



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:51 AM UTC

PDB ID : 5UHB / pdb_00005uhb
Title : Crystal structure of Mycobacterium tuberculosis transcription initiation complex in complex with Rifampin
Authors : Lin, W.; Das, K.; Feng, Y.; Ebright, R.H.
Deposited on : 2017-01-11
Resolution : 4.29 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

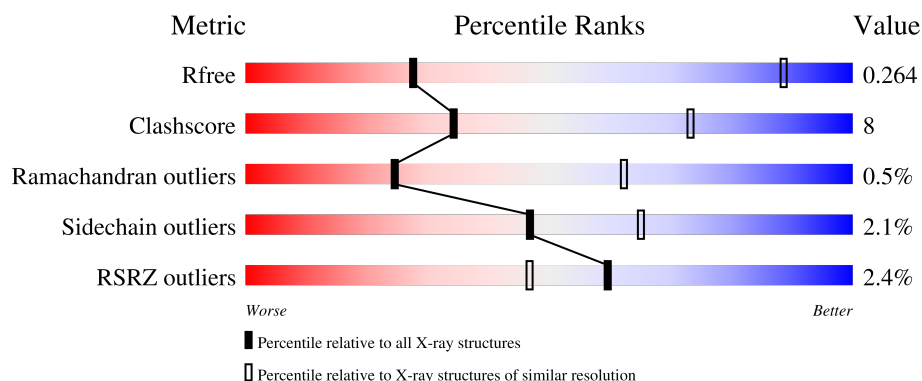
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.29 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1052 (4.70-3.90)
Clashscore	190562	1097 (4.70-3.90)
Ramachandran outliers	187476	1001 (4.70-3.90)
Sidechain outliers	187428	1007 (4.72-3.88)
RSRZ outliers	180081	1049 (4.70-3.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	347	% 51% 13% 35%
1	B	347	4% 53% 12% 35%
2	C	1178	2% 77% 18% • •
3	D	1316	% 78% 17% • •
4	E	110	3% 57% 16% 26%

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Mol	Chain	Length	Quality of chain
5	F	528	3% 46% 13% 39%
6	H	23	57% 43%
7	G	16	25% 44% 25% 6% 25%

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 25979 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	224	Total	C	N	O	S	0	0	0
			1704	1072	295	335	2			
1	B	227	Total	C	N	O	S	0	0	0
			1715	1080	291	342	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
			8714	5454	1528	1693	39			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1265	Total	C	N	O	S	0	0	0
			9887	6188	1793	1866	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
			637	408	106	123			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	320	Total	C	N	O	S	0	0	0
			2543	1583	459	492	9			

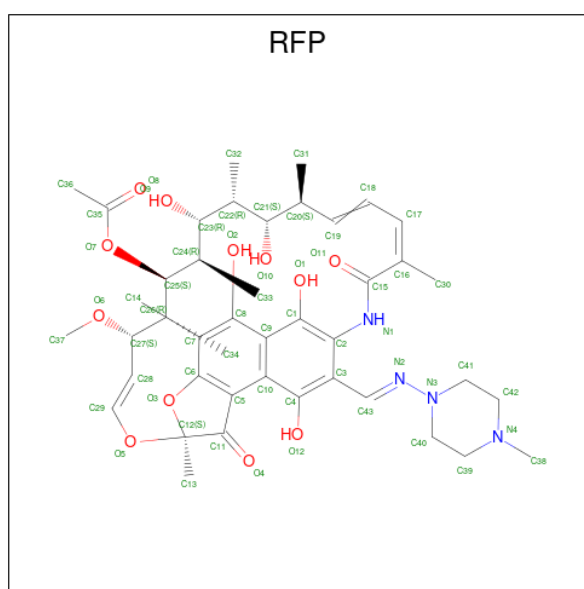
- Molecule 6 is a DNA chain called DNA (5'-D(*TP*AP*TP*AP*AP*TP*GP*GP*GP*AP*GP*CP*TP*GP*TP*CP*AP*CP*GP*GP*AP*TP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	H	23	Total	C	N	O	P	0	0	0
			476	227	91	136	22			

- Molecule 7 is a DNA chain called DNA (5'-D(*CP*AP*TP*CP*CP*GP*TP*GP*AP*GP*TP*CP*GP*AP*GP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	12	Total	C	N	O	P	0	0	0
			241	116	43	71	11			

- Molecule 8 is RIFAMPICIN (CCD ID: RFP) (formula: C₄₃H₅₈N₄O₁₂).



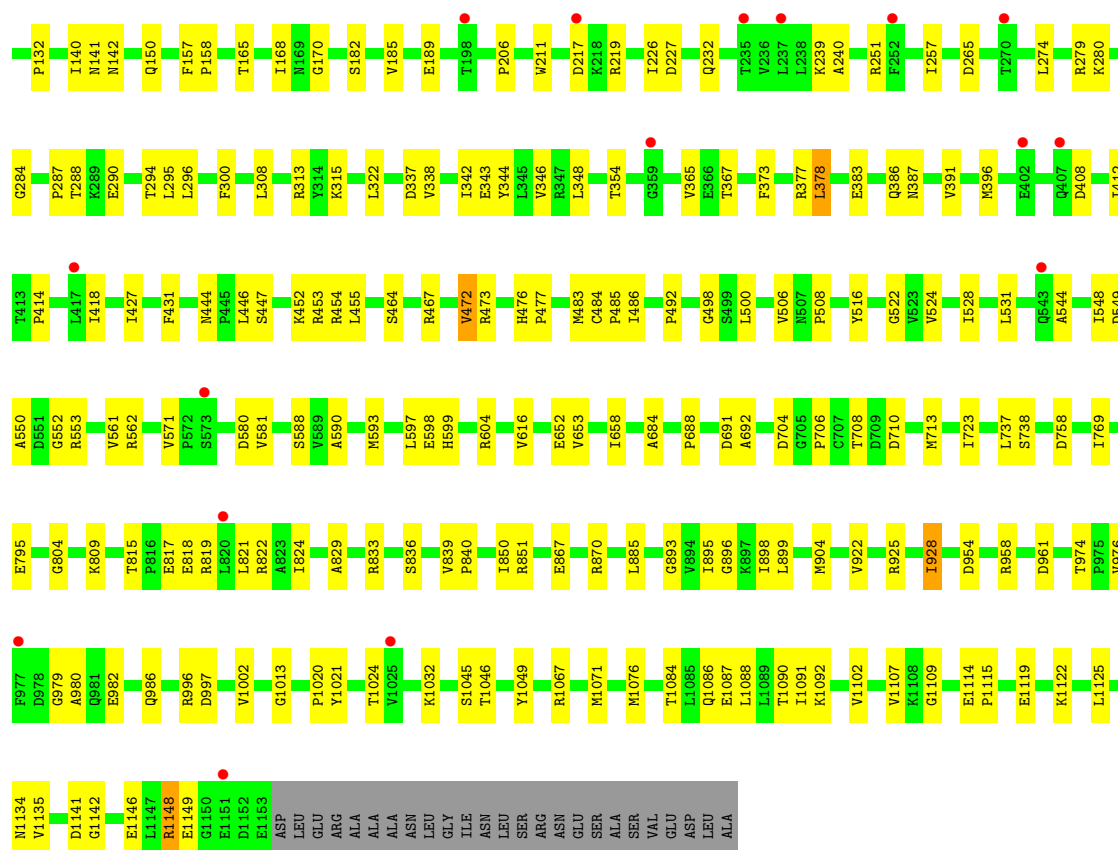
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	C	1	Total	C	N	O	0	0
			59	43	4	12		

- Molecule 9 is ZINC ION (CCD ID: ZN) (formula: Zn).

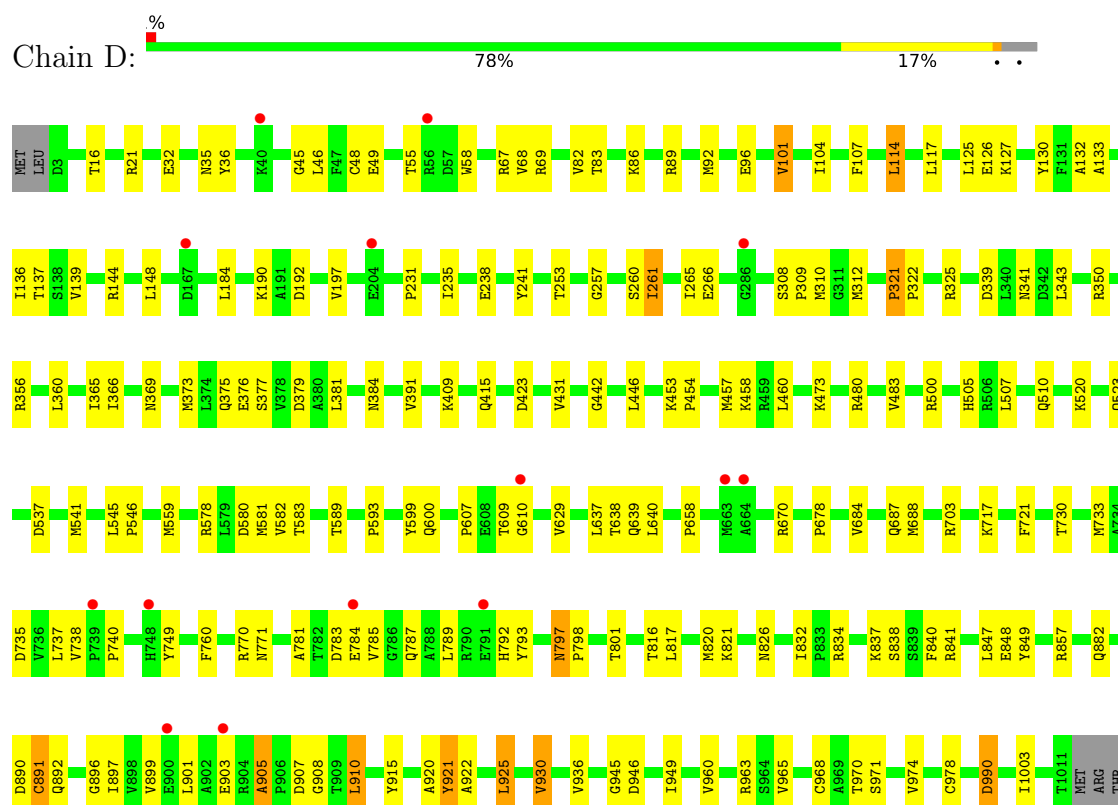
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	D	2	Total	Zn	0	0
			2	2		

- Molecule 10 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

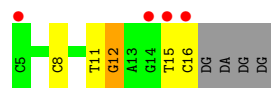
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	D	1	Total	Mg	0	0
			1	1		



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



- Molecule 7: DNA (5'-D(*CP*AP*TP*CP*CP*GP*TP*GP*AP*GP*TP*CP*GP*AP*GP*G)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	154.19Å 164.23Å 200.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.78 – 4.29 49.78 – 4.29	Depositor EDS
% Data completeness (in resolution range)	83.4 (49.78-4.29) 83.4 (49.78-4.29)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.67 (at 4.29Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.208 , 0.267 0.214 , 0.264	Depositor DCC
R_{free} test set	2006 reflections (6.78%)	wwPDB-VP
Wilson B-factor (Å ²)	31.8	Xtriage
Anisotropy	0.545	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 61.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.79	EDS
Total number of atoms	25979	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 2.62% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: RFP, MG, ZN

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	0.32	0/1730	0.80	2/2354 (0.1%)
1	B	0.32	0/1741	0.80	2/2371 (0.1%)
2	C	0.30	0/8873	0.76	2/12031 (0.0%)
3	D	0.32	1/10052 (0.0%)	0.81	16/13591 (0.1%)
4	E	0.32	0/650	0.76	0/886
5	F	0.32	0/2572	0.76	0/3466
6	H	0.20	0/535	0.38	0/826
7	G	0.21	0/269	0.64	1/413 (0.2%)
All	All	0.31	1/26422 (0.0%)	0.78	23/35938 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	910	LEU	C-N	6.40	1.42	1.33

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	910	LEU	CA-C-N	-14.92	102.25	122.99
3	D	910	LEU	C-N-CA	-14.92	102.25	122.99
3	D	910	LEU	O-C-N	13.87	140.44	122.96
7	G	12	DG	P-O3'-C3'	9.00	133.70	120.20
3	D	903	GLU	O-C-N	-8.72	112.91	122.85
3	D	1213	ALA	N-CA-C	-7.44	103.25	111.36
3	D	1126	GLY	CA-C-N	6.17	126.62	119.47
3	D	1126	GLY	C-N-CA	6.17	126.62	119.47
3	D	1213	ALA	N-CA-CB	5.96	118.97	110.16
3	D	321	PRO	CA-C-N	5.91	125.61	119.05
3	D	321	PRO	C-N-CA	5.91	125.61	119.05
3	D	797	ASN	CA-C-N	5.49	125.32	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	797	ASN	C-N-CA	5.49	125.32	119.28
1	A	147	VAL	CA-C-N	5.44	125.38	119.78
1	A	147	VAL	C-N-CA	5.44	125.38	119.78
3	D	905	ALA	CA-C-N	5.39	124.58	118.97
3	D	905	ALA	C-N-CA	5.39	124.58	118.97
3	D	1212	LYS	N-CA-C	5.32	117.99	111.82
1	B	14	LEU	N-CA-C	5.26	118.17	109.85
3	D	1211	THR	N-CA-C	5.26	116.70	110.97
2	C	46	GLU	CA-C-N	-5.19	113.35	119.84
2	C	46	GLU	C-N-CA	-5.19	113.35	119.84
1	B	184	GLU	CB-CA-C	-5.10	110.29	117.23

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	1704	0	1741	31	0
1	B	1715	0	1739	24	0
2	C	8714	0	8636	142	0
3	D	9887	0	9943	166	0
4	E	637	0	635	11	0
5	F	2543	0	2571	56	0
6	H	476	0	261	10	0
7	G	241	0	137	8	0
8	C	59	0	58	6	0
9	D	2	0	0	0	0
10	D	1	0	0	0	0
All	All	25979	0	25721	391	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 (391) 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:562:ARG:NH2	3:D:847:LEU:CD1	2.05	1.19
2:C:562:ARG:NH2	3:D:847:LEU:HD11	1.62	1.11
3:D:891:CYS:SG	3:D:970:THR:OG1	2.09	1.09
2:C:562:ARG:HH22	3:D:847:LEU:HD11	1.23	0.93
7:G:11:DT:H2''	7:G:12:DG:H8	1.32	0.92
3:D:968:CYS:SG	3:D:978:CYS:HB3	2.11	0.90
2:C:562:ARG:HH21	3:D:847:LEU:CD1	1.83	0.87
3:D:970:THR:HG22	3:D:971:SER:H	1.38	0.86
7:G:11:DT:H2''	7:G:12:DG:C8	2.11	0.84
2:C:113:ASP:HB2	2:C:132:PRO:HG2	1.69	0.75
2:C:562:ARG:HH21	3:D:847:LEU:HD13	1.50	0.75
2:C:284:GLY:H	5:F:219:ALA:HB1	1.53	0.74
3:D:970:THR:HG22	3:D:971:SER:N	2.02	0.72
2:C:454:ARG:HH22	8:C:1201:RFP:H19C	1.55	0.72
1:A:11:GLU:HB2	1:A:22:VAL:HB	1.74	0.70
2:C:562:ARG:HH22	3:D:847:LEU:CD1	1.87	0.70
5:F:522:VAL:HG23	5:F:523:LEU:HD12	1.74	0.69
3:D:46:LEU:O	3:D:325:ARG:NH2	2.20	0.69
3:D:1090:LYS:HB3	3:D:1092:GLU:HG2	1.75	0.69
1:B:75:GLU:O	1:B:79:ASN:ND2	2.26	0.68
5:F:470:ARG:HB3	5:F:506:ILE:HD13	1.76	0.68
2:C:101:GLY:O	2:C:142:ASN:ND2	2.27	0.68
2:C:1024:THR:H	3:D:730:THR:HG21	1.59	0.67
1:A:107:ALA:HB2	1:A:123:MET:HE2	1.77	0.67
2:C:1119:GLU:OE2	3:D:89:ARG:NH2	2.28	0.66
1:B:170:PRO:HA	1:B:199:LYS:HD2	1.79	0.65
5:F:401:LYS:HA	5:F:405:ILE:HA	1.79	0.65
7:G:11:DT:C2'	7:G:12:DG:C8	2.79	0.65
3:D:356:ARG:HH21	3:D:360:LEU:HD11	1.62	0.64
3:D:1030:ARG:HH21	3:D:1137:GLU:HG2	1.63	0.64
2:C:1122:LYS:HE2	2:C:1148:ARG:HG2	1.80	0.64
3:D:637:LEU:HD13	3:D:640:LEU:HD12	1.80	0.63
2:C:561:VAL:HG21	2:C:571:VAL:HB	1.80	0.63
3:D:832:ILE:HG22	3:D:834:ARG:H	1.63	0.63
5:F:477:LEU:HD13	5:F:492:ILE:HG23	1.79	0.63
2:C:104:SER:HB3	2:C:140:ILE:HB	1.80	0.63
2:C:168:ILE:HG12	2:C:431:PHE:HB3	1.80	0.62
6:H:15:DT:H2''	6:H:16:DC:H5'	1.81	0.62
3:D:473:LYS:HD2	5:F:448:VAL:HG21	1.82	0.62
3:D:107:PHE:HZ	3:D:126:GLU:HG2	1.64	0.62
1:A:40:ARG:NH1	2:C:1013:GLY:O	2.31	0.62
3:D:137:THR:OG1	3:D:253:THR:O	2.18	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:48:LEU:HD12	2:C:528:ILE:HD13	1.81	0.62
3:D:238:GLU:OE1	5:F:237:LYS:NZ	2.32	0.62
2:C:815:THR:HG22	2:C:817:GLU:H	1.65	0.61
2:C:396:MET:HE1	2:C:418:ILE:HG23	1.83	0.61
2:C:562:ARG:NH2	3:D:847:LEU:HD13	2.04	0.61
3:D:589:THR:HG21	3:D:688:MET:HG2	1.83	0.61
3:D:891:CYS:O	3:D:892:GLN:HB2	1.99	0.61
1:A:87:SER:O	1:A:142:ARG:NH1	2.31	0.60
1:A:152:ASN:HB3	1:A:163:PRO:HB3	1.82	0.60
5:F:499:THR:OG1	5:F:500:ARG:N	2.31	0.60
2:C:899:LEU:HB2	2:C:904:MET:HE1	1.82	0.60
3:D:737:LEU:N	3:D:793:TYR:OH	2.32	0.60
3:D:442:GLY:HA3	3:D:523:GLN:HB2	1.83	0.60
7:G:11:DT:C1'	7:G:12:DG:C8	2.85	0.60
3:D:365:ILE:HG21	5:F:297:GLU:HG2	1.84	0.59
3:D:1265:ASN:OD1	3:D:1268:ARG:NH2	2.35	0.59
2:C:182:SER:HB2	2:C:377:ARG:HB2	1.85	0.59
1:A:214:THR:HA	1:B:230:GLU:HG2	1.83	0.59
2:C:189:GLU:HB2	2:C:367:THR:HG21	1.84	0.59
3:D:454:PRO:HA	3:D:457:MET:HE2	1.84	0.58
3:D:930:VAL:HG22	3:D:936:VAL:HG12	1.85	0.58
2:C:821:LEU:HD22	5:F:456:LEU:HD11	1.85	0.58
3:D:1092:GLU:HG3	3:D:1094:GLY:H	1.67	0.58
2:C:239:LYS:NZ	2:C:265:ASP:OD2	2.36	0.58
2:C:1148:ARG:NH1	3:D:86:LYS:O	2.37	0.58
8:C:1201:RFP:HN1	8:C:1201:RFP:C18	2.17	0.58
8:C:1201:RFP:H28C	8:C:1201:RFP:C5	2.32	0.58
2:C:737:LEU:HB2	2:C:898:ILE:HG12	1.85	0.58
3:D:1247:GLY:O	3:D:1251:ASN:ND2	2.36	0.57
2:C:43:LYS:NZ	2:C:544:ALA:O	2.36	0.57
2:C:604:ARG:HG3	2:C:925:ARG:HB3	1.86	0.57
3:D:1090:LYS:HG2	3:D:1091:HIS:H	1.69	0.57
3:D:638:THR:HG23	3:D:639:GLN:HG2	1.87	0.57
2:C:279:ARG:HD3	5:F:215:ALA:HB1	1.85	0.57
3:D:578:ARG:H	3:D:581:MET:HE3	1.70	0.56
3:D:1089:PHE:HA	3:D:1095:SER:HA	1.87	0.56
3:D:257:GLY:O	3:D:260:SER:OG	2.23	0.56
3:D:114:LEU:HB3	3:D:125:LEU:HD21	1.88	0.56
2:C:485:PRO:O	3:D:857:ARG:NH2	2.38	0.56
2:C:758:ASP:N	2:C:758:ASP:OD1	2.36	0.56
2:C:1087:GLU:HG2	2:C:1092:LYS:HG3	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:658:ILE:HD11	2:C:688:PRO:HB3	1.89	0.55
2:C:684:ALA:HA	2:C:706:PRO:HG3	1.88	0.55
2:C:974:THR:HG23	2:C:980:ALA:H	1.71	0.55
1:B:100:GLN:HG3	1:B:133:LYS:HA	1.88	0.55
2:C:41:PHE:HB2	2:C:979:GLY:HA2	1.88	0.55
3:D:373:MET:SD	5:F:318:LEU:HB3	2.46	0.55
3:D:921:TYR:HE1	3:D:946:ASP:HA	1.72	0.55
2:C:653:VAL:HG12	2:C:692:ALA:HB2	1.87	0.55
3:D:897:ILE:HD13	3:D:1128:ARG:HH11	1.71	0.55
2:C:1107:VAL:HG21	5:F:451:VAL:HG11	1.89	0.55
3:D:915:TYR:HA	3:D:1143:ARG:HH12	1.72	0.55
5:F:315:MET:HE2	5:F:359:MET:HE3	1.87	0.55
3:D:507:LEU:HB3	3:D:510:GLN:HE21	1.71	0.55
3:D:965:VAL:HG13	3:D:974:VAL:HG11	1.88	0.55
3:D:970:THR:CG2	3:D:971:SER:H	2.15	0.54
5:F:345:THR:HB	6:H:4:DA:H8	1.73	0.54
3:D:890:ASP:OD1	3:D:963:ARG:NH2	2.40	0.54
1:A:213:LYS:HD3	1:B:227:VAL:HG23	1.90	0.54
5:F:506:ILE:HA	5:F:509:LYS:HD2	1.89	0.54
2:C:348:LEU:HD13	2:C:365:VAL:HG12	1.88	0.54
2:C:1045:SER:OG	2:C:1046:THR:N	2.41	0.54
5:F:505:GLN:HG3	5:F:509:LYS:HE3	1.89	0.53
1:A:18:ARG:NH1	2:C:997:ASP:OD1	2.41	0.53
1:B:27:GLU:HG3	1:B:28:PRO:HD2	1.90	0.53
2:C:107:PHE:HE1	2:C:418:ILE:HD11	1.73	0.53
2:C:484:CYS:HB2	2:C:588:SER:HB3	1.90	0.53
5:F:256:GLY:HA3	5:F:288:GLY:HA3	1.89	0.53
3:D:266:GLU:HA	3:D:310:MET:HE1	1.89	0.53
3:D:49:GLU:OE2	3:D:55:THR:N	2.40	0.52
1:A:223:ARG:HD3	1:B:213:LYS:HB2	1.91	0.52
3:D:1055:LEU:HB2	3:D:1101:ASP:HB3	1.92	0.52
3:D:1051:GLY:HA2	3:D:1069:ASP:HB2	1.91	0.52
3:D:1165:VAL:HG12	3:D:1205:PRO:HA	1.91	0.52
2:C:483:MET:HE3	2:C:498:GLY:HA3	1.90	0.52
5:F:302:LEU:O	5:F:305:SER:OG	2.20	0.52
2:C:986:GLN:HB2	3:D:733:MET:HE1	1.91	0.52
2:C:1091:ILE:HB	2:C:1102:VAL:HG21	1.91	0.52
3:D:1273:GLN:O	4:E:105:GLU:N	2.36	0.52
4:E:70:GLN:O	4:E:74:GLY:N	2.32	0.51
2:C:378:LEU:HD21	2:C:455:LEU:HD22	1.92	0.51
5:F:515:ARG:O	5:F:519:ARG:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:893:GLY:HA2	3:D:537:ASP:HA	1.92	0.51
3:D:738:VAL:HG13	3:D:841:ARG:HD3	1.92	0.51
2:C:738:SER:HA	2:C:904:MET:HE3	1.92	0.51
2:C:704:ASP:HB2	2:C:708:THR:HB	1.93	0.51
2:C:1020:PRO:HB2	2:C:1021:TYR:CD2	2.46	0.51
2:C:287:PRO:HD2	5:F:216:ARG:HG3	1.93	0.51
2:C:815:THR:O	2:C:819:ARG:N	2.42	0.51
5:F:231:TYR:CE2	5:F:235:ILE:HD11	2.46	0.51
2:C:982:GLU:HG3	3:D:841:ARG:HH12	1.76	0.51
1:B:95:MET:HE3	1:B:140:VAL:HG21	1.92	0.50
2:C:232:GLN:OE1	2:C:280:LYS:HG3	2.12	0.50
1:B:97:LEU:HD22	1:B:110:ILE:HG12	1.94	0.50
2:C:524:VAL:HG21	2:C:548:ILE:HD13	1.92	0.50
2:C:1148:ARG:NH1	3:D:86:LYS:HG3	2.26	0.50
5:F:240:LEU:HD21	5:F:301:ARG:HD2	1.92	0.50
5:F:492:ILE:HG22	5:F:503:ILE:HG21	1.93	0.50
3:D:970:THR:CG2	3:D:971:SER:N	2.73	0.50
3:D:1038:ARG:NH1	6:H:18:DC:O3'	2.44	0.50
3:D:339:ASP:OD1	5:F:422:SER:OG	2.27	0.50
4:E:33:LEU:HD23	4:E:33:LEU:H	1.77	0.50
3:D:350:ARG:NH1	3:D:373:MET:HB3	2.27	0.50
3:D:990:ASP:OD1	3:D:990:ASP:N	2.45	0.50
2:C:206:PRO:HA	2:C:308:LEU:HD23	1.93	0.50
2:C:516:TYR:HD2	2:C:531:LEU:HD13	1.76	0.49
3:D:376:GLU:OE2	5:F:227:SER:HB3	2.12	0.49
3:D:770:ARG:NH1	3:D:771:ASN:OD1	2.45	0.49
3:D:1245:LEU:HD13	3:D:1254:ILE:HD13	1.93	0.49
3:D:816:THR:HG23	3:D:821:LYS:HA	1.92	0.49
2:C:896:GLY:HA2	3:D:431:VAL:HG13	1.94	0.49
3:D:1274:PRO:HB3	4:E:82:LEU:HD11	1.93	0.49
2:C:616:VAL:N	2:C:1032:LYS:O	2.44	0.49
3:D:350:ARG:HH11	3:D:373:MET:HB3	1.78	0.49
5:F:492:ILE:HA	5:F:495:VAL:HG12	1.95	0.49
3:D:735:ASP:O	3:D:797:ASN:ND2	2.40	0.49
6:H:18:DC:H2''	6:H:19:DG:C8	2.47	0.49
1:A:153:ARG:HD3	2:C:795:GLU:CB	2.43	0.49
2:C:822:ARG:NE	2:C:829:ALA:HB2	2.28	0.49
2:C:290:GLU:O	2:C:294:THR:OG1	2.24	0.49
3:D:749:TYR:OH	3:D:784:GLU:OE1	2.24	0.49
3:D:545:LEU:HD12	3:D:546:PRO:HD2	1.95	0.49
3:D:882:GLN:HE22	3:D:1249:LYS:HG3	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:600:GLN:HB2	3:D:609:THR:HB	1.94	0.48
5:F:266:LEU:HA	5:F:269:ARG:HG2	1.95	0.48
2:C:1109:GLY:HA3	3:D:458:LYS:HE3	1.95	0.48
3:D:67:ARG:HD2	3:D:69:ARG:NE	2.29	0.48
3:D:104:ILE:HD12	3:D:379:ASP:HB3	1.95	0.48
1:A:37:SER:O	1:A:41:THR:OG1	2.30	0.48
1:B:72:ASP:OD1	1:B:73:VAL:N	2.45	0.48
2:C:885:LEU:HD12	2:C:895:ILE:HD11	1.95	0.48
3:D:500:ARG:HB2	3:D:541:MET:HE2	1.96	0.48
3:D:589:THR:HG22	3:D:670:ARG:HG2	1.96	0.48
2:C:549:ASP:HB3	2:C:553:ARG:H	1.78	0.48
1:A:136:VAL:HG12	1:A:137:GLU:H	1.78	0.48
5:F:242:ASN:OD1	5:F:243:ALA:N	2.47	0.48
7:G:11:DT:H1'	7:G:12:DG:C8	2.49	0.47
2:C:344:TYR:OH	2:C:365:VAL:HA	2.13	0.47
3:D:740:PRO:HD3	3:D:792:HIS:ND1	2.29	0.47
3:D:820:MET:HE3	3:D:837:LYS:HA	1.97	0.47
3:D:1170:SER:O	3:D:1173:THR:OG1	2.31	0.47
5:F:470:ARG:HH11	5:F:506:ILE:HD11	1.80	0.47
5:F:499:THR:HG23	5:F:500:ARG:HD2	1.96	0.47
3:D:505:HIS:CD2	3:D:507:LEU:HB2	2.48	0.47
2:C:211:TRP:HB2	2:C:227:ASP:HA	1.97	0.47
3:D:907:ASP:OD1	3:D:907:ASP:N	2.47	0.47
1:A:129:ASN:ND2	2:C:652:GLU:HG3	2.29	0.47
2:C:115:VAL:HG11	2:C:129:TYR:CE1	2.50	0.47
3:D:144:ARG:O	3:D:148:LEU:HB2	2.15	0.47
5:F:345:THR:HA	6:H:5:DA:N7	2.30	0.47
5:F:446:VAL:HB	5:F:449:ASP:HB2	1.97	0.47
2:C:1049:TYR:OH	3:D:423:ASP:OD2	2.30	0.47
3:D:896:GLY:O	3:D:1128:ARG:NH1	2.35	0.47
3:D:922:ALA:HB3	3:D:1150:HIS:CE1	2.50	0.47
3:D:130:TYR:OH	3:D:379:ASP:OD2	2.32	0.47
3:D:325:ARG:NH1	3:D:341:ASN:OD1	2.46	0.47
3:D:409:LYS:NZ	7:G:15:DT:OP2	2.40	0.47
1:B:84:VAL:HG12	1:B:199:LYS:HD3	1.98	0.46
1:B:77:ILE:HG22	1:B:81:LYS:HE3	1.97	0.46
3:D:580:ASP:HB2	3:D:721:PHE:CE1	2.50	0.46
3:D:580:ASP:HB2	3:D:721:PHE:HE1	1.80	0.46
4:E:60:ARG:NE	4:E:98:GLU:OE2	2.49	0.46
1:A:18:ARG:NH2	1:A:195:ASP:OD1	2.41	0.46
1:A:62:GLU:HG3	1:A:77:ILE:HD12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:261:ILE:O	3:D:265:ILE:HG13	2.15	0.46
3:D:369:ASN:O	3:D:373:MET:HG3	2.16	0.46
5:F:489:LEU:H	5:F:489:LEU:HD23	1.80	0.46
1:A:97:LEU:HD21	1:A:105:VAL:HG21	1.98	0.46
2:C:522:GLY:O	2:C:553:ARG:HA	2.16	0.46
3:D:1087:ARG:HG2	3:D:1098:VAL:HG22	1.98	0.46
3:D:1139:GLN:O	3:D:1143:ARG:HG2	2.15	0.46
3:D:35:ASN:OD1	3:D:36:TYR:N	2.49	0.46
3:D:453:LYS:O	3:D:457:MET:HG3	2.16	0.46
1:B:95:MET:HB3	1:B:113:PRO:HD3	1.98	0.46
2:C:1141:ASP:OD1	2:C:1142:GLY:N	2.48	0.46
1:B:171:VAL:HG22	1:B:198:THR:HG22	1.98	0.45
2:C:313:ARG:HH22	2:C:337:ASP:CG	2.24	0.45
2:C:599:HIS:HB3	2:C:928:ILE:HD12	1.99	0.45
8:C:1201:RFP:O4	8:C:1201:RFP:O12	2.33	0.45
2:C:126:ASP:HA	2:C:170:GLY:HA3	1.98	0.45
6:H:19:DG:H2''	6:H:20:DG:C8	2.51	0.45
3:D:783:ASP:O	3:D:787:GLN:HG2	2.17	0.45
2:C:1076:MET:HE1	3:D:559:MET:HE1	1.98	0.45
5:F:342:LYS:HE2	5:F:342:LYS:HB3	1.79	0.45
2:C:544:ALA:HB2	2:C:580:ASP:HB2	1.99	0.45
1:A:120:ASN:OD1	1:A:120:ASN:N	2.48	0.45
1:A:175:THR:OG1	1:A:176:TYR:N	2.50	0.45
8:C:1201:RFP:H342	8:C:1201:RFP:H24C	1.67	0.45
1:B:157:ALA:C	1:B:159:ILE:H	2.25	0.45
2:C:817:GLU:N	2:C:817:GLU:OE1	2.50	0.45
3:D:343:LEU:HD13	3:D:381:LEU:HA	1.98	0.45
3:D:365:ILE:HG23	3:D:366:ILE:HG13	1.98	0.45
3:D:717:LYS:HB3	3:D:717:LYS:HE2	1.71	0.45
3:D:905:ALA:HB3	3:D:908:GLY:O	2.16	0.45
6:H:19:DG:O6	7:G:8:DC:N4	2.49	0.44
2:C:41:PHE:O	2:C:979:GLY:HA2	2.17	0.44
2:C:444:ASN:H	2:C:447:SER:HB3	1.83	0.44
3:D:58:TRP:CD2	3:D:68:VAL:HG13	2.53	0.44
7:G:15:DT:H2'	7:G:16:DC:C6	2.53	0.44
2:C:315:LYS:HD2	2:C:315:LYS:HA	1.85	0.44
2:C:1067:ARG:NH2	3:D:415:GLN:O	2.50	0.44
3:D:581:MET:HG3	3:D:721:PHE:CE1	2.52	0.44
3:D:733:MET:HE2	3:D:733:MET:HB3	1.88	0.44
1:B:39:ARG:HH21	1:B:173:LYS:NZ	2.14	0.44
2:C:928:ILE:H	2:C:928:ILE:HG13	1.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:954:ASP:O	2:C:958:ARG:NH1	2.51	0.44
1:A:130:ASP:O	1:A:131:LYS:HG2	2.18	0.44
2:C:288:THR:HG22	2:C:290:GLU:H	1.82	0.44
2:C:590:ALA:HA	2:C:593:MET:HE3	1.99	0.44
3:D:798:PRO:HA	3:D:801:THR:HB	1.98	0.44
5:F:364:ARG:HG3	5:F:368:ILE:HG12	1.99	0.44
2:C:824:ILE:HG12	5:F:514:LEU:HD13	2.00	0.44
3:D:1219:SER:OG	3:D:1243:ASP:OD2	2.32	0.44
3:D:117:LEU:HD22	3:D:312:MET:HE1	1.99	0.44
5:F:347:ALA:O	5:F:351:ILE:HG13	2.18	0.44
1:A:181:THR:O	1:A:188:ASP:HA	2.17	0.44
1:A:208:LEU:O	1:B:222:ALA:HB1	2.18	0.44
1:A:100:GLN:HG2	1:A:101:GLY:H	1.83	0.44
2:C:476:HIS:CG	2:C:477:PRO:HD2	2.53	0.44
2:C:851:ARG:HB3	2:C:870:ARG:HB2	2.00	0.44
3:D:190:LYS:HE3	3:D:192:ASP:HB3	1.99	0.44
3:D:446:LEU:HD12	3:D:520:LYS:HG2	1.99	0.44
3:D:945:GLY:O	3:D:949:ILE:HG12	2.18	0.44
3:D:1220:TRP:CD1	3:D:1243:ASP:HB2	2.52	0.44
2:C:928:ILE:HG12	3:D:817:LEU:CD1	2.48	0.43
3:D:127:LYS:O	3:D:133:ALA:N	2.47	0.43
3:D:235:ILE:HD12	3:D:241:TYR:HD1	1.83	0.43
3:D:21:ARG:NH2	3:D:96:GLU:OE2	2.50	0.43
6:H:11:DG:H5"	6:H:12:DC:C4	2.53	0.43
2:C:446:LEU:HD13	2:C:593:MET:HE1	2.00	0.43
2:C:1125:LEU:HD22	2:C:1135:VAL:HG11	2.01	0.43
3:D:899:VAL:HG11	3:D:920:ALA:HB2	2.01	0.43
3:D:925:LEU:HD11	3:D:960:VAL:HG11	2.01	0.43
1:B:45:SER:OG	1:B:214:THR:HG21	2.18	0.43
2:C:47:PRO:HB2	2:C:581:VAL:HG13	2.01	0.43
5:F:474:VAL:HA	5:F:477:LEU:HB2	1.99	0.43
3:D:45:GLY:H	3:D:48:CYS:HB2	1.84	0.43
5:F:262:LEU:O	5:F:266:LEU:HG	2.18	0.43
2:C:815:THR:HG21	5:F:453:PHE:CE1	2.54	0.43
8:C:1201:RFP:H28C	8:C:1201:RFP:H341	1.58	0.43
3:D:104:ILE:HB	3:D:379:ASP:OD1	2.19	0.43
3:D:127:LYS:HA	3:D:132:ALA:HB3	2.00	0.43
3:D:599:TYR:HA	3:D:610:GLY:HA3	2.00	0.43
3:D:781:ALA:O	3:D:785:VAL:HG23	2.18	0.43
3:D:834:ARG:NH2	3:D:847:LEU:HG	2.34	0.43
2:C:251:ARG:NH2	2:C:343:GLU:OE1	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1247:GLY:H	3:D:1251:ASN:ND2	2.16	0.43
5:F:231:TYR:O	5:F:235:ILE:HG13	2.19	0.43
4:E:32:PRO:HB2	4:E:37:ASN:HB2	2.00	0.43
4:E:40:ILE:O	4:E:44:LEU:HG	2.19	0.43
4:E:56:TYR:HE2	4:E:99:ILE:HG12	1.84	0.43
2:C:150:GLN:HG2	2:C:414:PRO:HG2	2.01	0.43
2:C:211:TRP:HH2	6:H:14:DG:OP1	2.02	0.43
2:C:598:GLU:HA	3:D:849:TYR:CE1	2.53	0.43
3:D:1039:VAL:HA	3:D:1040:PRO:HD3	1.86	0.43
2:C:396:MET:HE3	2:C:396:MET:HB2	1.94	0.42
2:C:809:LYS:HD2	2:C:833:ARG:HD3	2.00	0.42
1:A:56:ILE:HG12	1:A:136:VAL:HG13	2.01	0.42
2:C:295:LEU:HD12	2:C:296:LEU:HD12	2.02	0.42
3:D:69:ARG:HE	5:F:485:GLN:HB2	1.84	0.42
3:D:1221:LEU:HD12	3:D:1221:LEU:HA	1.91	0.42
1:A:14:LEU:HD23	1:A:19:SER:HB2	2.00	0.42
1:A:100:GLN:HG3	1:A:133:LYS:HB2	2.02	0.42
5:F:371:HIS:O	5:F:375:VAL:HG23	2.20	0.42
1:A:197:GLU:OE1	2:C:996:ARG:NH1	2.49	0.42
2:C:549:ASP:OD2	2:C:550:ALA:N	2.52	0.42
3:D:760:PHE:CD2	3:D:770:ARG:HD2	2.54	0.42
3:D:832:ILE:HG22	3:D:834:ARG:N	2.33	0.42
1:A:10:SER:HA	1:A:23:ILE:HG12	2.02	0.42
2:C:599:HIS:ND1	3:D:840:PHE:O	2.46	0.42
2:C:769:ILE:HD12	2:C:867:GLU:HB3	2.02	0.42
3:D:101:VAL:HG23	3:D:375:GLN:CD	2.44	0.42
3:D:1220:TRP:NE1	3:D:1243:ASP:HB2	2.35	0.42
5:F:269:ARG:NH1	5:F:271:GLU:OE1	2.53	0.42
2:C:408:ASP:O	2:C:412:ILE:HG13	2.19	0.42
2:C:604:ARG:NH1	2:C:925:ARG:HD2	2.35	0.42
2:C:47:PRO:HG2	2:C:581:VAL:O	2.20	0.42
3:D:32:GLU:HG3	5:F:367:ARG:HB2	2.02	0.42
3:D:1218:ASP:OD1	3:D:1218:ASP:N	2.44	0.42
5:F:330:ARG:HH21	5:F:350:TRP:HZ3	1.67	0.42
1:A:11:GLU:N	1:A:22:VAL:O	2.42	0.42
1:B:182:ARG:HA	1:B:187:THR:HA	2.01	0.42
2:C:257:ILE:HD11	2:C:346:VAL:HG23	2.01	0.42
2:C:46:GLU:N	2:C:47:PRO:HD3	2.35	0.41
3:D:308:SER:HA	3:D:309:PRO:HD3	1.82	0.41
2:C:104:SER:N	2:C:140:ILE:O	2.52	0.41
2:C:804:GLY:HA2	2:C:836:SER:OG	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:818:GLU:OE2	2:C:822:ARG:NH1	2.51	0.41
2:C:839:VAL:HA	2:C:840:PRO:HD3	1.95	0.41
3:D:136:ILE:HD11	3:D:235:ILE:HD11	2.02	0.41
1:B:42:LEU:HD22	1:B:171:VAL:HG21	2.01	0.41
2:C:338:VAL:O	2:C:342:ILE:HG13	2.20	0.41
2:C:464:SER:HB3	2:C:467:ARG:HG3	2.02	0.41
2:C:1114:GLU:HA	2:C:1115:PRO:HD3	1.93	0.41
3:D:139:VAL:HG12	3:D:231:PRO:HD3	2.02	0.41
3:D:760:PHE:CG	3:D:770:ARG:HD2	2.55	0.41
1:B:208:LEU:O	1:B:212:GLY:N	2.53	0.41
2:C:446:LEU:HB2	2:C:713:MET:HE2	2.02	0.41
5:F:503:ILE:HD12	5:F:503:ILE:HA	1.80	0.41
2:C:157:PHE:HA	2:C:158:PRO:HD3	1.96	0.41
2:C:472:VAL:HG22	6:H:14:DG:N2	2.35	0.41
3:D:589:THR:HB	3:D:687:GLN:HA	2.02	0.41
2:C:165:THR:HG22	2:C:452:LYS:HE2	2.02	0.41
2:C:377:ARG:HH22	2:C:383:GLU:CD	2.29	0.41
3:D:321:PRO:HA	3:D:322:PRO:HD3	1.78	0.41
5:F:378:LYS:HD3	5:F:381:ARG:HH11	1.85	0.41
2:C:1086:GLN:O	2:C:1090:THR:OG1	2.34	0.41
3:D:384:ASN:HD21	3:D:391:VAL:H	1.68	0.41
3:D:789:LEU:HD23	3:D:789:LEU:HA	1.93	0.41
4:E:84:GLU:CD	4:E:84:GLU:H	2.29	0.41
5:F:273:LEU:HD13	5:F:277:GLN:HB3	2.03	0.41
2:C:226:ILE:HG23	2:C:300:PHE:HZ	1.86	0.41
2:C:383:GLU:HA	2:C:386:GLN:HB3	2.02	0.41
2:C:486:ILE:HD11	3:D:849:TYR:HE2	1.86	0.41
2:C:597:LEU:HB3	2:C:976:VAL:HG13	2.02	0.41
2:C:723:ILE:O	3:D:730:THR:HG23	2.20	0.41
2:C:1084:THR:O	2:C:1088:LEU:HG	2.21	0.41
3:D:125:LEU:HD12	3:D:125:LEU:HA	1.84	0.41
3:D:184:LEU:HD12	3:D:197:VAL:HG21	2.02	0.41
3:D:990:ASP:HB3	4:E:49:SER:HB2	2.03	0.41
3:D:1003:ILE:HA	3:D:1149:ILE:HD13	2.03	0.41
5:F:392:ARG:NH1	5:F:398:GLU:OE2	2.53	0.41
5:F:474:VAL:HA	5:F:477:LEU:HD12	2.03	0.41
1:B:147:VAL:HA	1:B:148:PRO:HD3	1.91	0.41
2:C:473:ARG:NH2	2:C:492:PRO:O	2.54	0.41
2:C:32:VAL:H	2:C:33:PRO:HD3	1.85	0.40
3:D:826:ASN:HD22	3:D:832:ILE:HD11	1.86	0.40
5:F:502:ARG:O	5:F:506:ILE:HG13	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:387:ASN:O	2:C:391:VAL:HG23	2.21	0.40
3:D:480:ARG:O	3:D:483:VAL:HG22	2.21	0.40
3:D:1054:ARG:HB3	3:D:1065:THR:HB	2.02	0.40
4:E:37:ASN:HA	4:E:38:PRO:C	2.46	0.40
1:A:105:VAL:HG12	1:A:126:ALA:O	2.22	0.40
1:B:212:GLY:O	1:B:216:VAL:HG23	2.21	0.40
2:C:102:SER:O	2:C:141:ASN:ND2	2.54	0.40
2:C:217:ASP:HB3	2:C:219:ARG:H	1.86	0.40
3:D:365:ILE:HD11	5:F:234:GLN:HB3	2.04	0.40
3:D:460:LEU:HD23	3:D:460:LEU:HA	1.94	0.40
5:F:403:MET:HE3	5:F:403:MET:HB2	1.93	0.40
5:F:496:TYR:CD1	5:F:503:ILE:HD13	2.56	0.40
1:A:173:LYS:HD2	2:C:996:ARG:HH11	1.85	0.40
2:C:240:ALA:HB1	2:C:274:LEU:HD23	2.04	0.40
2:C:453:ARG:NH2	2:C:500:LEU:HD23	2.37	0.40
3:D:67:ARG:HB3	3:D:69:ARG:HG2	2.02	0.40
3:D:797:ASN:HA	3:D:798:PRO:HD3	1.78	0.40
3:D:834:ARG:HH21	3:D:848:GLU:HA	1.87	0.40
1:A:214:THR:OG1	1:B:230:GLU:OE1	2.37	0.40
2:C:1146:GLU:HB2	2:C:1149:GLU:O	2.21	0.40
3:D:350:ARG:HD2	3:D:377:SER:OG	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	222/347 (64%)	210 (95%)	11 (5%)	1 (0%)	24	62
1	B	225/347 (65%)	208 (92%)	15 (7%)	2 (1%)	14	49
2	C	1124/1178 (95%)	1053 (94%)	63 (6%)	8 (1%)	18	55
3	D	1261/1316 (96%)	1197 (95%)	59 (5%)	5 (0%)	30	66

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	E	79/110 (72%)	77 (98%)	2 (2%)	0	100	100
5	F	316/528 (60%)	302 (96%)	13 (4%)	1 (0%)	36	71
All	All	3227/3826 (84%)	3047 (94%)	163 (5%)	17 (0%)	24	62

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	678	PRO
1	A	184	GLU
2	C	1148	ARG
5	F	405	ILE
1	B	158	GLU
2	C	47	PRO
2	C	922	VAL
2	C	1134	ASN
3	D	607	PRO
3	D	658	PRO
3	D	703	ARG
1	B	35	GLY
2	C	508	PRO
3	D	593	PRO
2	C	32	VAL
2	C	33	PRO
2	C	552	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	192/297 (65%)	189 (98%)	3 (2%)	55	69
1	B	192/297 (65%)	192 (100%)	0	100	100
2	C	948/998 (95%)	930 (98%)	18 (2%)	50	66
3	D	1048/1095 (96%)	1023 (98%)	25 (2%)	43	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	E	68/90 (76%)	66 (97%)	2 (3%)	37	58
5	F	270/427 (63%)	262 (97%)	8 (3%)	36	57
All	All	2718/3204 (85%)	2662 (98%)	56 (2%)	47	65

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	136	VAL
1	A	159	ILE
1	A	225	LEU
2	C	39	VAL
2	C	48	LEU
2	C	80	VAL
2	C	185	VAL
2	C	322	LEU
2	C	354	THR
2	C	373	PHE
2	C	378	LEU
2	C	427	ILE
2	C	472	VAL
2	C	506	VAL
2	C	691	ASP
2	C	710	ASP
2	C	850	ILE
2	C	928	ILE
2	C	961	ASP
2	C	1002	VAL
2	C	1071	MET
3	D	16	THR
3	D	82	VAL
3	D	83	THR
3	D	92	MET
3	D	101	VAL
3	D	114	LEU
3	D	261	ILE
3	D	582	VAL
3	D	583	THR
3	D	629	VAL
3	D	684	VAL
3	D	838	SER
3	D	891	CYS

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Mol	Chain	Res	Type
3	D	901	LEU
3	D	910	LEU
3	D	921	TYR
3	D	925	LEU
3	D	930	VAL
3	D	990	ASP
3	D	1098	VAL
3	D	1099	LEU
3	D	1194	VAL
3	D	1206	VAL
3	D	1212	LYS
3	D	1249	LYS
4	E	48	SER
4	E	75	ILE
5	F	241	LEU
5	F	269	ARG
5	F	306	LEU
5	F	367	ARG
5	F	370	VAL
5	F	448	VAL
5	F	503	ILE
5	F	527	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	124	HIS
2	C	37	ASN
2	C	200	HIS
2	C	372	HIS
2	C	388	GLN
2	C	451	HIS
2	C	729	HIS
2	C	969	ASN
3	D	303	GLN
3	D	465	HIS
3	D	467	GLN
3	D	510	GLN
3	D	639	GLN
3	D	687	GLN
3	D	767	HIS
3	D	1160	GLN

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Mol	Chain	Res	Type
4	E	70	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	RFP	C	1201	-	63,63,63	2.72	12 (19%)	94,94,94	2.16	19 (20%)

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	RFP	C	1201	-	-	21/60/85/85	0/5/5/5

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	1201	RFP	O4-C11	12.42	1.40	1.21
8	C	1201	RFP	C43-N2	8.22	1.50	1.27
8	C	1201	RFP	C17-C16	7.74	1.55	1.34
8	C	1201	RFP	C15-N1	5.27	1.46	1.35
8	C	1201	RFP	O7-C25	-5.07	1.37	1.44
8	C	1201	RFP	C3-C43	4.82	1.56	1.46
8	C	1201	RFP	C12-C11	-3.60	1.40	1.54
8	C	1201	RFP	C18-C17	3.54	1.54	1.43
8	C	1201	RFP	C6-C7	3.03	1.45	1.39
8	C	1201	RFP	C29-C28	2.15	1.41	1.30
8	C	1201	RFP	O9-C23	-2.07	1.37	1.43
8	C	1201	RFP	O6-C27	-2.01	1.38	1.43

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	1201	RFP	C43-N2-N3	-8.48	108.44	120.55
8	C	1201	RFP	C30-C16-C17	-7.42	105.63	123.67
8	C	1201	RFP	C38-N4-C42	6.64	123.28	110.63
8	C	1201	RFP	C2-C3-C43	-6.27	117.33	123.99
8	C	1201	RFP	O3-C6-C7	5.23	130.03	121.16
8	C	1201	RFP	O4-C11-C5	-4.48	123.37	131.63
8	C	1201	RFP	O7-C35-C36	4.28	118.73	111.09
8	C	1201	RFP	C23-C24-C25	4.17	118.54	110.58
8	C	1201	RFP	C12-O5-C29	3.42	126.26	117.84
8	C	1201	RFP	C37-O6-C27	3.01	119.89	112.99
8	C	1201	RFP	C25-O7-C35	2.72	121.94	117.72
8	C	1201	RFP	C5-C10-C4	-2.72	121.44	124.08
8	C	1201	RFP	C20-C19-C18	-2.71	120.50	126.11
8	C	1201	RFP	O5-C12-C13	2.48	113.41	106.98
8	C	1201	RFP	C3-C2-C1	2.45	122.42	120.68
8	C	1201	RFP	C5-C6-C7	-2.35	119.62	125.29
8	C	1201	RFP	C25-C26-C27	2.30	118.26	111.99
8	C	1201	RFP	C33-C24-C25	-2.20	107.53	111.40
8	C	1201	RFP	C34-C26-C25	-2.08	107.74	111.40

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	C	1201	RFP	C4-C3-C43-N2
8	C	1201	RFP	C15-C16-C17-C18

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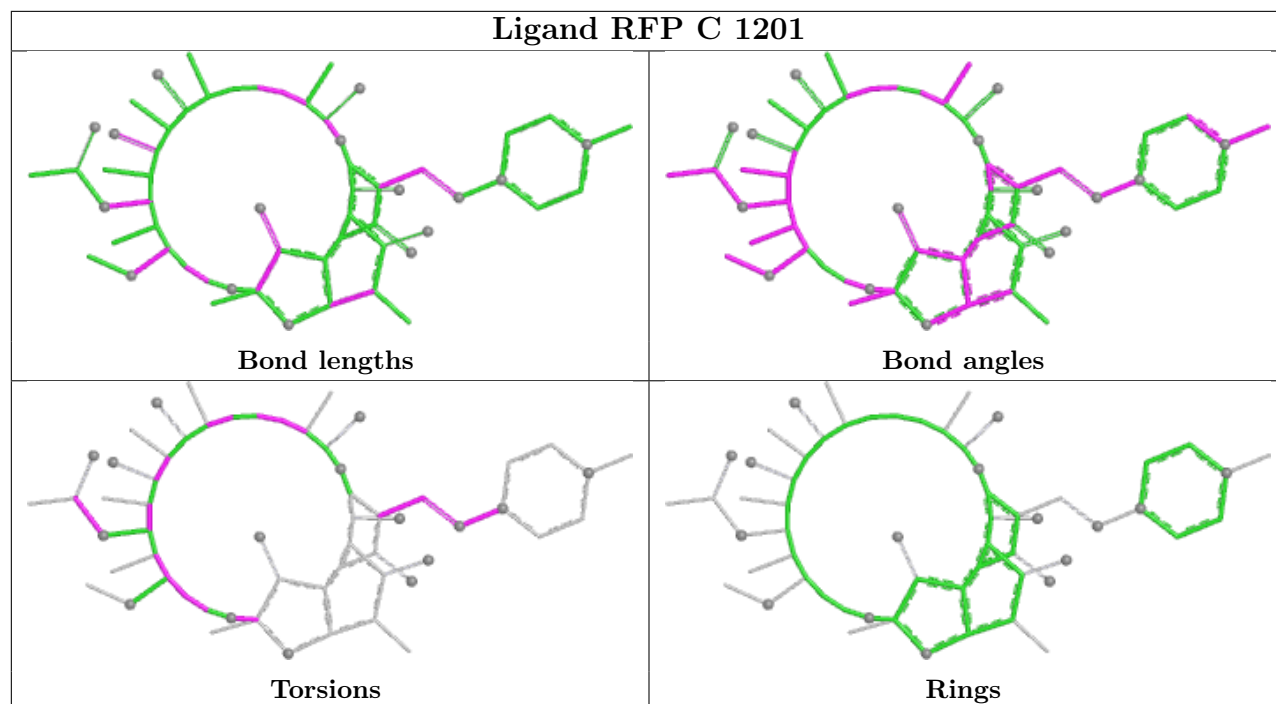
Mol	Chain	Res	Type	Atoms
8	C	1201	RFP	C26-C27-C28-C29
8	C	1201	RFP	O6-C27-C28-C29
8	C	1201	RFP	C43-N2-N3-C40
8	C	1201	RFP	C3-C43-N2-N3
8	C	1201	RFP	C36-C35-O7-C25
8	C	1201	RFP	C16-C17-C18-C19
8	C	1201	RFP	C34-C26-C27-C28
8	C	1201	RFP	C34-C26-C27-O6
8	C	1201	RFP	C25-C26-C27-O6
8	C	1201	RFP	C27-C28-C29-O5
8	C	1201	RFP	C30-C16-C17-C18
8	C	1201	RFP	C18-C19-C20-C31
8	C	1201	RFP	C11-C12-O5-C29
8	C	1201	RFP	O3-C12-O5-C29
8	C	1201	RFP	C2-C3-C43-N2
8	C	1201	RFP	C32-C22-C23-C24
8	C	1201	RFP	C21-C22-C23-C24
8	C	1201	RFP	C33-C24-C25-C26
8	C	1201	RFP	C23-C24-C25-C26

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	1201	RFP	6	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	224/347 (64%)	0.54	5 (2%) 62 48	23, 64, 126, 150	0
1	B	227/347 (65%)	0.81	15 (6%) 24 25	48, 102, 161, 204	0
2	C	1126/1178 (95%)	0.39	19 (1%) 69 54	8, 47, 127, 163	0
3	D	1265/1316 (96%)	0.31	16 (1%) 75 59	7, 39, 111, 155	0
4	E	81/110 (73%)	0.50	3 (3%) 45 37	28, 59, 94, 129	0
5	F	320/528 (60%)	0.59	17 (5%) 32 30	10, 64, 159, 190	0
6	H	23/23 (100%)	0.89	0 100 100	21, 139, 179, 194	0
7	G	12/16 (75%)	1.63	4 (33%) 1 3	126, 169, 396, 396	0
All	All	3278/3865 (84%)	0.43	79 (2%) 59 47	7, 51, 135, 396	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	F	500	ARG	5.3
5	F	389	ASP	4.6
5	F	503	ILE	4.5
1	B	201	SER	3.9
4	E	44	LEU	3.5
2	C	235	THR	3.5
3	D	903	GLU	3.4
5	F	393	GLU	3.3
2	C	28	SER	3.2
4	E	72	GLY	3.2
1	A	196	VAL	3.2
1	B	154	ALA	3.2
5	F	512	SER	3.1
2	C	237	LEU	3.0
3	D	900	GLU	3.0
2	C	1151	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	155	SER	3.0
1	A	194	LEU	2.9
5	F	516	HIS	2.8
3	D	663	MET	2.8
3	D	56	ARG	2.8
5	F	431	GLY	2.8
1	B	140	VAL	2.7
7	G	14	DG	2.7
2	C	402	GLU	2.7
2	C	359	GLY	2.7
2	C	44	LEU	2.6
3	D	1281	ALA	2.6
5	F	502	ARG	2.6
5	F	207	ASP	2.6
1	B	159	ILE	2.6
2	C	217	ASP	2.5
3	D	610	GLY	2.5
1	B	156	GLY	2.5
3	D	664	ALA	2.5
1	A	34	LEU	2.5
3	D	1080	ILE	2.5
5	F	265	GLU	2.4
2	C	270	THR	2.4
1	B	90	ASP	2.4
3	D	748	HIS	2.4
7	G	16	DC	2.4
2	C	417	LEU	2.3
2	C	820	LEU	2.3
1	B	71	GLU	2.3
2	C	1025	VAL	2.3
5	F	501	GLU	2.3
2	C	198	THR	2.3
2	C	252	PHE	2.3
4	E	28	GLY	2.3
3	D	204	GLU	2.2
1	A	152	ASN	2.2
3	D	286	GLY	2.2
5	F	528	ASP	2.2
5	F	258	TYR	2.2
5	F	509	LYS	2.2
3	D	791	GLU	2.2
3	D	167	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
3	D	784	GLU	2.1
2	C	977	PHE	2.1
3	D	40	LYS	2.1
1	B	87	SER	2.1
2	C	573	SER	2.1
5	F	489	LEU	2.1
2	C	407	GLN	2.1
1	B	167	ILE	2.1
3	D	739	PRO	2.1
2	C	79	ASP	2.1
1	A	225	LEU	2.1
1	B	54	ILE	2.1
2	C	543	GLN	2.1
1	B	227	VAL	2.1
7	G	15	DT	2.1
1	B	158	GLU	2.1
1	B	150	VAL	2.0
7	G	5	DC	2.0
1	B	60	LEU	2.0
5	F	513	LYS	2.0
5	F	482	THR	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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.

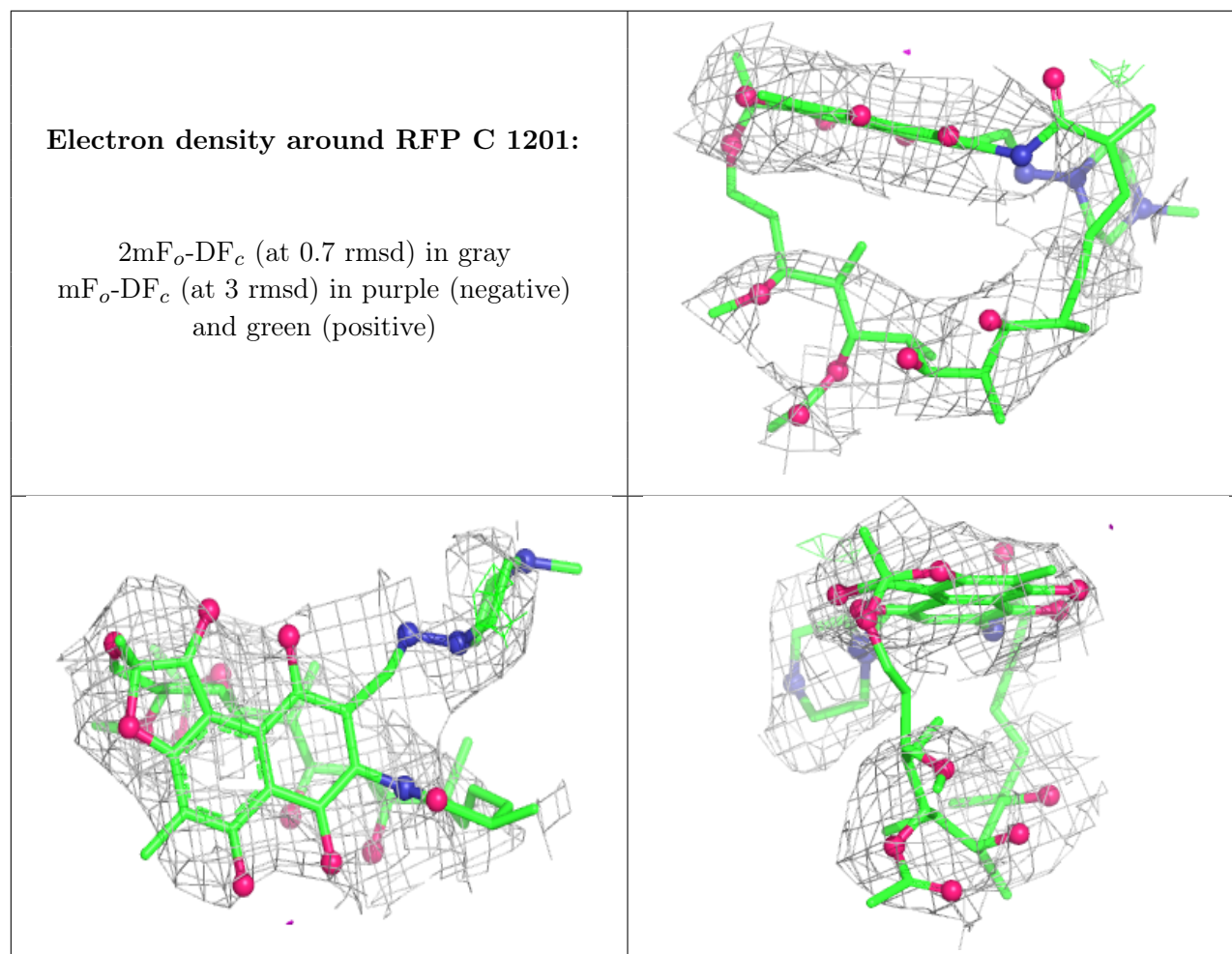
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
10	MG	D	1403	1/1	0.90	0.22	5,5,5,5	0
8	RFP	C	1201	59/59	0.92	0.14	13,27,57,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	ZN	D	1401	1/1	0.99	0.04	33,33,33,33	0
9	ZN	D	1402	1/1	1.00	0.03	28,28,28,28	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.



6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.