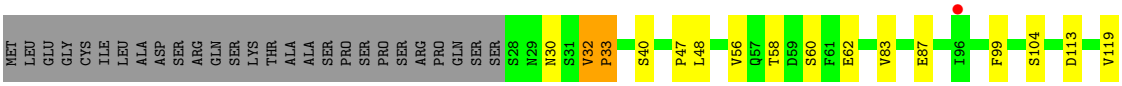
Chain B:

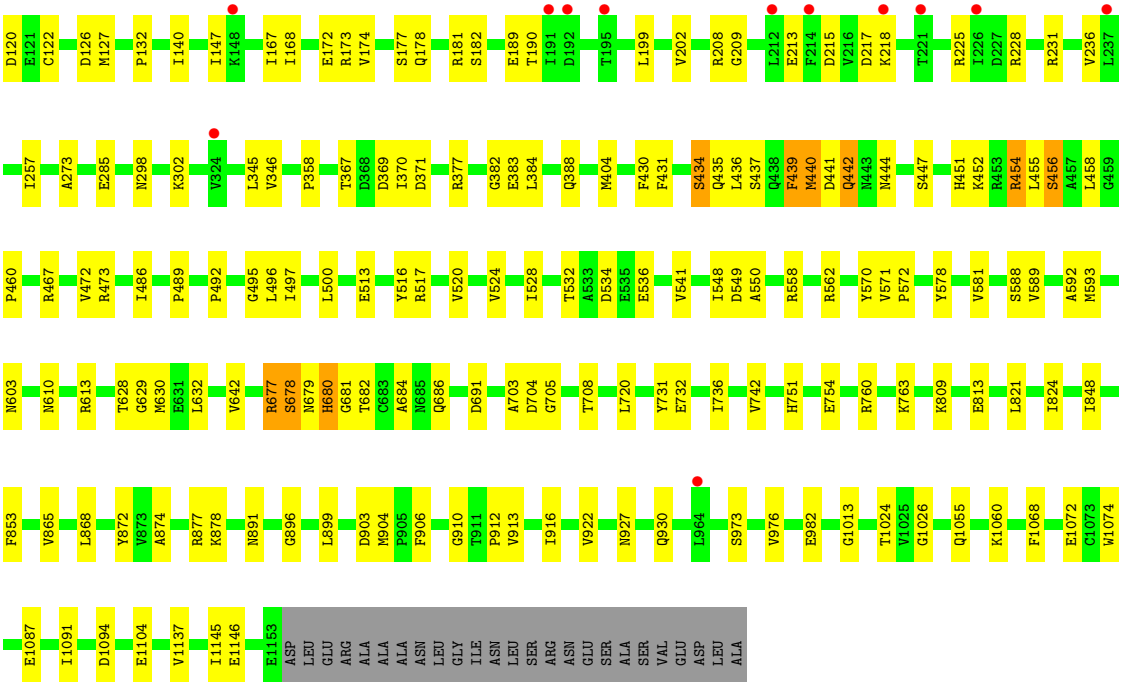


• Molecule 2: DNA-directed RNA polymerase subunit beta

Chain C:

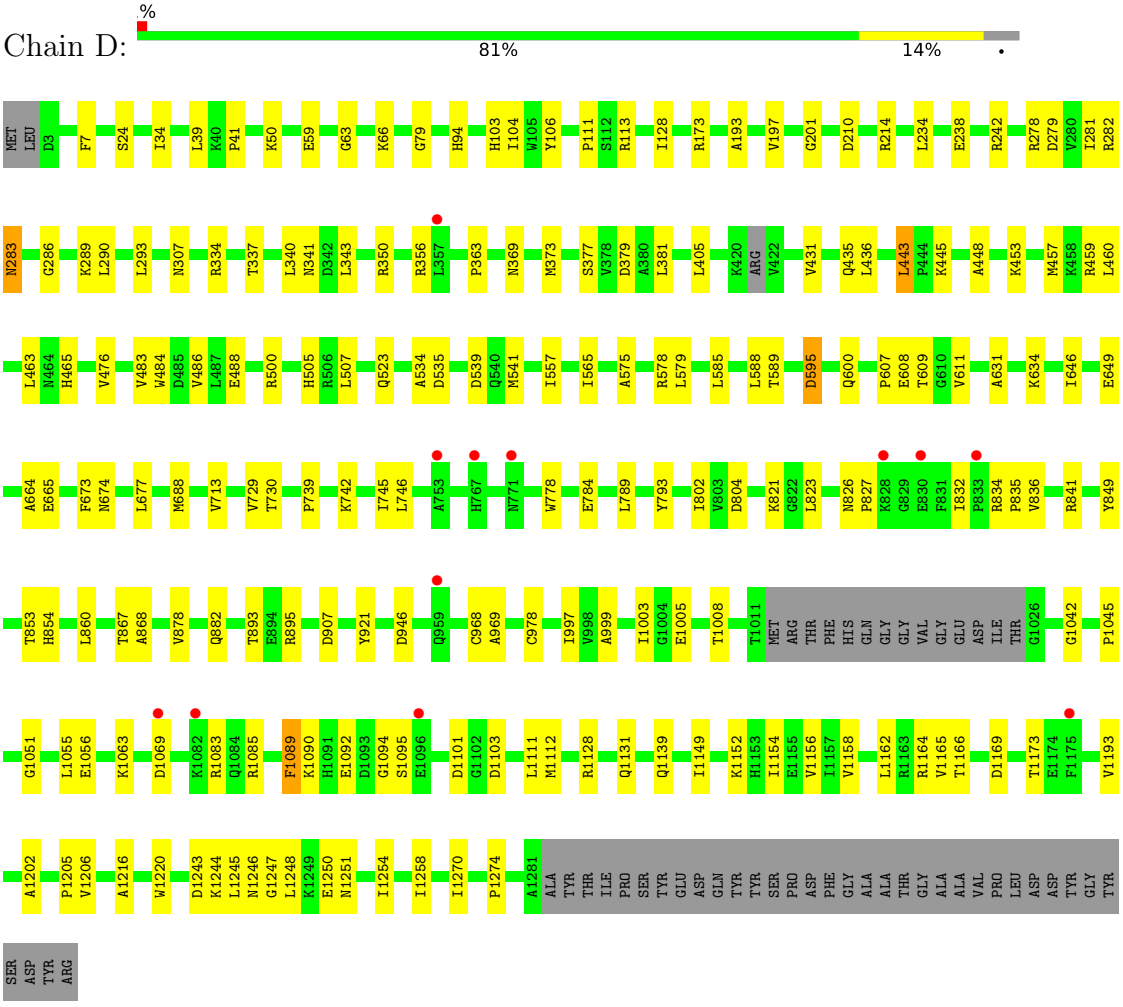






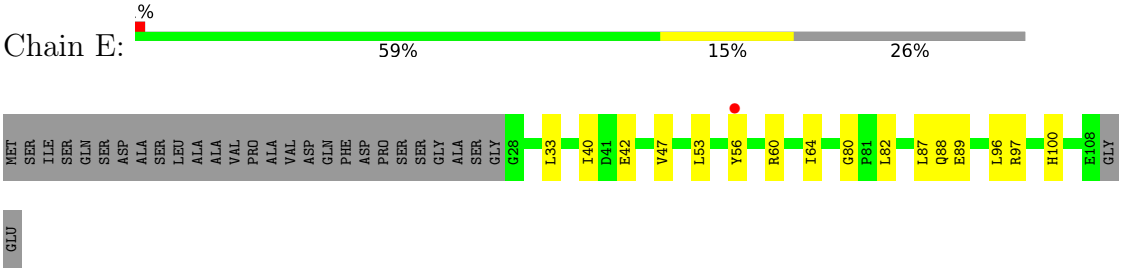
• Molecule 3: DNA-directed RNA polymerase subunit beta'

Chain D:



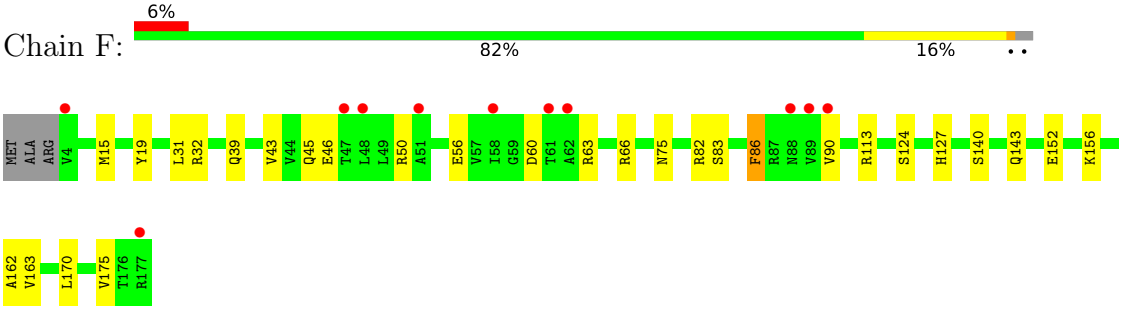
• Molecule 4: DNA-directed RNA polymerase subunit omega

Chain E:



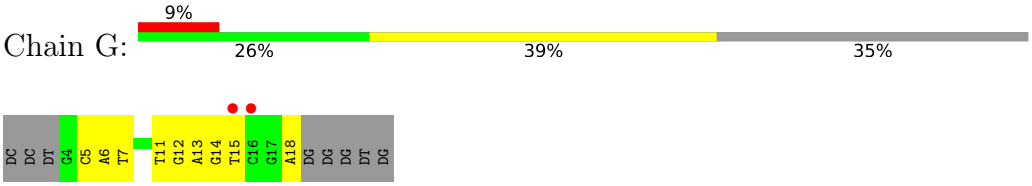
• Molecule 5: RNA polymerase sigma factor

Chain F:



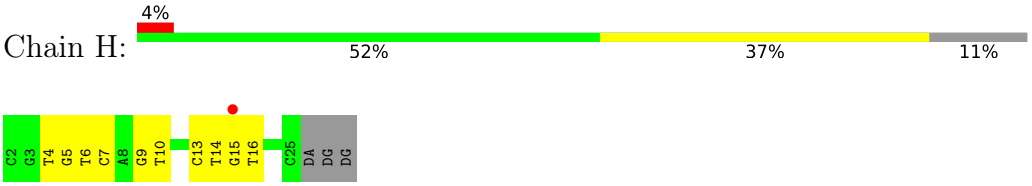
• Molecule 6: T DNA

Chain G:



• Molecule 7: NT DNA

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	142.77Å 160.61Å 238.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.71 – 3.70 48.71 – 3.70	Depositor EDS
% Data completeness (in resolution range)	97.1 (48.71-3.70) 97.1 (48.71-3.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.53 (at 3.67Å)	Xtriage
Refinement program	PHENIX 1.19_4092, PHENIX 1.19_4092	Depositor
R, R_{free}	0.208 , 0.245 0.207 , 0.244	Depositor DCC
R_{free} test set	1997 reflections (3.48%)	wwPDB-VP
Wilson B-factor (Å^2)	132.1	Xtriage
Anisotropy	0.612	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 97.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	24903	wwPDB-VP
Average B, all atoms (Å^2)	167.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.51% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 7US

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	0.26	0/1742	0.56	0/2370
1	B	0.26	0/1758	0.55	0/2397
2	C	0.25	0/8883	0.51	1/12043 (0.0%)
3	D	0.25	0/10049	0.50	0/13583
4	E	0.24	0/643	0.45	0/877
5	F	0.25	0/1374	0.52	0/1869
6	G	0.44	0/343	0.84	0/528
7	H	0.54	0/550	0.93	0/848
All	All	0.26	0/25342	0.53	1/34515 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	677	ARG	O-C-N	-5.96	113.16	122.70

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	1716	0	1756	42	0
1	B	1732	0	1754	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	8724	0	8651	160	0
3	D	9884	0	9947	124	0
4	E	630	0	622	11	0
5	F	1352	0	1346	20	0
6	G	306	0	170	10	0
7	H	491	0	272	18	0
8	C	68	0	0	10	0
All	All	24903	0	24518	369	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 (369) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:442:GLN:HG3	2:C:679:ASN:ND2	1.37	1.36
2:C:442:GLN:CG	2:C:679:ASN:HD22	1.43	1.30
2:C:430:PHE:O	2:C:434:SER:HB2	1.26	1.25
2:C:454:ARG:HH22	8:C:1201:7US:C19	1.53	1.22
2:C:442:GLN:CB	2:C:679:ASN:HD22	1.60	1.13
2:C:442:GLN:CG	2:C:679:ASN:ND2	2.13	0.99
2:C:454:ARG:NH2	8:C:1201:7US:C19	2.26	0.97
1:A:40:ARG:HE	1:B:33:THR:HG22	1.29	0.97
2:C:384:LEU:CD1	2:C:436:LEU:HD23	1.95	0.96
2:C:384:LEU:HD13	2:C:436:LEU:HD23	1.47	0.95
2:C:178:GLN:HB2	2:C:436:LEU:HD21	1.48	0.95
1:A:4:SER:HB3	1:B:144:ARG:HH12	1.29	0.94
2:C:489:PRO:HB3	8:C:1201:7US:C30	1.98	0.93
2:C:430:PHE:O	2:C:434:SER:CB	2.20	0.89
2:C:442:GLN:HG3	2:C:679:ASN:HD21	1.37	0.86
2:C:174:VAL:HG23	2:C:440:MET:HB3	1.59	0.85
2:C:454:ARG:HH12	8:C:1201:7US:C16	1.91	0.83
2:C:442:GLN:CB	2:C:679:ASN:ND2	2.39	0.82
2:C:456:SER:OG	2:C:497:ILE:HG12	1.83	0.78
2:C:593:MET:HA	2:C:628:THR:HG21	1.66	0.77
2:C:384:LEU:HD13	2:C:436:LEU:CD2	2.16	0.75
1:A:56:ILE:HB	1:A:59:VAL:HG22	1.67	0.74
2:C:442:GLN:OE1	2:C:678:SER:OG	2.05	0.74
3:D:832:ILE:HG22	3:D:834:ARG:H	1.54	0.73
5:F:50:ARG:NH1	7:H:4:DT:O4	2.22	0.73
2:C:442:GLN:HB2	2:C:679:ASN:ND2	2.05	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:185:GLN:O	3:D:445:LYS:NZ	2.21	0.72
3:D:1090:LYS:HB3	3:D:1092:GLU:HG2	1.72	0.71
2:C:454:ARG:HH12	8:C:1201:7US:C15	2.02	0.71
3:D:1173:THR:HG22	3:D:1193:VAL:HG21	1.72	0.71
2:C:435:GLN:HG3	2:C:460:PRO:HD3	1.73	0.71
2:C:174:VAL:HG21	2:C:440:MET:HB2	1.72	0.70
3:D:674:ASN:HA	3:D:677:LEU:HD21	1.72	0.70
2:C:467:ARG:HG3	7:H:16:DT:H5'	1.74	0.70
3:D:1090:LYS:HE2	3:D:1103:ASP:HA	1.74	0.70
2:C:1024:THR:H	3:D:730:THR:HG21	1.56	0.69
1:B:24:GLU:HB2	1:B:191:LYS:HG3	1.74	0.69
2:C:384:LEU:CD1	2:C:436:LEU:CD2	2.71	0.69
2:C:384:LEU:HD11	2:C:436:LEU:HD23	1.73	0.68
2:C:442:GLN:CB	2:C:679:ASN:HB2	2.23	0.68
2:C:558:ARG:HB3	2:C:570:TYR:HB3	1.75	0.68
3:D:1248:LEU:HD22	3:D:1258:ILE:HB	1.76	0.68
2:C:467:ARG:NH1	7:H:14:DT:OP1	2.27	0.67
5:F:75:ASN:ND2	7:H:4:DT:O2	2.28	0.67
2:C:541:VAL:HG12	2:C:578:TYR:HB2	1.79	0.65
1:B:84:VAL:HG12	1:B:199:LYS:HD2	1.79	0.65
2:C:896:GLY:HA2	3:D:431:VAL:HG13	1.80	0.64
2:C:113:ASP:HB3	2:C:132:PRO:HG2	1.80	0.63
3:D:50:LYS:HE2	3:D:79:GLY:HA3	1.81	0.63
3:D:460:LEU:HD11	3:D:483:VAL:HG12	1.81	0.62
2:C:174:VAL:CG2	2:C:440:MET:CB	2.78	0.62
3:D:363:PRO:HG2	5:F:15:MET:HG3	1.82	0.62
2:C:458:LEU:HD21	2:C:496:LEU:HD13	1.82	0.62
2:C:824:ILE:HA	5:F:163:VAL:HG13	1.82	0.61
3:D:557:ILE:HG23	4:E:40:ILE:HD11	1.82	0.61
3:D:1247:GLY:O	3:D:1251:ASN:ND2	2.25	0.61
2:C:30:ASN:ND2	2:C:629:GLY:O	2.34	0.61
2:C:442:GLN:HB3	2:C:679:ASN:HB2	1.83	0.61
2:C:174:VAL:HG23	2:C:440:MET:CB	2.30	0.61
1:A:144:ARG:NH2	1:B:27:GLU:OE2	2.34	0.61
2:C:83:VAL:HG13	2:C:87:GLU:HB2	1.82	0.60
1:B:100:GLN:HG3	1:B:133:LYS:HB2	1.83	0.60
2:C:442:GLN:HB2	2:C:679:ASN:HD22	1.52	0.60
3:D:1045:PRO:HG2	3:D:1111:LEU:HB2	1.84	0.60
1:A:40:ARG:NE	1:B:33:THR:HG22	2.09	0.59
2:C:228:ARG:HD3	7:H:14:DT:H72	1.85	0.59
2:C:454:ARG:HH22	8:C:1201:7US:C18	2.13	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:ILE:HG12	1:A:136:VAL:HG22	1.85	0.58
2:C:174:VAL:CG2	2:C:440:MET:HB3	2.32	0.58
2:C:377:ARG:NH2	2:C:383:GLU:OE1	2.34	0.58
2:C:442:GLN:HB2	2:C:679:ASN:HB2	1.83	0.58
1:A:186:ARG:HG3	1:A:187:THR:HG23	1.86	0.58
2:C:1104:GLU:OE2	5:F:113:ARG:NH1	2.37	0.58
2:C:168:ILE:HG12	2:C:431:PHE:HB3	1.85	0.58
2:C:1087:GLU:HG3	2:C:1091:ILE:HD11	1.85	0.58
1:A:216:VAL:HG13	1:B:216:VAL:HG13	1.85	0.57
2:C:440:MET:HA	2:C:451:HIS:CE1	2.40	0.57
2:C:473:ARG:NH2	2:C:492:PRO:O	2.37	0.57
2:C:181:ARG:NH1	7:H:15:DG:OP2	2.37	0.57
1:A:183:VAL:O	1:A:185:GLN:N	2.38	0.57
3:D:500:ARG:HD2	3:D:534:ALA:HB2	1.86	0.57
4:E:87:LEU:HG	4:E:88:GLN:HG3	1.87	0.57
5:F:60:ASP:OD1	5:F:63:ARG:HB3	2.03	0.57
1:A:22:VAL:HG12	1:A:193:ILE:HG12	1.87	0.57
2:C:628:THR:HG23	2:C:630:MET:H	1.70	0.56
2:C:182:SER:HB2	2:C:377:ARG:HB2	1.86	0.56
3:D:111:PRO:O	3:D:113:ARG:NH1	2.37	0.56
3:D:1051:GLY:HA2	3:D:1069:ASP:HB2	1.86	0.56
2:C:388:GLN:HG3	2:C:430:PHE:CD1	2.41	0.56
2:C:173:ARG:HA	2:C:439:PHE:HA	1.87	0.56
1:B:55:ARG:NH2	1:B:137:GLU:OE1	2.35	0.55
6:G:18:DA:H8	6:G:18:DA:P	2.28	0.55
3:D:173:ARG:HH21	3:D:201:GLY:HA2	1.72	0.55
6:G:11:DT:H2'	6:G:12:DG:C8	2.41	0.55
2:C:257:ILE:HD11	2:C:346:VAL:HG23	1.88	0.55
1:B:97:LEU:HB2	1:B:110:ILE:HG13	1.88	0.55
3:D:104:ILE:HD12	3:D:379:ASP:HB3	1.89	0.55
3:D:907:ASP:OD1	3:D:907:ASP:N	2.38	0.55
1:A:2:LEU:O	1:A:2:LEU:HD12	2.06	0.55
3:D:505:HIS:CD2	3:D:507:LEU:HB2	2.42	0.55
3:D:742:LYS:HE2	3:D:746:LEU:HD11	1.89	0.55
2:C:168:ILE:HB	2:C:173:ARG:HD2	1.90	0.54
3:D:34:ILE:HA	3:D:41:PRO:HA	1.88	0.54
2:C:47:PRO:HG2	2:C:581:VAL:HG13	1.89	0.54
3:D:882:GLN:HG3	3:D:997:ILE:HD11	1.89	0.54
4:E:60:ARG:NH2	4:E:80:GLY:O	2.40	0.54
3:D:1055:LEU:H	3:D:1101:ASP:HB3	1.72	0.54
3:D:826:ASN:HB3	3:D:832:ILE:HD11	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1085:ARG:HA	3:D:1112:MET:HA	1.90	0.54
2:C:285:GLU:OE2	7:H:9:DG:N2	2.41	0.54
2:C:536:GLU:OE2	2:C:562:ARG:NH1	2.41	0.54
3:D:356:ARG:NH2	5:F:46:GLU:OE2	2.41	0.54
3:D:867:THR:HG22	3:D:1008:THR:HG23	1.90	0.53
3:D:849:TYR:O	3:D:853:THR:HG23	2.08	0.53
7:H:14:DT:H4'	7:H:15:DG:O5'	2.09	0.53
1:A:62:GLU:O	1:A:73:VAL:HB	2.09	0.53
2:C:369:ASP:C	2:C:371:ASP:H	2.11	0.53
3:D:1164:ARG:NH2	3:D:1216:ALA:O	2.42	0.53
1:B:81:LYS:HD3	1:B:165:ASP:HB2	1.90	0.53
3:D:1165:VAL:HG12	3:D:1205:PRO:HA	1.91	0.52
2:C:571:VAL:HG22	2:C:572:PRO:HD2	1.90	0.52
3:D:128:ILE:HD11	3:D:234:LEU:HD11	1.90	0.52
1:B:182:ARG:CZ	3:D:488:GLU:HG2	2.40	0.52
2:C:174:VAL:CG2	2:C:440:MET:HB2	2.35	0.52
3:D:334:ARG:HD3	5:F:90:VAL:HG21	1.91	0.52
3:D:369:ASN:ND2	5:F:45:GLN:OE1	2.42	0.52
3:D:1270:ILE:HD13	4:E:56:TYR:HE1	1.73	0.52
5:F:140:SER:HB3	5:F:143:GLN:HG3	1.91	0.52
2:C:442:GLN:HB2	2:C:679:ASN:CB	2.40	0.52
3:D:674:ASN:HA	3:D:677:LEU:CD2	2.40	0.52
1:B:84:VAL:HG23	1:B:119:HIS:HB2	1.91	0.51
2:C:209:GLY:O	7:H:13:DC:N4	2.44	0.51
2:C:140:ILE:HA	2:C:147:ILE:HG12	1.92	0.51
1:A:9:LEU:HD11	1:A:21:PHE:HB3	1.93	0.51
2:C:982:GLU:HG3	3:D:841:ARG:HH12	1.76	0.51
2:C:120:ASP:OD1	2:C:120:ASP:N	2.44	0.51
5:F:32:ARG:HD2	7:H:9:DG:O3'	2.11	0.51
3:D:1152:LYS:O	3:D:1156:VAL:HG23	2.11	0.51
1:A:30:PHE:HE2	1:B:41:THR:HA	1.76	0.51
2:C:122:CYS:HA	2:C:127:MET:HG3	1.93	0.51
1:B:98:ARG:HG2	1:B:135:GLU:HG2	1.93	0.50
2:C:679:ASN:C	2:C:681:GLY:H	2.13	0.50
2:C:213:GLU:OE2	2:C:225:ARG:NH1	2.45	0.50
2:C:218:LYS:NZ	6:G:7:DT:OP2	2.43	0.50
2:C:678:SER:HB2	2:C:684:ALA:HB2	1.93	0.50
3:D:778:TRP:CD2	3:D:835:PRO:HG3	2.46	0.50
2:C:524:VAL:HG21	2:C:548:ILE:HD13	1.93	0.50
1:B:176:TYR:HB3	1:B:194:LEU:HD23	1.93	0.50
3:D:600:GLN:HB2	3:D:609:THR:HB	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:101:GLY:N	1:B:132:GLY:O	2.39	0.50
2:C:217:ASP:OD2	2:C:231:ARG:NH2	2.45	0.50
3:D:1042:GLY:O	3:D:1083:ARG:NH2	2.42	0.50
3:D:1045:PRO:HB2	3:D:1111:LEU:HD12	1.94	0.50
4:E:89:GLU:OE2	4:E:97:ARG:NH1	2.44	0.50
5:F:152:GLU:HG3	5:F:156:LYS:HE3	1.93	0.50
2:C:440:MET:HA	2:C:451:HIS:ND1	2.27	0.50
2:C:441:ASP:OD1	2:C:680:HIS:CD2	2.65	0.50
2:C:848:ILE:HD13	2:C:874:ALA:HB2	1.93	0.49
1:A:45:SER:HG	1:B:30:PHE:HZ	1.60	0.49
3:D:1247:GLY:H	3:D:1251:ASN:ND2	2.10	0.49
6:G:12:DG:H2'	6:G:13:DA:C8	2.47	0.49
3:D:611:VAL:HG22	3:D:634:LYS:HB2	1.94	0.49
3:D:739:PRO:HG3	3:D:789:LEU:HG	1.94	0.49
2:C:99:PHE:HB3	7:H:7:DC:H1'	1.94	0.49
1:A:214:THR:OG1	1:B:230:GLU:HG3	2.12	0.49
3:D:369:ASN:O	3:D:373:MET:HG3	2.13	0.49
2:C:441:ASP:OD1	2:C:680:HIS:HD2	1.96	0.49
3:D:968:CYS:HB2	3:D:978:CYS:SG	2.53	0.49
1:B:77:ILE:HD11	1:B:162:ILE:HD12	1.94	0.49
2:C:172:GLU:O	2:C:439:PHE:HB2	2.13	0.49
2:C:440:MET:SD	2:C:452:LYS:HE3	2.52	0.49
3:D:453:LYS:HG3	3:D:476:VAL:HG11	1.94	0.49
1:A:40:ARG:HD2	2:C:1013:GLY:O	2.13	0.49
1:B:182:ARG:NH2	3:D:488:GLU:HG2	2.27	0.49
3:D:443:LEU:HD13	3:D:448:ALA:HB2	1.94	0.49
3:D:1274:PRO:HB3	4:E:82:LEU:HD11	1.94	0.48
1:B:17:ASN:OD1	1:B:17:ASN:N	2.45	0.48
3:D:1154:ILE:O	3:D:1158:VAL:HG23	2.13	0.48
4:E:42:GLU:OE1	4:E:100:HIS:NE2	2.38	0.48
1:A:89:GLU:HB3	1:A:91:GLU:HG2	1.95	0.48
1:A:185:GLN:HG2	1:A:186:ARG:H	1.78	0.48
2:C:454:ARG:NH1	8:C:1201:7US:C16	2.70	0.48
2:C:720:LEU:HD23	2:C:913:VAL:HA	1.96	0.48
3:D:59:GLU:HG2	3:D:66:LYS:HD3	1.95	0.48
2:C:58:THR:O	2:C:62:GLU:HG3	2.14	0.48
2:C:435:GLN:CG	2:C:460:PRO:HD3	2.42	0.48
2:C:440:MET:SD	2:C:452:LYS:CE	3.02	0.48
3:D:463:LEU:HB2	3:D:465:HIS:HD2	1.79	0.48
3:D:677:LEU:HD23	3:D:677:LEU:H	1.78	0.48
3:D:337:THR:HG1	3:D:341:ASN:HD22	1.56	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:14:DT:H2"	7:H:15:DG:H5"	1.95	0.48
1:B:45:SER:HA	1:B:144:ARG:HD2	1.96	0.47
2:C:33:PRO:HG2	2:C:632:LEU:HD21	1.96	0.47
2:C:1055:GLN:HG2	2:C:1094:ASP:HB3	1.95	0.47
1:A:56:ILE:HB	1:A:59:VAL:CG2	2.40	0.47
4:E:33:LEU:HD23	4:E:33:LEU:H	1.80	0.47
4:E:47:VAL:HG11	4:E:53:LEU:HB2	1.96	0.47
2:C:388:GLN:HG3	2:C:430:PHE:HB2	1.96	0.47
3:D:827:PRO:HD3	3:D:854:HIS:HB3	1.96	0.47
2:C:190:THR:HG23	2:C:199:LEU:HB2	1.96	0.47
2:C:473:ARG:HB3	2:C:495:GLY:HA3	1.97	0.47
3:D:286:GLY:HA2	3:D:289:LYS:HB3	1.96	0.47
2:C:592:ALA:HA	2:C:976:VAL:HG21	1.97	0.47
1:A:2:LEU:HD11	1:B:168:TYR:CE2	2.50	0.47
3:D:290:LEU:HD23	3:D:293:LEU:HD12	1.97	0.47
3:D:343:LEU:HD13	3:D:381:LEU:HA	1.96	0.47
3:D:453:LYS:O	3:D:457:MET:HG3	2.14	0.47
3:D:1166:THR:HB	3:D:1206:VAL:HG21	1.97	0.47
2:C:704:ASP:HB2	2:C:708:THR:HB	1.96	0.47
3:D:340:LEU:HD11	3:D:405:LEU:HD11	1.97	0.47
1:A:149:ALA:HB1	1:A:163:PRO:HB2	1.97	0.47
1:A:40:ARG:NH1	2:C:903:ASP:OD1	2.39	0.47
2:C:489:PRO:HG3	8:C:1201:7US:O11	2.15	0.46
3:D:1220:TRP:CD1	3:D:1243:ASP:HB2	2.50	0.46
1:B:74:THR:HG21	3:D:608:GLU:HB2	1.95	0.46
3:D:1169:ASP:H	3:D:1202:ALA:HB3	1.79	0.46
2:C:104:SER:HB3	2:C:140:ILE:HB	1.97	0.46
2:C:435:GLN:CB	2:C:460:PRO:HD3	2.45	0.46
2:C:32:VAL:H	2:C:33:PRO:HD3	1.80	0.46
3:D:290:LEU:HA	3:D:293:LEU:HD12	1.98	0.46
3:D:1131:GLN:HE21	3:D:1162:LEU:HD12	1.80	0.46
2:C:298:ASN:HA	2:C:302:LYS:HB2	1.97	0.46
2:C:441:ASP:H	2:C:451:HIS:CD2	2.33	0.46
3:D:63:GLY:HA2	3:D:66:LYS:HE2	1.98	0.46
1:A:86:SER:O	1:A:116:VAL:HA	2.15	0.46
3:D:729:VAL:HG11	3:D:802:ILE:HD11	1.98	0.46
2:C:236:VAL:HG13	2:C:273:ALA:HB1	1.98	0.46
2:C:48:LEU:HB2	2:C:528:ILE:HD13	1.97	0.46
3:D:1131:GLN:HG2	3:D:1158:VAL:HG12	1.98	0.46
3:D:1250:GLU:O	3:D:1254:ILE:HG12	2.16	0.46
3:D:565:ILE:HG23	3:D:575:ALA:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1056:GLU:HB2	3:D:1063:LYS:HG3	1.97	0.45
1:B:92:PRO:HB3	1:B:141:GLU:HG2	1.99	0.45
1:B:228:GLU:HG2	1:B:229:ALA:H	1.81	0.45
3:D:595:ASP:HB3	3:D:631:ALA:HB2	1.98	0.45
2:C:549:ASP:OD1	2:C:550:ALA:N	2.50	0.45
2:C:742:VAL:HG13	2:C:878:LYS:HD3	1.99	0.45
2:C:927:ASN:O	2:C:930:GLN:HG2	2.17	0.45
7:H:6:DT:H3'	7:H:7:DC:H5"	1.98	0.45
1:A:2:LEU:N	1:A:186:ARG:HH21	2.15	0.45
3:D:436:LEU:HD11	3:D:523:GLN:HB3	1.98	0.45
1:A:90:ASP:OD1	1:A:142:ARG:HD3	2.16	0.45
3:D:281:ILE:HD13	3:D:293:LEU:HD23	1.99	0.45
2:C:1060:LYS:HB2	6:G:18:DA:H5"	1.99	0.45
2:C:1074:TRP:CE2	3:D:878:VAL:HG11	2.52	0.45
3:D:1092:GLU:HG3	3:D:1094:GLY:H	1.82	0.45
5:F:83:SER:HA	5:F:86:PHE:HB2	1.98	0.45
1:A:29:GLY:N	1:A:190:ASP:OD2	2.44	0.45
3:D:283:ASN:O	3:D:283:ASN:ND2	2.50	0.45
2:C:47:PRO:HG3	2:C:517:ARG:HD2	1.99	0.45
3:D:24:SER:HB2	3:D:94:HIS:HB3	1.99	0.45
1:A:95:MET:HG2	1:A:112:PRO:HA	1.99	0.44
1:B:2:LEU:O	1:B:231:GLY:HA3	2.16	0.44
2:C:754:GLU:HG3	2:C:872:TYR:HE1	1.82	0.44
6:G:5:DC:H2"	6:G:6:DA:C8	2.52	0.44
7:H:9:DG:N3	7:H:9:DG:H2'	2.32	0.44
2:C:32:VAL:H	2:C:33:PRO:CD	2.30	0.44
2:C:686:GLN:HA	2:C:705:GLY:HA2	1.99	0.44
1:B:30:PHE:HA	1:B:33:THR:HG23	2.00	0.44
2:C:440:MET:O	2:C:440:MET:HG2	2.17	0.44
3:D:334:ARG:CD	5:F:90:VAL:HG21	2.48	0.44
2:C:189:GLU:HB2	2:C:367:THR:HG21	1.99	0.44
3:D:1244:LYS:O	3:D:1246:ASN:N	2.49	0.44
5:F:170:LEU:HD22	5:F:175:VAL:HG21	1.99	0.44
6:G:18:DA:OP2	6:G:18:DA:C8	2.71	0.44
1:A:95:MET:HB3	1:A:95:MET:HE2	1.94	0.44
2:C:603:ASN:ND2	3:D:860:LEU:HD21	2.33	0.44
3:D:103:HIS:HB3	3:D:106:TYR:HD2	1.82	0.44
1:A:175:THR:HB	2:C:910:GLY:HA3	2.00	0.44
1:B:75:GLU:O	1:B:79:ASN:ND2	2.50	0.44
2:C:228:ARG:O	2:C:228:ARG:HG3	2.18	0.44
2:C:440:MET:HA	2:C:451:HIS:CG	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:809:LYS:HE2	2:C:813:GLU:HB2	2.00	0.44
3:D:677:LEU:HD23	3:D:677:LEU:N	2.33	0.43
2:C:173:ARG:NH1	2:C:437:SER:O	2.51	0.43
2:C:215:ASP:OD1	2:C:231:ARG:NH1	2.51	0.43
2:C:751:HIS:CD2	2:C:877:ARG:HD2	2.53	0.43
2:C:760:ARG:HG2	2:C:865:VAL:HG22	2.01	0.43
2:C:853:PHE:HD2	2:C:868:LEU:HD23	1.84	0.43
3:D:745:ILE:HD13	3:D:784:GLU:HG2	1.99	0.43
3:D:445:LYS:HB3	3:D:484:TRP:CZ3	2.54	0.43
2:C:404:MET:HB2	2:C:404:MET:HE2	1.88	0.43
3:D:634:LYS:HA	3:D:664:ALA:O	2.18	0.43
3:D:646:ILE:O	3:D:649:GLU:HG3	2.19	0.43
3:D:893:THR:HG21	3:D:969:ALA:HB3	2.01	0.43
2:C:720:LEU:HD12	2:C:1026:GLY:O	2.18	0.43
2:C:891:ASN:OD1	2:C:891:ASN:N	2.45	0.43
2:C:906:PHE:HA	2:C:912:PRO:HA	2.00	0.43
3:D:350:ARG:HD2	3:D:377:SER:OG	2.18	0.43
3:D:589:THR:HG21	3:D:688:MET:HG2	2.00	0.43
3:D:921:TYR:HE1	3:D:946:ASP:HA	1.84	0.43
5:F:124:SER:OG	5:F:127:HIS:ND1	2.39	0.43
2:C:642:VAL:HB	2:C:703:ALA:HB3	2.00	0.43
3:D:193:ALA:O	3:D:197:VAL:HG23	2.19	0.43
5:F:31:LEU:HD21	7:H:10:DT:C6	2.54	0.43
2:C:678:SER:CB	2:C:684:ALA:HB2	2.48	0.43
1:A:69:VAL:HG12	1:A:128:LEU:HG	2.00	0.43
1:A:99:LYS:HG2	1:A:105:VAL:HG22	2.01	0.43
1:B:28:PRO:HA	1:B:29:GLY:HA2	1.50	0.43
2:C:982:GLU:HG3	3:D:841:ARG:NH1	2.34	0.43
3:D:823:LEU:HD23	3:D:835:PRO:HB3	2.01	0.43
1:A:4:SER:HB3	1:B:144:ARG:NH1	2.13	0.43
3:D:575:ALA:O	3:D:713:VAL:HG21	2.19	0.42
4:E:96:LEU:HD12	4:E:96:LEU:HA	1.85	0.42
2:C:202:VAL:HG21	2:C:345:LEU:HB2	2.01	0.42
3:D:634:LYS:HG2	3:D:665:GLU:HG2	2.00	0.42
3:D:868:ALA:HA	6:G:14:DG:O4'	2.19	0.42
1:A:218:LEU:HD12	1:A:218:LEU:HA	1.85	0.42
2:C:56:VAL:HG21	2:C:500:LEU:HD22	2.01	0.42
2:C:588:SER:OG	2:C:589:VAL:N	2.53	0.42
3:D:1139:GLN:NE2	3:D:1149:ILE:O	2.49	0.42
2:C:763:LYS:HE2	3:D:39:LEU:HG	2.02	0.42
3:D:789:LEU:HD22	3:D:793:TYR:HE2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:119:VAL:HG23	2:C:167:ILE:HD11	2.02	0.42
2:C:439:PHE:CD1	2:C:439:PHE:O	2.72	0.42
3:D:238:GLU:HG2	3:D:242:ARG:HH12	1.84	0.42
4:E:60:ARG:O	4:E:64:ILE:HG13	2.18	0.42
2:C:444:ASN:O	2:C:447:SER:OG	2.26	0.42
2:C:610:ASN:OD1	2:C:613:ARG:NH1	2.52	0.42
2:C:678:SER:N	2:C:682:THR:O	2.47	0.42
3:D:585:LEU:HD13	3:D:673:PHE:HE1	1.84	0.42
6:G:5:DC:H2"	6:G:6:DA:N7	2.34	0.42
3:D:821:LYS:HB3	3:D:836:VAL:HB	2.01	0.42
3:D:1101:ASP:N	3:D:1101:ASP:OD1	2.51	0.42
7:H:14:DT:H6	7:H:14:DT:H2'	1.67	0.42
1:A:34:LEU:HD11	1:B:218:LEU:HD13	2.02	0.42
1:A:219:PHE:CE1	1:B:215:LEU:HD13	2.54	0.42
1:B:99:LYS:NZ	1:B:104:GLU:O	2.45	0.42
1:A:81:LYS:NZ	1:A:165:ASP:HB2	2.35	0.42
2:C:177:SER:HB2	2:C:455:LEU:HD23	2.02	0.42
2:C:454:ARG:NH1	8:C:1201:7US:C15	2.78	0.42
2:C:571:VAL:CG2	2:C:572:PRO:HD2	2.50	0.42
2:C:821:LEU:HA	2:C:824:ILE:HG12	2.01	0.42
3:D:210:ASP:O	3:D:214:ARG:HG3	2.19	0.42
3:D:505:HIS:ND1	3:D:1005:GLU:HG3	2.35	0.42
5:F:82:ARG:HB3	5:F:83:SER:H	1.69	0.42
2:C:40:SER:HA	2:C:973:SER:HB2	2.02	0.41
2:C:60:SER:OG	2:C:382:GLY:N	2.36	0.41
1:A:66:VAL:O	1:A:69:VAL:HG22	2.20	0.41
2:C:486:ILE:HD11	3:D:849:TYR:HE1	1.84	0.41
5:F:39:GLN:O	5:F:43:VAL:HG23	2.20	0.41
1:A:68:GLY:HA3	1:A:132:GLY:HA2	2.02	0.41
1:A:77:ILE:O	1:A:81:LYS:HG3	2.20	0.41
1:B:124:HIS:HE1	1:B:127:THR:HG23	1.85	0.41
3:D:457:MET:HE2	3:D:457:MET:HB2	1.74	0.41
3:D:579:LEU:HD23	3:D:579:LEU:HA	1.93	0.41
5:F:127:HIS:HB3	5:F:162:ALA:HB2	2.03	0.41
6:G:14:DG:H2'	6:G:15:DT:C6	2.56	0.41
3:D:500:ARG:HB2	3:D:541:MET:HG2	2.02	0.41
2:C:736:ILE:HB	2:C:916:ILE:HB	2.03	0.41
2:C:1068:PHE:CZ	2:C:1072:GLU:HB3	2.56	0.41
3:D:278:ARG:O	3:D:282:ARG:HG3	2.21	0.41
3:D:435:GLN:OE1	3:D:435:GLN:N	2.43	0.41
3:D:895:ARG:HD2	3:D:1128:ARG:HH22	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1245:LEU:HD13	3:D:1254:ILE:HD13	2.03	0.41
2:C:472:VAL:HG22	7:H:15:DG:C2	2.56	0.41
1:A:221:LEU:O	1:A:224:GLU:HG2	2.21	0.40
2:C:1146:GLU:H	2:C:1146:GLU:HG2	1.76	0.40
1:A:84:VAL:HG12	1:A:120:ASN:ND2	2.36	0.40
2:C:1137:VAL:HG23	2:C:1145:ILE:HG13	2.03	0.40
3:D:999:ALA:O	3:D:1003:ILE:HG13	2.21	0.40
2:C:516:TYR:HB3	2:C:578:TYR:HB3	2.04	0.40
3:D:460:LEU:HD23	3:D:486:VAL:HG21	2.03	0.40
2:C:513:GLU:HG2	2:C:532:THR:HG22	2.02	0.40
2:C:731:TYR:HE1	3:D:579:LEU:HB2	1.87	0.40
2:C:451:HIS:NE2	8:C:1201:7US:O10	2.54	0.40
2:C:899:LEU:HB2	2:C:904:MET:CE	2.52	0.40
3:D:1089:PHE:HA	3:D:1095:SER:HA	2.04	0.40
7:H:5:DG:H5'	7:H:6:DT:OP2	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	223/347 (64%)	213 (96%)	9 (4%)	1 (0%)	34	69
1	B	230/347 (66%)	217 (94%)	10 (4%)	3 (1%)	12	47
2	C	1124/1178 (95%)	1061 (94%)	54 (5%)	9 (1%)	19	56
3	D	1258/1316 (96%)	1206 (96%)	50 (4%)	2 (0%)	47	78
4	E	79/110 (72%)	76 (96%)	3 (4%)	0	100	100
5	F	172/177 (97%)	167 (97%)	5 (3%)	0	100	100
All	All	3086/3475 (89%)	2940 (95%)	131 (4%)	15 (0%)	29	66

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	184	GLU
1	B	159	ILE
2	C	370	ILE
2	C	677	ARG
2	C	680	HIS
2	C	732	GLU
2	C	32	VAL
3	D	1089	PHE
1	B	6	ARG
3	D	607	PRO
2	C	520	VAL
2	C	922	VAL
2	C	358	PRO
1	B	227	VAL
2	C	33	PRO

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	194/297 (65%)	194 (100%)	0	100	100
1	B	191/297 (64%)	189 (99%)	2 (1%)	76	86
2	C	950/998 (95%)	939 (99%)	11 (1%)	71	84
3	D	1049/1095 (96%)	1037 (99%)	12 (1%)	73	85
4	E	66/90 (73%)	66 (100%)	0	100	100
5	F	134/136 (98%)	130 (97%)	4 (3%)	41	66
All	All	2584/2913 (89%)	2555 (99%)	29 (1%)	73	85

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

Mol	Chain	Res	Type
1	B	79	ASN
1	B	90	ASP
2	C	126	ASP
2	C	208	ARG

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Mol	Chain	Res	Type
2	C	434	SER
2	C	439	PHE
2	C	440	MET
2	C	442	GLN
2	C	454	ARG
2	C	456	SER
2	C	534	ASP
2	C	678	SER
2	C	691	ASP
3	D	7	PHE
3	D	279	ASP
3	D	283	ASN
3	D	307	ASN
3	D	443	LEU
3	D	459	ARG
3	D	535	ASP
3	D	539	ASP
3	D	578	ARG
3	D	588	LEU
3	D	595	ASP
3	D	804	ASP
5	F	19	TYR
5	F	56	GLU
5	F	66	ARG
5	F	86	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	679	ASN
2	C	680	HIS

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)

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	$\#\|Z\| > 2$
8	7US	C	1201	-	65,74,74	4.15	18 (27%)	80,113,113	3.54	26 (32%)

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
8	7US	C	1201	-	-	20/60/121/121	1/6/7/7

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	1201	7US	C4-N2	23.52	1.46	1.29
8	C	1201	7US	C43-N4	-11.73	1.20	1.47
8	C	1201	7US	O3-C6	9.85	1.56	1.37
8	C	1201	7US	C10-C4	9.39	1.58	1.46
8	C	1201	7US	C15-N1	7.26	1.49	1.36
8	C	1201	7US	O7-C25	-4.99	1.37	1.44
8	C	1201	7US	C9-C1	4.30	1.57	1.46
8	C	1201	7US	C3-N3	4.03	1.46	1.35
8	C	1201	7US	O5-C29	3.70	1.55	1.43
8	C	1201	7US	C12-C11	-3.40	1.41	1.54
8	C	1201	7US	C6-C7	3.01	1.44	1.39
8	C	1201	7US	O12-N7	-2.67	1.18	1.22
8	C	1201	7US	C44-C43	2.67	1.60	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	1201	7US	C28-C29	-2.60	1.41	1.50
8	C	1201	7US	C2-N1	2.27	1.46	1.41
8	C	1201	7US	O9-C23	-2.25	1.37	1.43
8	C	1201	7US	C5-C6	2.09	1.42	1.39
8	C	1201	7US	C18-C19	-2.02	1.43	1.52

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	C	1201	7US	C39-C38-N2	21.37	130.87	111.42
8	C	1201	7US	O3-C6-C5	-9.96	107.56	114.36
8	C	1201	7US	C29-C28-C27	7.50	125.28	113.24
8	C	1201	7US	C16-C15-N1	6.73	121.42	114.45
8	C	1201	7US	C5-C6-C7	-6.46	120.25	125.33
8	C	1201	7US	O3-C6-C7	6.43	132.19	121.14
8	C	1201	7US	C29-O5-C12	5.22	126.08	116.42
8	C	1201	7US	C42-C38-N2	-4.75	107.10	111.42
8	C	1201	7US	C18-C17-C16	4.39	123.81	114.82
8	C	1201	7US	O7-C35-C36	4.12	118.66	111.09
8	C	1201	7US	C3-C2-C1	-4.10	117.61	121.44
8	C	1201	7US	C23-C24-C25	4.06	118.54	110.61
8	C	1201	7US	C43-C44-N5	-3.78	104.41	110.97
8	C	1201	7US	O4-C11-C5	-3.34	122.94	130.66
8	C	1201	7US	C34-C26-C27	-2.88	107.22	111.43
8	C	1201	7US	C25-O7-C35	2.74	121.96	117.72
8	C	1201	7US	O11-C15-N1	-2.74	118.26	122.57
8	C	1201	7US	C1-C2-N1	2.56	121.28	115.28
8	C	1201	7US	C30-C16-C17	-2.27	105.60	111.33
8	C	1201	7US	C33-C24-C25	-2.18	107.48	111.40
8	C	1201	7US	C8-C7-C6	2.18	119.83	116.78
8	C	1201	7US	C37-O6-C27	2.15	119.81	114.03
8	C	1201	7US	C10-C4-C3	-2.13	121.36	123.42
8	C	1201	7US	C41-N4-C40	2.08	113.52	108.83
8	C	1201	7US	C39-C40-N4	2.05	113.26	111.23
8	C	1201	7US	C34-C26-C25	-2.03	107.76	111.40

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	C	1201	7US	N1-C15-C16-C17
8	C	1201	7US	O11-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
8	C	1201	7US	C15-C16-C17-C18
8	C	1201	7US	C25-C26-C27-O6
8	C	1201	7US	C27-C28-C29-O5
8	C	1201	7US	C28-C29-O5-C12
8	C	1201	7US	C43-C44-N5-C45
8	C	1201	7US	C36-C35-O7-C25
8	C	1201	7US	C18-C19-C20-C31
8	C	1201	7US	N4-C43-C44-N5
8	C	1201	7US	C16-C17-C18-C19
8	C	1201	7US	C18-C19-C20-C21
8	C	1201	7US	C34-C26-C27-C28
8	C	1201	7US	C34-C26-C27-O6
8	C	1201	7US	C32-C22-C23-C24
8	C	1201	7US	C21-C22-C23-C24
8	C	1201	7US	C44-C43-N4-C41
8	C	1201	7US	C33-C24-C25-C26
8	C	1201	7US	C43-C44-N5-C48
8	C	1201	7US	C23-C24-C25-C26

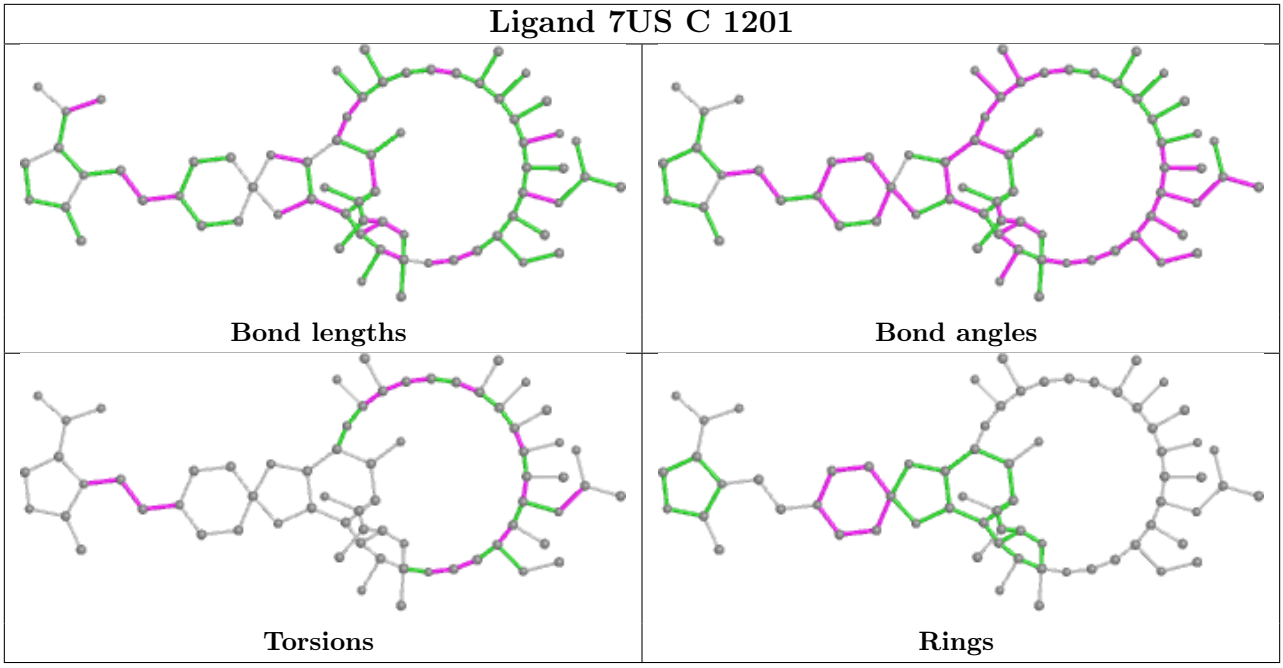
All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	C	1201	7US	C38-C39-C40-C41-C42-N4

1 monomer is involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	1201	7US	10	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.



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, 95^{th} 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	225/347 (64%)	-0.30	3 (1%)	77	67	88, 125, 198, 262	0
1	B	232/347 (66%)	-0.24	5 (2%)	62	50	102, 152, 228, 274	0
2	C	1126/1178 (95%)	-0.15	13 (1%)	79	69	86, 145, 242, 291	0
3	D	1264/1316 (96%)	-0.13	12 (0%)	84	76	83, 163, 270, 312	0
4	E	81/110 (73%)	0.03	1 (1%)	79	69	122, 161, 232, 285	0
5	F	174/177 (98%)	-0.01	11 (6%)	20	13	111, 173, 251, 294	0
6	G	15/23 (65%)	0.07	2 (13%)	3	3	212, 245, 280, 283	0
7	H	24/27 (88%)	0.04	1 (4%)	36	27	224, 263, 294, 310	0
All	All	3141/3525 (89%)	-0.15	48 (1%)	73	63	83, 155, 256, 312	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	157	ALA	6.6
1	B	156	GLY	5.7
5	F	89	VAL	4.5
2	C	192	ASP	4.1
1	B	158	GLU	4.0
3	D	767	HIS	4.0
2	C	214	PHE	4.0
2	C	212	LEU	3.4
5	F	177	ARG	3.4
1	B	155	SER	3.3
1	A	226	ASN	3.1
2	C	195	THR	3.1
5	F	61	THR	3.1
2	C	148	LYS	3.0
3	D	833	PRO	3.0
5	F	4	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
3	D	830	GLU	3.0
5	F	90	VAL	2.9
2	C	96	ILE	2.7
3	D	1175	PHE	2.7
3	D	959	GLN	2.7
5	F	51	ALA	2.6
2	C	191	ILE	2.6
3	D	771	ASN	2.5
2	C	237	LEU	2.4
5	F	48	LEU	2.4
5	F	58	ILE	2.4
3	D	357	LEU	2.4
5	F	88	ASN	2.3
2	C	324	VAL	2.3
3	D	753	ALA	2.3
7	H	15	DG	2.2
5	F	47	THR	2.2
1	B	5	GLN	2.2
2	C	221	THR	2.2
5	F	62	ALA	2.2
3	D	1082	LYS	2.2
3	D	828	LYS	2.2
2	C	964	LEU	2.1
2	C	226	ILE	2.1
1	A	186	ARG	2.1
3	D	1096	GLU	2.1
4	E	56	TYR	2.1
6	G	16	DC	2.1
6	G	15	DT	2.1
3	D	1069	ASP	2.0
1	A	221	LEU	2.0
2	C	218	LYS	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)

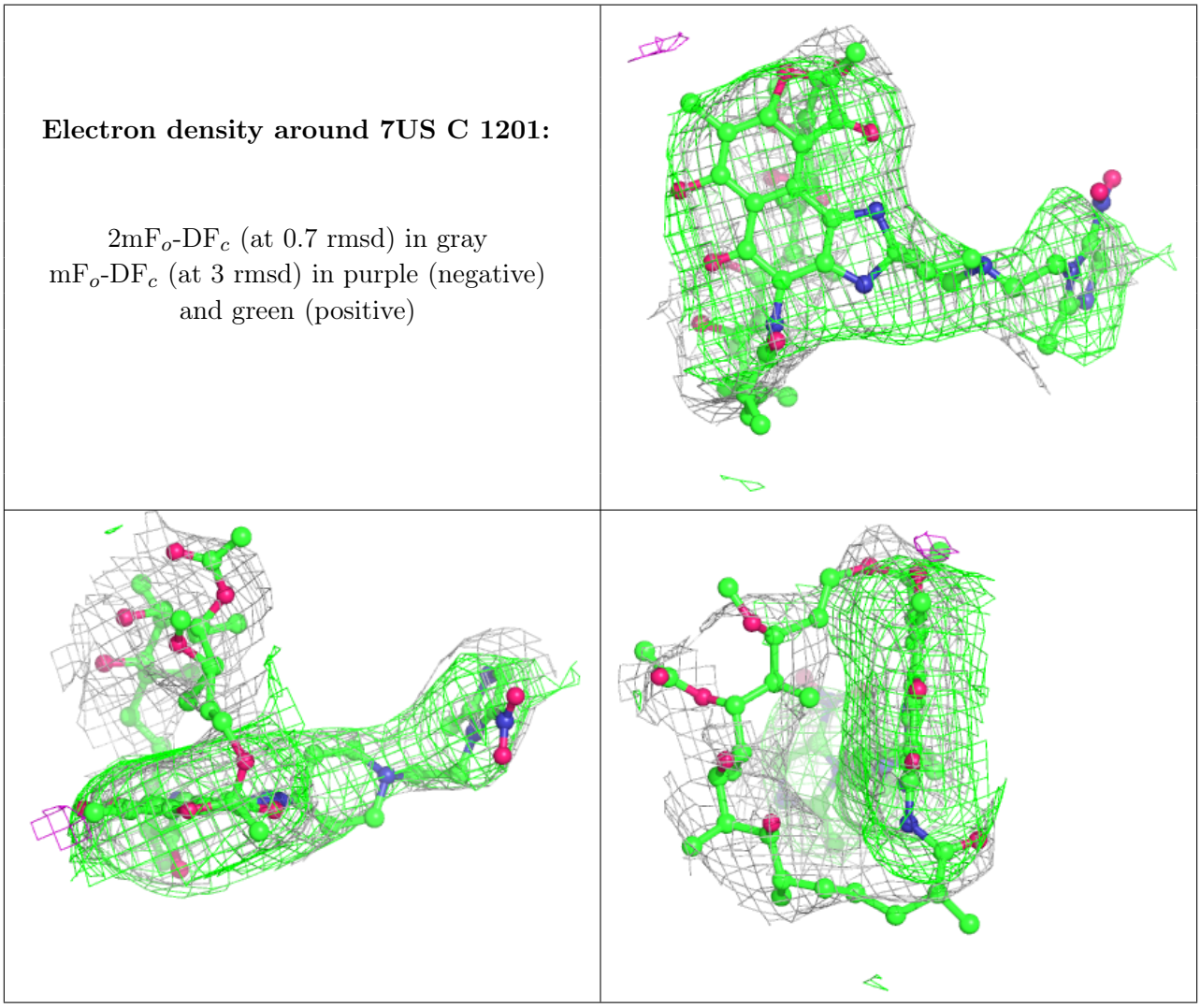
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
8	7US	C	1201	68/68	0.82	0.32	80,161,189,211	38

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 7US C 1201:

$2mF_o$-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.