



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:09 AM UTC

PDB ID : 5UH6 / pdb_00005uh6
Title : Crystal structure of Mycobacterium tuberculosis transcription initiation complex containing 2ntRNA in complex with Rifampin
Authors : Lin, W.; Das, K.; Feng, Y.; Ebright, R.H.
Deposited on : 2017-01-11
Resolution : 3.84 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

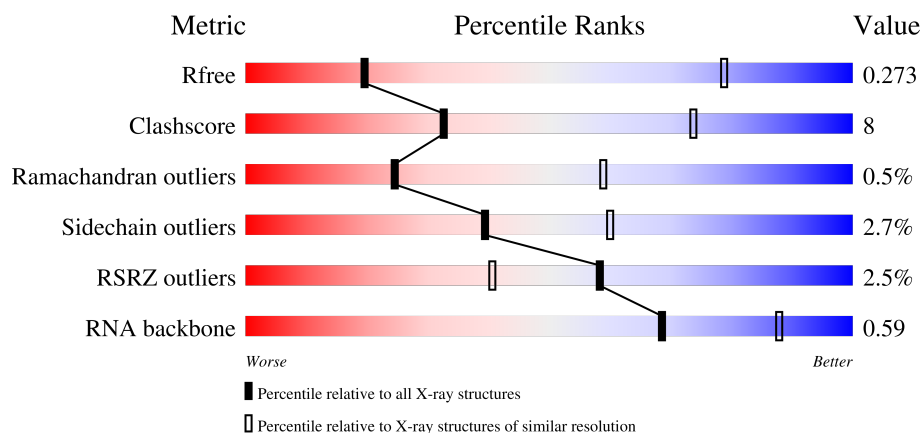
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.84 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	1169 (4.00-3.68)
Clashscore	190562	1211 (4.00-3.68)
Ramachandran outliers	187476	1156 (4.00-3.68)
Sidechain outliers	187428	1149 (4.00-3.68)
RSRZ outliers	180081	1168 (4.00-3.68)
RNA backbone	3983	1010 (4.56-3.10)

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	2% 52% 12% 35%
1	B	347	3% 51% 13% 35%
2	C	1178	2% 75% 20% . .
3	D	1316	% 75% 20% . .

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Mol	Chain	Length	Quality of chain
4	E	110	% 55% 18% 26%
5	F	528	5% 47% 14% 39%
6	H	23	17% 43% 57%
7	G	16	19% 69% 19% 6% 6%
8	I	2	100%

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 26085 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	225	Total	C	N	O	S	0	0	0
			1705	1075	289	339	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	322	Total	C	N	O	S	0	0	0
			2555	1589	461	496	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			

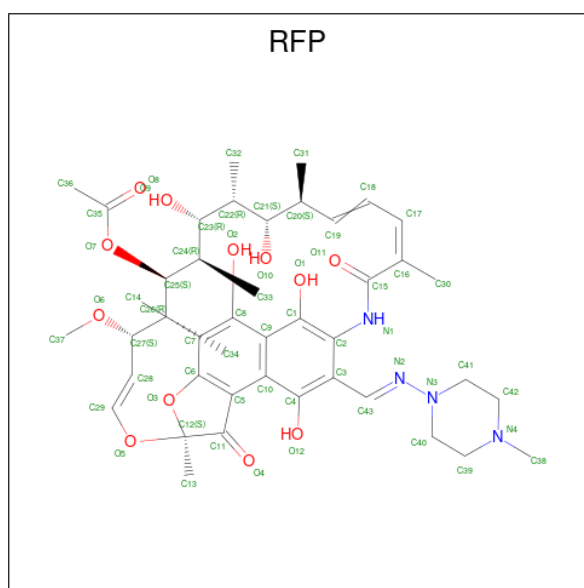
- Molecule 7 is a DNA chain called DNA (5'-D(*CP*AP*TP*CP*CP*GP*TP*GP*AP*GP*TP*CP*CP*AP*GP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	15	Total	C	N	O	P	0	0	0
			303	145	56	88	14			

- Molecule 8 is a RNA chain called RNA (5'-R(*GP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	2	Total	C	N	O	P	0	0	0
			42	20	10	11	1			

- Molecule 9 is RIFAMPICIN (CCD ID: RFP) (formula: C₄₃H₅₈N₄O₁₂).



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

- Molecule 10 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

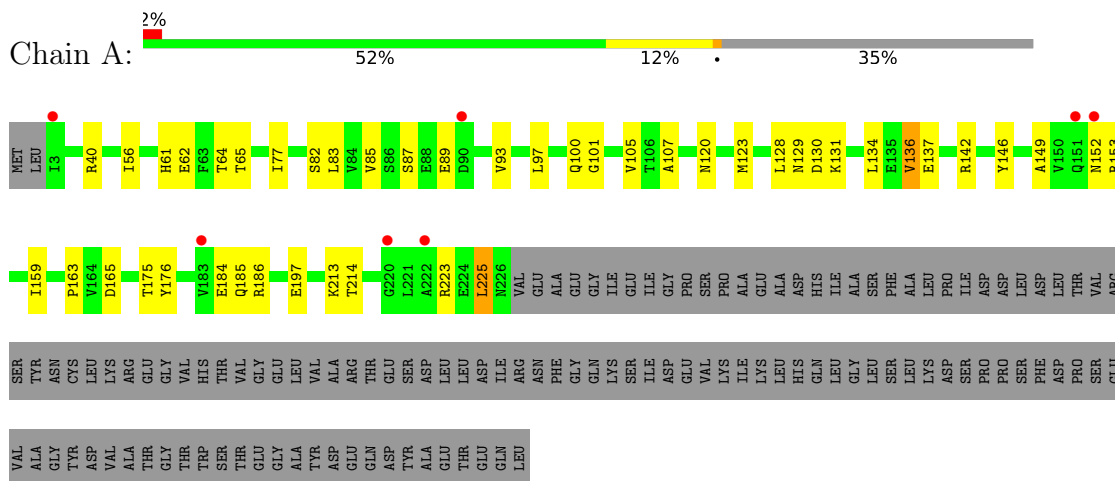
- Molecule 11 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

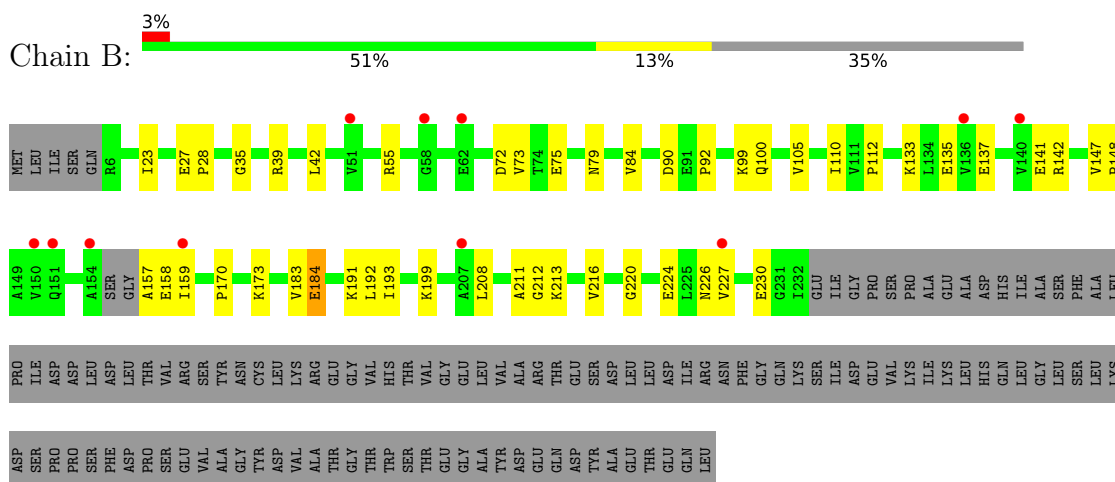
3 Residue-property plots

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.

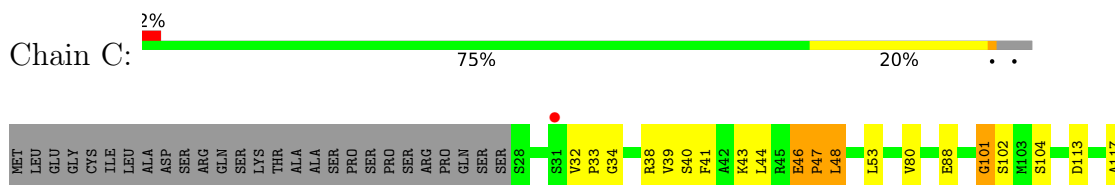
- Molecule 1: DNA-directed RNA polymerase subunit alpha

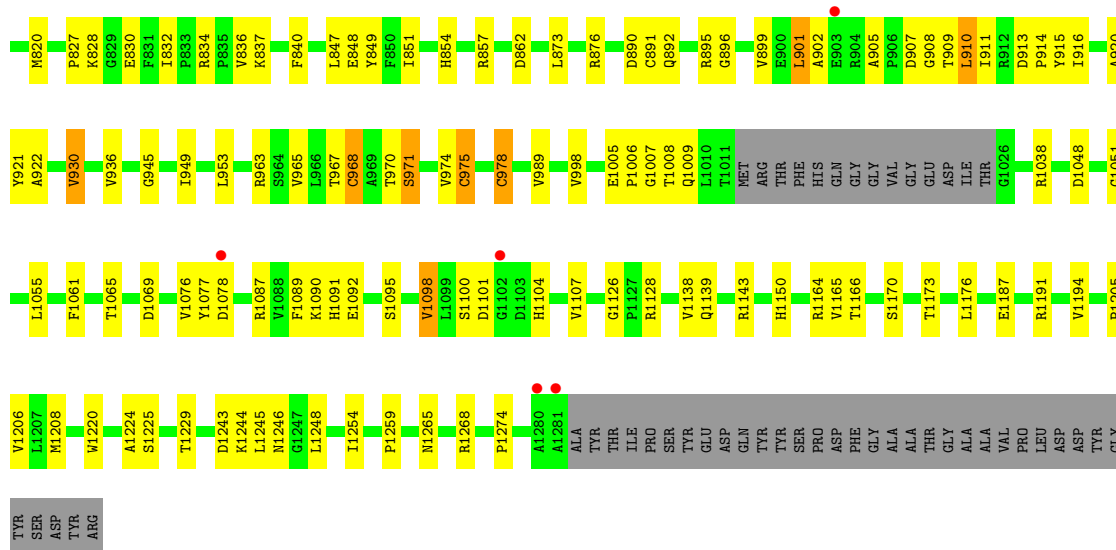


- Molecule 1: DNA-directed RNA polymerase subunit alpha

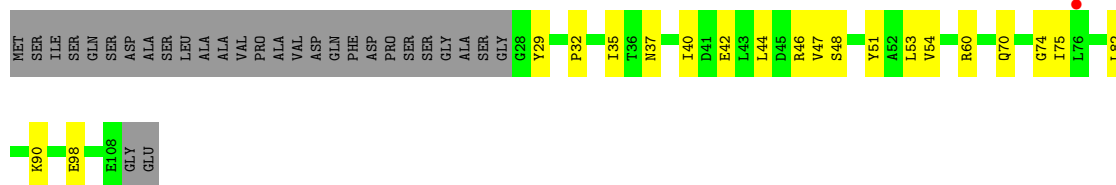


- Molecule 2: DNA-directed RNA polymerase subunit beta

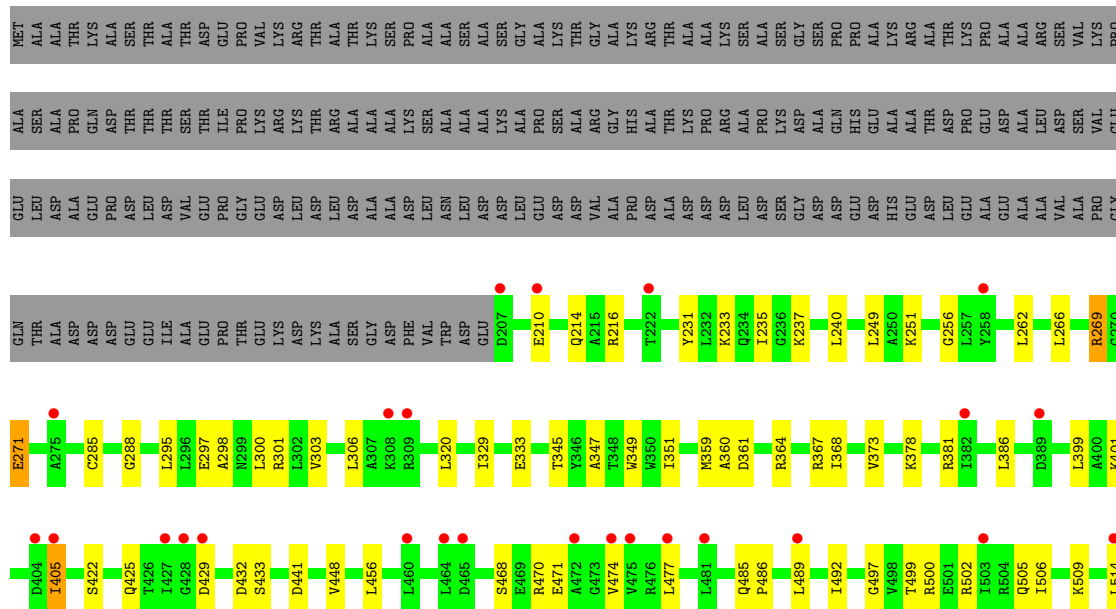




• Molecule 4: DNA-directed RNA polymerase subunit omega

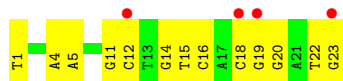
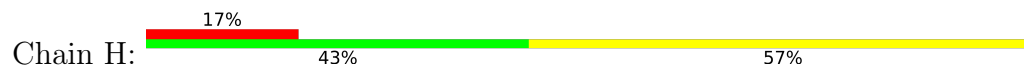


• Molecule 5: RNA polymerase sigma factor SigA

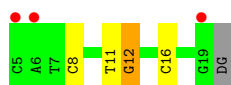




- Molecule 6: DNA (5'-D(*TP*AP*TP*AP*AP*TP*GP*GP*GP*AP*GP*CP*TP*GP*TP*CP*AP*CP*GP*GP*AP*TP*G)-3')



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



- Molecule 8: RNA (5'-R(*GP*A)-3')



There are no outlier residues recorded for this chain.

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	153.24Å 164.89Å 199.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.09 – 3.84 50.09 – 3.84	Depositor EDS
% Data completeness (in resolution range)	81.0 (50.09-3.84) 80.9 (50.09-3.84)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.61 (at 3.88Å)	Xtriage
Refinement program	REFMAC, PHENIX	Depositor
R, R_{free}	0.212 , 0.264 0.230 , 0.273	Depositor DCC
R_{free} test set	1997 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	27.5	Xtriage
Anisotropy	0.493	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 45.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	26085	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.97% 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 ⓘ

5.1 Standard geometry ⓘ

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	0.31	0/1730	0.79	0/2354
1	B	0.32	0/1730	0.79	1/2355 (0.0%)
2	C	0.31	0/8873	0.76	3/12031 (0.0%)
3	D	0.34	0/10052	0.79	14/13591 (0.1%)
4	E	0.31	0/650	0.76	0/886
5	F	0.33	0/2585	0.75	0/3485
6	H	0.27	0/535	0.41	0/826
7	G	0.25	0/339	0.52	1/521 (0.2%)
8	I	0.11	0/47	0.17	0/72
All	All	0.32	0/26541	0.76	19/36121 (0.1%)

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1126	GLY	CA-C-N	6.09	126.26	119.32
3	D	1126	GLY	C-N-CA	6.09	126.26	119.32
2	C	46	GLU	CA-C-N	-5.90	112.46	119.84
2	C	46	GLU	C-N-CA	-5.90	112.46	119.84
3	D	797	ASN	CA-C-N	5.75	125.43	119.05
3	D	797	ASN	C-N-CA	5.75	125.43	119.05
3	D	1005	GLU	CA-C-N	-5.73	114.36	121.00
3	D	1005	GLU	C-N-CA	-5.73	114.36	121.00
3	D	453	LYS	CA-C-N	-5.70	113.89	120.04
3	D	453	LYS	C-N-CA	-5.70	113.89	120.04
3	D	286	GLY	N-CA-C	5.51	119.16	112.49
3	D	110	VAL	N-CA-C	5.44	114.47	108.05
2	C	101	GLY	N-CA-C	-5.27	108.05	115.32
3	D	433	GLY	CA-C-N	5.25	124.92	119.56
3	D	433	GLY	C-N-CA	5.25	124.92	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	184	GLU	CB-CA-C	-5.22	110.12	117.23
3	D	321	PRO	CA-C-N	5.13	124.31	118.97
3	D	321	PRO	C-N-CA	5.13	124.31	118.97
7	G	12	DG	P-O3'-C3'	5.10	127.85	120.20

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	29	0
1	B	1705	0	1730	28	0
2	C	8714	0	8636	151	0
3	D	9887	0	9943	173	0
4	E	637	0	635	13	0
5	F	2555	0	2579	50	0
6	H	476	0	261	12	0
7	G	303	0	170	6	0
8	I	42	0	23	0	0
9	C	59	0	58	4	0
10	D	2	0	0	0	0
11	D	1	0	0	0	0
All	All	26085	0	25776	411	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 (411) 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)
3:D:913:ASP:OD1	3:D:914:PRO:HD2	1.57	1.03
3:D:891:CYS:SG	3:D:970:THR:OG1	2.22	0.98
3:D:913:ASP:OD1	3:D:914:PRO:CD	2.20	0.89
3:D:908:GLY:O	3:D:909:THR:OG1	1.91	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:902:ALA:HB1	3:D:911:ILE:O	1.82	0.80
2:C:230:ARG:HH12	7:G:8:DC:H5''	1.53	0.74
2:C:974:THR:HG23	2:C:980:ALA:H	1.53	0.73
2:C:113:ASP:HB2	2:C:132:PRO:HG2	1.71	0.72
3:D:589:THR:HG22	3:D:670:ARG:HG2	1.72	0.72
3:D:905:ALA:HB3	3:D:908:GLY:O	1.91	0.70
2:C:101:GLY:O	2:C:142:ASN:ND2	2.24	0.70
3:D:901:LEU:HD13	3:D:901:LEU:O	1.93	0.69
3:D:891:CYS:O	3:D:892:GLN:HB2	1.93	0.69
1:B:75:GLU:O	1:B:79:ASN:ND2	2.25	0.68
3:D:442:GLY:HA3	3:D:523:GLN:HB2	1.75	0.68
5:F:522:VAL:HG23	5:F:523:LEU:HD12	1.76	0.68
3:D:1090:LYS:HB3	3:D:1092:GLU:HG2	1.75	0.68
7:G:11:DT:H2''	7:G:12:DG:H8	1.58	0.68
6:H:16:DC:O2	7:G:12:DG:N2	2.19	0.68
1:A:214:THR:HA	1:B:230:GLU:HG2	1.76	0.67
3:D:107:PHE:HZ	3:D:126:GLU:HG2	1.60	0.67
1:A:56:ILE:HG12	1:A:136:VAL:HG13	1.78	0.66
2:C:1024:THR:H	3:D:730:THR:HG21	1.59	0.66
3:D:638:THR:HG23	3:D:639:GLN:HG2	1.77	0.66
3:D:907:ASP:OD1	3:D:908:GLY:N	2.28	0.66
7:G:11:DT:H2''	7:G:12:DG:C8	2.29	0.66
5:F:477:LEU:HD13	5:F:492:ILE:HG23	1.78	0.65
3:D:454:PRO:HA	3:D:457:MET:HE2	1.77	0.65
1:A:107:ALA:HB2	1:A:123:MET:HE2	1.78	0.65
2:C:104:SER:HB3	2:C:140:ILE:HB	1.79	0.65
2:C:658:ILE:HD11	2:C:688:PRO:HB3	1.79	0.65
2:C:704:ASP:HB2	2:C:708:THR:HB	1.79	0.64
3:D:1245:LEU:HD13	3:D:1254:ILE:HD13	1.79	0.64
3:D:1274:PRO:HB3	4:E:82:LEU:HD11	1.79	0.64
1:A:197:GLU:OE1	2:C:996:ARG:NH1	2.30	0.64
5:F:269:ARG:NH1	5:F:271:GLU:OE1	2.31	0.64
2:C:1044:ARG:HH12	2:C:1048:PRO:HD2	1.61	0.64
6:H:15:DT:H2''	6:H:16:DC:H5'	1.80	0.64
2:C:396:MET:HE1	2:C:418:ILE:HG23	1.79	0.64
3:D:913:ASP:OD1	3:D:914:PRO:N	2.31	0.64
3:D:190:LYS:HE3	3:D:192:ASP:HB3	1.78	0.63
2:C:959:LEU:HD12	2:C:960:PRO:HD2	1.81	0.63
3:D:373:MET:O	3:D:377:SER:OG	2.14	0.63
1:B:90:ASP:HA	1:B:142:ARG:HD3	1.80	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:1122:LYS:HE2	2:C:1148:ARG:HG2	1.81	0.62
3:D:1051:GLY:HA2	3:D:1069:ASP:HB2	1.81	0.62
2:C:483:MET:HE3	2:C:498:GLY:HA3	1.81	0.62
3:D:910:LEU:HD12	3:D:910:LEU:O	2.00	0.62
3:D:1265:ASN:OD1	3:D:1268:ARG:NH2	2.32	0.62
3:D:930:VAL:HG22	3:D:936:VAL:HG12	1.82	0.62
3:D:970:THR:HG22	3:D:971:SER:N	2.14	0.61
5:F:470:ARG:HH11	5:F:506:ILE:HD11	1.66	0.61
5:F:505:GLN:HG3	5:F:509:LYS:HE3	1.83	0.60
2:C:815:THR:HG22	2:C:817:GLU:H	1.65	0.60
1:B:84:VAL:HG12	1:B:199:LYS:HD3	1.83	0.60
2:C:587:VAL:HB	2:C:591:THR:HB	1.84	0.60
3:D:965:VAL:HG13	3:D:974:VAL:HG11	1.83	0.60
2:C:899:LEU:HB2	2:C:904:MET:HE1	1.83	0.60
3:D:820:MET:HE3	3:D:837:LYS:HA	1.83	0.60
1:A:87:SER:O	1:A:142:ARG:NH1	2.35	0.59
2:C:561:VAL:HG21	2:C:571:VAL:HB	1.84	0.59
2:C:189:GLU:HB2	2:C:367:THR:HG21	1.83	0.59
3:D:1165:VAL:HG12	3:D:1205:PRO:HA	1.84	0.59
3:D:418:LEU:HD11	3:D:1225:SER:HB2	1.84	0.58
2:C:737:LEU:HB2	2:C:898:ILE:HG12	1.85	0.58
3:D:1089:PHE:HA	3:D:1095:SER:HA	1.85	0.58
1:A:152:ASN:HB3	1:A:163:PRO:HB3	1.85	0.58
1:A:213:LYS:HD3	1:B:227:VAL:HG23	1.86	0.58
2:C:658:ILE:HG21	2:C:702:ILE:HD12	1.86	0.58
2:C:43:LYS:NZ	2:C:544:ALA:O	2.37	0.57
2:C:348:LEU:HD13	2:C:365:VAL:HG12	1.84	0.57
3:D:320:ILE:HG22	3:D:344:TYR:HE2	1.68	0.57
5:F:256:GLY:HA3	5:F:288:GLY:HA3	1.87	0.57
2:C:1087:GLU:HG3	2:C:1091:ILE:HD11	1.86	0.57
5:F:231:TYR:CE2	5:F:235:ILE:HD11	2.40	0.57
1:A:62:GLU:HG3	1:A:77:ILE:HD12	1.85	0.57
2:C:599:HIS:HB3	2:C:928:ILE:HD12	1.85	0.57
3:D:363:PRO:HD2	3:D:366:ILE:HD12	1.86	0.57
9:C:1201:RFP:HN1	9:C:1201:RFP:C18	2.16	0.56
5:F:364:ARG:HG3	5:F:368:ILE:HG12	1.87	0.56
2:C:438:GLN:OE1	2:C:451:HIS:NE2	2.34	0.56
1:A:40:ARG:NH1	2:C:1013:GLY:O	2.37	0.56
2:C:168:ILE:HG12	2:C:431:PHE:HB3	1.86	0.56
2:C:41:PHE:HB2	2:C:979:GLY:HA2	1.87	0.56
3:D:384:ASN:HD21	3:D:391:VAL:H	1.54	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:27:GLU:HG3	1:B:28:PRO:HD2	1.88	0.56
3:D:968:CYS:SG	3:D:978:CYS:HB3	2.46	0.56
2:C:1067:ARG:NH1	7:G:16:DC:OP1	2.39	0.55
3:D:891:CYS:SG	3:D:975:CYS:HB3	2.46	0.55
2:C:475:VAL:O	3:D:854:HIS:ND1	2.39	0.55
3:D:707:ILE:HD11	4:E:32:PRO:HB3	1.88	0.55
2:C:377:ARG:NH2	2:C:383:GLU:OE1	2.38	0.55
2:C:817:GLU:N	2:C:817:GLU:OE1	2.39	0.55
5:F:240:LEU:HD21	5:F:301:ARG:HD2	1.88	0.55
2:C:489:PRO:HA	2:C:610:ASN:HD21	1.72	0.54
2:C:549:ASP:HB3	2:C:553:ARG:H	1.72	0.54
3:D:578:ARG:H	3:D:581:MET:HE3	1.71	0.54
3:D:595:ASP:HB3	3:D:631:ALA:HB2	1.90	0.54
2:C:731:TYR:HE1	3:D:579:LEU:HB2	1.72	0.54
1:A:64:THR:OG1	1:A:65:THR:N	2.40	0.54
3:D:130:TYR:OH	3:D:379:ASP:OD2	2.23	0.54
1:A:175:THR:OG1	1:A:176:TYR:N	2.41	0.54
2:C:446:LEU:HB2	2:C:713:MET:HE2	1.88	0.54
3:D:238:GLU:OE1	5:F:237:LYS:NZ	2.41	0.54
5:F:506:ILE:HA	5:F:509:LYS:HD2	1.88	0.54
1:A:136:VAL:HG12	1:A:137:GLU:H	1.73	0.54
1:B:23:ILE:HD12	1:B:192:LEU:HD23	1.89	0.54
1:B:99:LYS:HD3	1:B:105:VAL:HG22	1.89	0.54
4:E:70:GLN:O	4:E:74:GLY:N	2.38	0.54
3:D:49:GLU:OE2	3:D:55:THR:N	2.34	0.54
2:C:516:TYR:HD2	2:C:531:LEU:HD13	1.74	0.53
3:D:589:THR:HG21	3:D:688:MET:HG2	1.88	0.53
5:F:474:VAL:HA	5:F:477:LEU:HD12	1.91	0.53
2:C:1041:ILE:HD12	3:D:520:LYS:HB3	1.90	0.53
3:D:1055:LEU:HB2	3:D:1101:ASP:HB3	1.89	0.53
5:F:468:SER:HB3	5:F:471:GLU:HG3	1.91	0.53
1:B:170:PRO:HA	1:B:199:LYS:HD2	1.89	0.53
2:C:317:ASN:O	2:C:321:GLY:N	2.35	0.53
5:F:470:ARG:HB3	5:F:506:ILE:HD13	1.91	0.53
2:C:1119:GLU:OE2	3:D:89:ARG:NH2	2.42	0.52
2:C:1141:ASP:OD1	2:C:1142:GLY:N	2.43	0.52
5:F:386:LEU:HD12	5:F:399:LEU:HD23	1.91	0.52
1:B:220:GLY:O	1:B:224:GLU:HG3	2.08	0.52
2:C:467:ARG:NE	6:H:15:DT:OP2	2.42	0.52
3:D:832:ILE:HG22	3:D:834:ARG:H	1.74	0.52
5:F:499:THR:OG1	5:F:500:ARG:N	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:238:GLU:OE2	3:D:242:ARG:NH1	2.40	0.52
4:E:42:GLU:O	4:E:46:ARG:NH1	2.42	0.52
2:C:597:LEU:HD23	2:C:976:VAL:HG11	1.91	0.52
2:C:738:SER:HA	2:C:904:MET:HE3	1.92	0.52
2:C:150:GLN:HG2	2:C:414:PRO:HG2	1.90	0.52
1:B:72:ASP:OD1	1:B:73:VAL:N	2.39	0.52
3:D:770:ARG:NH1	3:D:771:ASN:OD1	2.43	0.52
3:D:350:ARG:HG2	3:D:353:ARG:HH12	1.75	0.51
3:D:970:THR:CG2	3:D:971:SER:N	2.73	0.51
1:A:129:ASN:ND2	2:C:652:GLU:HG3	2.25	0.51
2:C:601:ASP:OD2	2:C:602:ALA:N	2.43	0.51
3:D:353:ARG:NH1	3:D:370:GLU:OE1	2.40	0.51
3:D:1166:THR:HB	3:D:1206:VAL:HG21	1.93	0.51
5:F:515:ARG:O	5:F:519:ARG:N	2.42	0.51
3:D:827:PRO:HG3	3:D:854:HIS:NE2	2.25	0.51
2:C:737:LEU:HG	2:C:895:ILE:HD12	1.92	0.51
3:D:104:ILE:HD12	3:D:379:ASP:HB3	1.93	0.51
3:D:365:ILE:HG21	5:F:297:GLU:HG2	1.92	0.50
2:C:211:TRP:HB2	2:C:227:ASP:HA	1.92	0.50
2:C:720:LEU:HD23	2:C:913:VAL:HA	1.94	0.50
3:D:107:PHE:CZ	3:D:126:GLU:HG2	2.45	0.50
3:D:215:GLU:OE1	3:D:218:ARG:NH1	2.43	0.50
3:D:708:VAL:HG22	4:E:29:TYR:HB3	1.93	0.50
3:D:908:GLY:C	3:D:909:THR:HG1	2.03	0.50
5:F:401:LYS:HA	5:F:405:ILE:HA	1.93	0.50
2:C:252:PHE:HB3	2:C:258:MET:HG3	1.94	0.50
2:C:721:VAL:HG23	2:C:915:ILE:HG23	1.93	0.50
2:C:926:MET:HE1	3:D:817:LEU:HA	1.93	0.50
2:C:47:PRO:HG2	2:C:581:VAL:O	2.11	0.49
2:C:88:GLU:CD	2:C:310:ARG:HH12	2.19	0.49
2:C:653:VAL:HG12	2:C:692:ALA:HB2	1.94	0.49
2:C:1148:ARG:NH1	3:D:86:LYS:HG3	2.27	0.49
3:D:453:LYS:O	3:D:457:MET:HG3	2.12	0.49
3:D:901:LEU:HD13	3:D:901:LEU:C	2.36	0.49
3:D:915:TYR:HA	3:D:1143:ARG:HH12	1.76	0.49
3:D:1090:LYS:HG2	3:D:1091:HIS:H	1.77	0.49
2:C:401:ARG:HA	2:C:404:MET:HE2	1.93	0.49
3:D:98:ALA:HB3	3:D:354:LEU:HD23	1.94	0.49
5:F:432:ASP:OD1	5:F:433:SER:N	2.45	0.49
2:C:855:ARG:NH1	2:C:862:PRO:O	2.45	0.49
2:C:1133:LEU:HD11	3:D:105:TRP:HZ3	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:599:TYR:HA	3:D:610:GLY:HA3	1.95	0.49
1:A:223:ARG:HD3	1:B:213:LYS:HB2	1.94	0.49
2:C:53:LEU:HD13	2:C:449:LEU:HD21	1.95	0.49
2:C:599:HIS:ND1	3:D:840:PHE:O	2.38	0.49
3:D:459:ARG:HA	3:D:462:ASP:HB2	1.95	0.49
3:D:828:LYS:HE3	3:D:830:GLU:HB2	1.94	0.49
1:A:153:ARG:HD3	2:C:795:GLU:CB	2.42	0.49
5:F:345:THR:HB	6:H:4:DA:H8	1.77	0.49
2:C:46:GLU:N	2:C:47:PRO:HD3	2.28	0.49
2:C:513:GLU:HB3	2:C:530:TYR:HB3	1.95	0.49
2:C:762:THR:HG23	2:C:764:LEU:H	1.77	0.49
3:D:428:SER:HB3	3:D:522:ILE:HG13	1.94	0.49
3:D:556:ARG:HG3	4:E:35:ILE:HG12	1.95	0.49
3:D:1038:ARG:NH1	6:H:18:DC:O3'	2.42	0.48
2:C:465:ARG:HD3	2:C:492:PRO:HB2	1.95	0.48
2:C:485:PRO:O	3:D:857:ARG:NH2	2.45	0.48
3:D:46:LEU:O	3:D:325:ARG:NH2	2.36	0.48
2:C:287:PRO:HD2	5:F:216:ARG:HA	1.94	0.48
5:F:499:THR:HG23	5:F:500:ARG:HD2	1.95	0.48
1:A:83:LEU:HG	1:A:85:VAL:HG23	1.95	0.48
2:C:557:PRO:O	2:C:573:SER:N	2.46	0.48
4:E:32:PRO:HB2	4:E:37:ASN:HB2	1.94	0.48
2:C:344:TYR:OH	2:C:365:VAL:HA	2.13	0.48
3:D:1087:ARG:HG2	3:D:1098:VAL:HG22	1.96	0.48
3:D:201:GLY:O	3:D:205:MET:HG3	2.14	0.48
3:D:797:ASN:HA	3:D:798:PRO:HD3	1.76	0.48
3:D:1061:PHE:HE2	3:D:1078:ASP:HB3	1.78	0.48
2:C:797:ARG:HH22	3:D:479:GLN:CD	2.21	0.48
2:C:464:SER:HB3	2:C:467:ARG:HG3	1.96	0.48
2:C:944:TRP:NE1	2:C:963:LEU:O	2.45	0.48
3:D:482:GLN:OE1	3:D:482:GLN:N	2.41	0.48
2:C:1091:ILE:HB	2:C:1102:VAL:HG21	1.95	0.47
2:C:389:ILE:O	2:C:393:MET:HG2	2.14	0.47
2:C:617:PRO:HA	2:C:707:CYS:SG	2.54	0.47
2:C:1078:ALA:HB1	3:D:998:VAL:HG22	1.97	0.47
2:C:206:PRO:HA	2:C:308:LEU:HD23	1.96	0.47
2:C:396:MET:HE3	2:C:396:MET:HB2	1.76	0.47
3:D:901:LEU:C	3:D:901:LEU:CD1	2.87	0.47
3:D:910:LEU:HD21	3:D:953:LEU:O	2.15	0.47
5:F:347:ALA:O	5:F:351:ILE:HG13	2.14	0.47
2:C:1106:ILE:HD13	3:D:455:PHE:CE2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:GLN:HG2	1:A:186:ARG:H	1.80	0.47
2:C:251:ARG:NH2	2:C:343:GLU:OE1	2.43	0.47
9:C:1201:RFP:HN1	9:C:1201:RFP:H18C	1.79	0.47
3:D:597:GLY:HA3	3:D:627:LEU:HA	1.97	0.47
5:F:489:LEU:H	5:F:489:LEU:HD23	1.79	0.47
4:E:60:ARG:NE	4:E:98:GLU:OE2	2.43	0.47
2:C:200:HIS:CD2	2:C:348:LEU:HG	2.50	0.47
3:D:101:VAL:HG23	3:D:375:GLN:CD	2.40	0.47
3:D:913:ASP:HB3	3:D:916:ILE:HG13	1.97	0.47
3:D:676:LEU:HD23	3:D:716:LEU:HD23	1.96	0.46
3:D:896:GLY:O	3:D:1128:ARG:NH1	2.48	0.46
2:C:220:ASP:HB3	2:C:257:ILE:HG22	1.96	0.46
2:C:894:VAL:HG22	3:D:536:PHE:O	2.14	0.46
4:E:47:VAL:HG11	4:E:53:LEU:HB2	1.97	0.46
1:A:128:LEU:HD21	1:A:134:LEU:HB2	1.97	0.46
1:A:149:ALA:N	1:A:165:ASP:OD2	2.38	0.46
1:B:208:LEU:O	1:B:212:GLY:N	2.47	0.46
3:D:873:LEU:HA	3:D:876:ARG:HE	1.80	0.46
5:F:360:ALA:HB1	5:F:373:VAL:HG21	1.96	0.46
3:D:793:TYR:HB3	3:D:800:ILE:HG13	1.97	0.46
1:B:157:ALA:C	1:B:159:ILE:H	2.24	0.46
2:C:549:ASP:OD2	2:C:550:ALA:N	2.49	0.46
2:C:1084:THR:O	2:C:1088:LEU:HG	2.16	0.46
2:C:257:ILE:HD11	2:C:346:VAL:HG23	1.98	0.46
2:C:1019:PHE:HA	2:C:1020:PRO:HD3	1.83	0.46
3:D:83:THR:HG22	3:D:84:ARG:H	1.80	0.46
3:D:1048:ASP:H	3:D:1077:TYR:HH	1.63	0.46
1:A:225:LEU:HD13	1:A:225:LEU:H	1.81	0.46
3:D:545:LEU:HD12	3:D:546:PRO:HD2	1.98	0.46
3:D:1220:TRP:CD1	3:D:1243:ASP:HB2	2.50	0.46
2:C:38:ARG:HH11	2:C:712:GLU:CD	2.24	0.45
2:C:476:HIS:CG	2:C:477:PRO:HD2	2.50	0.45
2:C:311:VAL:HG21	2:C:377:ARG:HD2	1.99	0.45
3:D:1069:ASP:OD2	3:D:1104:HIS:NE2	2.48	0.45
3:D:717:LYS:HB3	3:D:717:LYS:HE2	1.75	0.45
2:C:408:ASP:O	2:C:412:ILE:HG13	2.17	0.45
3:D:308:SER:HA	3:D:309:PRO:HD3	1.81	0.45
3:D:367:VAL:HG12	3:D:371:LYS:HE3	1.98	0.45
3:D:1006:PRO:C	3:D:1008:THR:H	2.23	0.45
3:D:1164:ARG:HD2	3:D:1208:MET:HE1	1.97	0.45
5:F:231:TYR:O	5:F:235:ILE:HG13	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:111:PRO:O	3:D:113:ARG:HD2	2.17	0.45
3:D:785:VAL:HG21	3:D:820:MET:SD	2.56	0.45
3:D:1170:SER:O	3:D:1173:THR:OG1	2.34	0.45
3:D:1248:LEU:HD23	3:D:1259:PRO:HD2	1.98	0.45
3:D:125:LEU:HD12	3:D:125:LEU:HA	1.78	0.45
3:D:1187:GLU:O	3:D:1191:ARG:HB2	2.17	0.45
1:A:120:ASN:OD1	1:A:120:ASN:N	2.50	0.45
5:F:456:LEU:HD12	5:F:526:TYR:HB3	2.00	0.44
6:H:11:DG:H5''	6:H:12:DC:C4	2.52	0.44
2:C:891:ASN:OD1	2:C:891:ASN:N	2.46	0.44
9:C:1201:RFP:H342	9:C:1201:RFP:H24C	1.72	0.44
3:D:266:GLU:HA	3:D:310:MET:HE1	1.99	0.44
3:D:589:THR:HB	3:D:687:GLN:HA	1.99	0.44
5:F:249:LEU:HD12	5:F:295:LEU:HD13	1.99	0.44
1:A:130:ASP:O	1:A:131:LYS:HG2	2.17	0.44
2:C:104:SER:O	2:C:140:ILE:N	2.43	0.44
3:D:87:VAL:HB	3:D:91:ARG:HE	1.82	0.44
3:D:832:ILE:HG13	3:D:851:ILE:HD11	1.99	0.44
5:F:349:TRP:HB3	6:H:1:DT:H4'	1.99	0.44
2:C:484:CYS:HB2	2:C:588:SER:HB3	1.98	0.44
2:C:549:ASP:HB3	2:C:553:ARG:N	2.32	0.44
9:C:1201:RFP:O4	9:C:1201:RFP:O12	2.31	0.44
3:D:922:ALA:HB3	3:D:1150:HIS:CE1	2.52	0.44
1:B:100:GLN:HG3	1:B:133:LYS:HA	1.99	0.44
2:C:1148:ARG:NH1	3:D:86:LYS:O	2.51	0.44
3:D:827:PRO:HG3	3:D:854:HIS:CE1	2.53	0.44
3:D:945:GLY:O	3:D:949:ILE:HG12	2.17	0.44
5:F:477:LEU:HB3	5:F:492:ILE:HD13	1.99	0.44
2:C:1020:PRO:HB2	2:C:1021:TYR:CD2	2.53	0.44
3:D:445:LYS:NZ	3:D:518:GLU:OE2	2.48	0.44
2:C:239:LYS:HE2	2:C:245:SER:OG	2.18	0.43
2:C:875:GLN:NE2	2:C:877:ARG:HE	2.16	0.43
5:F:262:LEU:O	5:F:266:LEU:HG	2.17	0.43
2:C:486:ILE:HD11	3:D:849:TYR:HE2	1.82	0.43
2:C:597:LEU:HB3	2:C:976:VAL:HG13	2.00	0.43
3:D:363:PRO:O	3:D:367:VAL:HG23	2.19	0.43
3:D:588:LEU:HD12	3:D:589:THR:HG23	2.00	0.43
3:D:910:LEU:CD2	3:D:953:LEU:O	2.66	0.43
1:A:89:GLU:HG3	1:A:93:VAL:HG11	2.00	0.43
3:D:642:PRO:HB3	3:D:662:TRP:CD2	2.53	0.43
1:B:212:GLY:O	1:B:216:VAL:HG23	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:87:VAL:O	3:D:91:ARG:HG3	2.18	0.43
3:D:325:ARG:HD2	3:D:341:ASN:OD1	2.17	0.43
1:A:97:LEU:HD21	1:A:105:VAL:HG21	2.00	0.43
4:E:90:LYS:HD3	4:E:90:LYS:HA	1.81	0.43
2:C:546:SER:HA	2:C:547:PRO:HD3	1.88	0.43
3:D:554:GLU:HG3	4:E:54:VAL:HG11	2.01	0.43
5:F:329:ILE:O	5:F:333:GLU:HG2	2.18	0.43
1:B:226:ASN:O	1:B:226:ASN:ND2	2.49	0.43
2:C:377:ARG:HH22	2:C:383:GLU:CD	2.27	0.43
2:C:596:PHE:HB3	2:C:599:HIS:CD2	2.54	0.43
2:C:757:ILE:HD12	2:C:837:LEU:HB2	2.01	0.43
2:C:518:LYS:HA	2:C:578:TYR:HD1	1.84	0.43
2:C:818:GLU:OE2	2:C:822:ARG:NH1	2.51	0.43
3:D:114:LEU:HD23	3:D:114:LEU:HA	1.81	0.43
2:C:230:ARG:NH1	7:G:8:DC:OP1	2.52	0.43
3:D:890:ASP:OD1	3:D:963:ARG:NH2	2.51	0.43
6:H:22:DT:H1'	6:H:23:DG:H5'	2.00	0.43
2:C:315:LYS:HA	2:C:315:LYS:HD2	1.79	0.42
2:C:515:PRO:HB2	2:C:581:VAL:HG21	2.00	0.42
2:C:731:TYR:CE1	3:D:579:LEU:HB2	2.54	0.42
3:D:836:VAL:HG13	3:D:848:GLU:CD	2.44	0.42
5:F:210:GLU:O	5:F:214:GLN:HG2	2.18	0.42
1:B:39:ARG:HH21	1:B:173:LYS:NZ	2.18	0.42
1:B:92:PRO:HB3	1:B:141:GLU:HG2	2.02	0.42
1:B:110:ILE:O	1:B:112:PRO:HD3	2.19	0.42
2:C:40:SER:HB2	2:C:973:SER:HB2	2.00	0.42
3:D:106:TYR:CD2	3:D:312:MET:HG2	2.54	0.42
2:C:596:PHE:HB3	2:C:599:HIS:HD2	1.85	0.42
2:C:824:ILE:HG12	5:F:514:LEU:HD13	2.02	0.42
2:C:313:ARG:HH22	2:C:337:ASP:CG	2.27	0.42
2:C:540:VAL:HG13	2:C:561:VAL:HG13	2.02	0.42
2:C:730:ASN:HB3	2:C:736:ILE:HG13	2.02	0.42
2:C:737:LEU:HD22	2:C:741:LEU:HD12	2.02	0.42
2:C:1011:PHE:HA	2:C:1018:PRO:HA	2.00	0.42
3:D:117:LEU:HD12	3:D:299:VAL:HG22	2.02	0.42
2:C:1051:MET:HA	5:F:441:ASP:HB2	2.01	0.42
5:F:303:VAL:HG22	5:F:351:ILE:HD13	2.01	0.42
5:F:422:SER:O	5:F:425:GLN:HG2	2.19	0.42
2:C:809:LYS:HD2	2:C:833:ARG:HD3	2.01	0.42
3:D:278:ARG:O	3:D:282:ARG:HG2	2.20	0.42
3:D:1224:ALA:HB1	3:D:1229:THR:HG23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:183:VAL:HG12	1:B:184:GLU:HG2	2.02	0.42
3:D:1244:LYS:O	3:D:1246:ASN:N	2.52	0.42
3:D:176:LYS:NZ	3:D:180:ASP:OD2	2.52	0.42
6:H:19:DG:H2''	6:H:20:DG:C8	2.55	0.42
2:C:476:HIS:CD2	2:C:477:PRO:HD2	2.55	0.42
3:D:144:ARG:HG3	3:D:226:PHE:CZ	2.54	0.42
3:D:733:MET:HE2	3:D:733:MET:HB3	1.95	0.42
3:D:899:VAL:HG11	3:D:920:ALA:HB2	2.02	0.42
5:F:320:LEU:HD21	5:F:359:MET:HE3	2.02	0.42
2:C:472:VAL:HG22	6:H:14:DG:N2	2.34	0.41
3:D:740:PRO:HD3	3:D:792:HIS:ND1	2.34	0.41
3:D:760:PHE:CG	3:D:770:ARG:HD2	2.55	0.41
2:C:687:CYS:HA	2:C:688:PRO:HD3	1.91	0.41
2:C:958:ARG:N	2:C:958:ARG:HD2	2.34	0.41
3:D:103:HIS:CE1	3:D:105:TRP:HB2	2.54	0.41
4:E:40:ILE:O	4:E:44:LEU:HG	2.20	0.41
5:F:345:THR:HA	6:H:5:DA:N7	2.35	0.41
1:B:133:LYS:NZ	1:B:135:GLU:OE2	2.47	0.41
2:C:463:LEU:HD13	2:C:468:ALA:HB2	2.01	0.41
2:C:600:ASP:OD2	2:C:889:HIS:ND1	2.32	0.41
2:C:822:ARG:NE	2:C:829:ALA:HB2	2.36	0.41
3:D:1065:THR:HG23	3:D:1076:VAL:HB	2.03	0.41
5:F:298:ALA:C	5:F:300:LEU:H	2.28	0.41
5:F:429:ASP:N	5:F:429:ASP:OD1	2.53	0.41
2:C:48:LEU:HD12	2:C:528:ILE:HD13	2.02	0.41
2:C:239:LYS:NZ	2:C:265:ASP:OD2	2.52	0.41
3:D:400:LYS:HD3	3:D:400:LYS:HA	1.87	0.41
3:D:895:ARG:NH1	3:D:967:THR:O	2.53	0.41
2:C:427:ILE:H	2:C:427:ILE:HG13	1.72	0.41
3:D:356:ARG:HH21	3:D:360:LEU:HD11	1.84	0.41
3:D:737:LEU:N	3:D:793:TYR:OH	2.41	0.41
2:C:229:LYS:HA	2:C:229:LYS:HD3	1.91	0.41
2:C:723:ILE:O	3:D:730:THR:HG23	2.20	0.41
3:D:343:LEU:HD23	3:D:343:LEU:HA	1.94	0.41
1:A:100:GLN:HG2	1:A:101:GLY:H	1.86	0.41
1:A:129:ASN:HD21	2:C:652:GLU:HG3	1.85	0.41
2:C:642:VAL:HB	2:C:703:ALA:HB3	2.03	0.41
3:D:392:THR:HB	3:D:396:ASN:HA	2.02	0.41
6:H:15:DT:C2'	6:H:16:DC:H5'	2.50	0.41
1:B:173:LYS:HE2	3:D:619:ILE:HD13	2.02	0.41
1:B:191:LYS:HE2	1:B:193:ILE:HD11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:69:ARG:HE	5:F:485:GLN:CB	2.34	0.41
3:D:1055:LEU:HD12	3:D:1100:SER:HA	2.03	0.41
3:D:1061:PHE:CE2	3:D:1078:ASP:HB3	2.55	0.41
3:D:1176:LEU:H	3:D:1176:LEU:HD12	1.85	0.41
5:F:485:GLN:HA	5:F:486:PRO:HD3	1.98	0.41
5:F:515:ARG:HA	5:F:518:SER:HB3	2.02	0.41
2:C:421:ARG:HB3	2:C:422:PRO:HD3	2.03	0.41
2:C:1080:GLY:HA3	4:E:51:TYR:HE1	1.85	0.41
2:C:1112:ILE:HG13	3:D:548:SER:HA	2.03	0.41
3:D:486:VAL:O	3:D:490:VAL:HG23	2.21	0.41
3:D:580:ASP:HB2	3:D:721:PHE:CE1	2.56	0.41
5:F:235:ILE:HG23	5:F:300:LEU:HB3	2.02	0.41
5:F:502:ARG:HA	5:F:502:ARG:HD3	1.93	0.41
1:A:61:HIS:HB2	2:C:846:LYS:HD3	2.03	0.40
1:A:214:THR:OG1	1:B:230:GLU:OE1	2.33	0.40
1:B:147:VAL:HA	1:B:148:PRO:HD3	1.91	0.40
2:C:568:VAL:HG21	3:D:847:LEU:HD23	2.03	0.40
3:D:104:ILE:HB	3:D:379:ASP:OD1	2.22	0.40
3:D:1139:GLN:O	3:D:1143:ARG:HG2	2.20	0.40
3:D:1208:MET:HE3	3:D:1208:MET:HB2	1.93	0.40
1:B:55:ARG:HB2	1:B:137:GLU:HB3	2.01	0.40
2:C:102:SER:O	2:C:141:ASN:ND2	2.52	0.40
2:C:232:GLN:OE1	2:C:280:LYS:HG3	2.20	0.40
2:C:650:ILE:HB	2:C:693:GLY:H	1.87	0.40
2:C:735:ILE:O	2:C:896:GLY:N	2.49	0.40
3:D:567:SER:HB2	3:D:574:LEU:HD11	2.02	0.40
3:D:584:GLY:O	3:D:587:TYR:HB3	2.22	0.40
1:A:146:TYR:CD2	2:C:743:GLU:HG2	2.56	0.40
2:C:658:ILE:HG13	2:C:672:MET:HE3	2.03	0.40
1:B:42:LEU:HD23	1:B:211:ALA:HB2	2.03	0.40
3:D:54:PRO:HG3	3:D:81:GLU:O	2.22	0.40
3:D:125:LEU:O	3:D:129:ILE:HG13	2.22	0.40
5:F:474:VAL:HA	5:F:477:LEU:HB2	2.03	0.40
2:C:117:ALA:HA	2:C:118:PRO:HD3	1.98	0.40
2:C:355:MET:HB3	2:C:355:MET:HE2	1.90	0.40
3:D:69:ARG:HH21	5:F:485:GLN:HB2	1.86	0.40
3:D:666:THR:HG21	3:D:683:PHE:CE2	2.56	0.40
5:F:378:LYS:HD3	5:F:381:ARG:HH11	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	209 (94%)	12 (5%)	1 (0%)	24	59
1	B	221/347 (64%)	202 (91%)	17 (8%)	2 (1%)	14	47
2	C	1124/1178 (95%)	1054 (94%)	64 (6%)	6 (0%)	24	59
3	D	1261/1316 (96%)	1191 (94%)	64 (5%)	6 (0%)	24	59
4	E	79/110 (72%)	76 (96%)	3 (4%)	0	100	100
5	F	320/528 (61%)	302 (94%)	16 (5%)	2 (1%)	21	55
All	All	3227/3826 (84%)	3034 (94%)	176 (6%)	17 (0%)	24	59

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	678	PRO
3	D	971	SER
1	A	184	GLU
1	B	35	GLY
2	C	33	PRO
2	C	34	GLY
3	D	593	PRO
1	B	158	GLU
2	C	47	PRO
2	C	508	PRO
2	C	922	VAL
3	D	607	PRO
3	D	658	PRO
2	C	32	VAL
3	D	1007	GLY
5	F	405	ILE
5	F	497	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%)	188 (98%)	4 (2%)	47	64
1	B	191/297 (64%)	191 (100%)	0	100	100
2	C	948/998 (95%)	924 (98%)	24 (2%)	42	62
3	D	1048/1095 (96%)	1015 (97%)	33 (3%)	35	57
4	E	68/90 (76%)	66 (97%)	2 (3%)	37	58
5	F	271/427 (64%)	261 (96%)	10 (4%)	30	54
All	All	2718/3204 (85%)	2645 (97%)	73 (3%)	39	60

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	82	SER
1	A	136	VAL
1	A	159	ILE
1	A	225	LEU
2	C	39	VAL
2	C	44	LEU
2	C	48	LEU
2	C	80	VAL
2	C	185	VAL
2	C	322	LEU
2	C	332	THR
2	C	354	THR
2	C	373	PHE
2	C	379	ARG
2	C	427	ILE
2	C	447	SER
2	C	506	VAL
2	C	540	VAL
2	C	649	VAL
2	C	691	ASP
2	C	708	THR
2	C	850	ILE

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Mol	Chain	Res	Type
2	C	875	GLN
2	C	928	ILE
2	C	961	ASP
2	C	1002	VAL
2	C	1079	TYR
2	C	1137	VAL
3	D	16	THR
3	D	60	CYS
3	D	76	GLU
3	D	82	VAL
3	D	83	THR
3	D	101	VAL
3	D	261	ILE
3	D	317	VAL
3	D	491	ILE
3	D	505	HIS
3	D	582	VAL
3	D	583	THR
3	D	589	THR
3	D	629	VAL
3	D	676	LEU
3	D	684	VAL
3	D	713	VAL
3	D	714	ASP
3	D	810	ASN
3	D	862	ASP
3	D	901	LEU
3	D	910	LEU
3	D	921	TYR
3	D	930	VAL
3	D	968	CYS
3	D	975	CYS
3	D	978	CYS
3	D	989	VAL
3	D	1009	GLN
3	D	1098	VAL
3	D	1107	VAL
3	D	1138	VAL
3	D	1194	VAL
4	E	48	SER
4	E	75	ILE
5	F	233	LYS

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Mol	Chain	Res	Type
5	F	251	LYS
5	F	269	ARG
5	F	271	GLU
5	F	285	CYS
5	F	306	LEU
5	F	361	ASP
5	F	367	ARG
5	F	448	VAL
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	A	5	GLN
1	B	226	ASN
2	C	37	ASN
2	C	200	HIS
2	C	232	GLN
2	C	539	HIS
2	C	543	GLN
2	C	610	ASN
2	C	612	GLN
3	D	303	GLN
3	D	368	ASN
3	D	499	ASN
3	D	1109	GLN
3	D	1119	HIS
3	D	1153	HIS
4	E	70	GLN
5	F	415	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	I	1/2 (50%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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
9	RFP	C	1201	-	63,63,63	2.69	12 (19%)	94,94,94	2.25	21 (22%)

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
9	RFP	C	1201	-	-	24/60/85/85	0/5/5/5

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	1201	RFP	O4-C11	12.22	1.40	1.21
9	C	1201	RFP	C43-N2	8.17	1.49	1.27
9	C	1201	RFP	C17-C16	7.56	1.55	1.34
9	C	1201	RFP	C15-N1	5.30	1.46	1.35
9	C	1201	RFP	O7-C25	-5.14	1.37	1.44
9	C	1201	RFP	C3-C43	4.74	1.56	1.46
9	C	1201	RFP	C12-C11	-3.68	1.40	1.54
9	C	1201	RFP	C18-C17	3.45	1.53	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	1201	RFP	C6-C7	3.17	1.45	1.39
9	C	1201	RFP	C29-C28	2.17	1.41	1.30
9	C	1201	RFP	O9-C23	-2.08	1.37	1.43
9	C	1201	RFP	O3-C6	2.01	1.41	1.37

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	C	1201	RFP	C43-N2-N3	-8.22	108.81	120.55
9	C	1201	RFP	C2-C3-C43	-7.51	116.02	123.99
9	C	1201	RFP	C30-C16-C17	-7.42	105.64	123.67
9	C	1201	RFP	C38-N4-C42	6.33	122.70	110.63
9	C	1201	RFP	O3-C6-C7	5.34	130.22	121.16
9	C	1201	RFP	O7-C35-C36	4.63	119.34	111.09
9	C	1201	RFP	O4-C11-C5	-4.61	123.14	131.63
9	C	1201	RFP	C23-C24-C25	4.15	118.51	110.58
9	C	1201	RFP	C37-O6-C27	3.61	121.25	112.99
9	C	1201	RFP	C12-O5-C29	3.27	125.89	117.84
9	C	1201	RFP	C20-C19-C18	-3.10	119.70	126.11
9	C	1201	RFP	C5-C10-C4	-3.05	121.11	124.08
9	C	1201	RFP	C4-C3-C43	3.00	120.48	116.63
9	C	1201	RFP	C33-C24-C25	-2.99	106.14	111.40
9	C	1201	RFP	C25-O7-C35	2.93	122.27	117.72
9	C	1201	RFP	O5-C12-C13	2.65	113.85	106.98
9	C	1201	RFP	C3-C43-N2	-2.43	117.61	121.58
9	C	1201	RFP	C25-C26-C27	2.43	118.60	111.99
9	C	1201	RFP	C3-C2-C1	2.27	122.30	120.68
9	C	1201	RFP	C5-C6-C7	-2.23	119.90	125.29
9	C	1201	RFP	C34-C26-C27	-2.16	106.58	110.95

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	C	1201	RFP	C4-C3-C43-N2
9	C	1201	RFP	C26-C27-C28-C29
9	C	1201	RFP	O6-C27-C28-C29
9	C	1201	RFP	C43-N2-N3-C40
9	C	1201	RFP	C3-C43-N2-N3
9	C	1201	RFP	C16-C17-C18-C19
9	C	1201	RFP	C18-C19-C20-C31
9	C	1201	RFP	C28-C27-O6-C37

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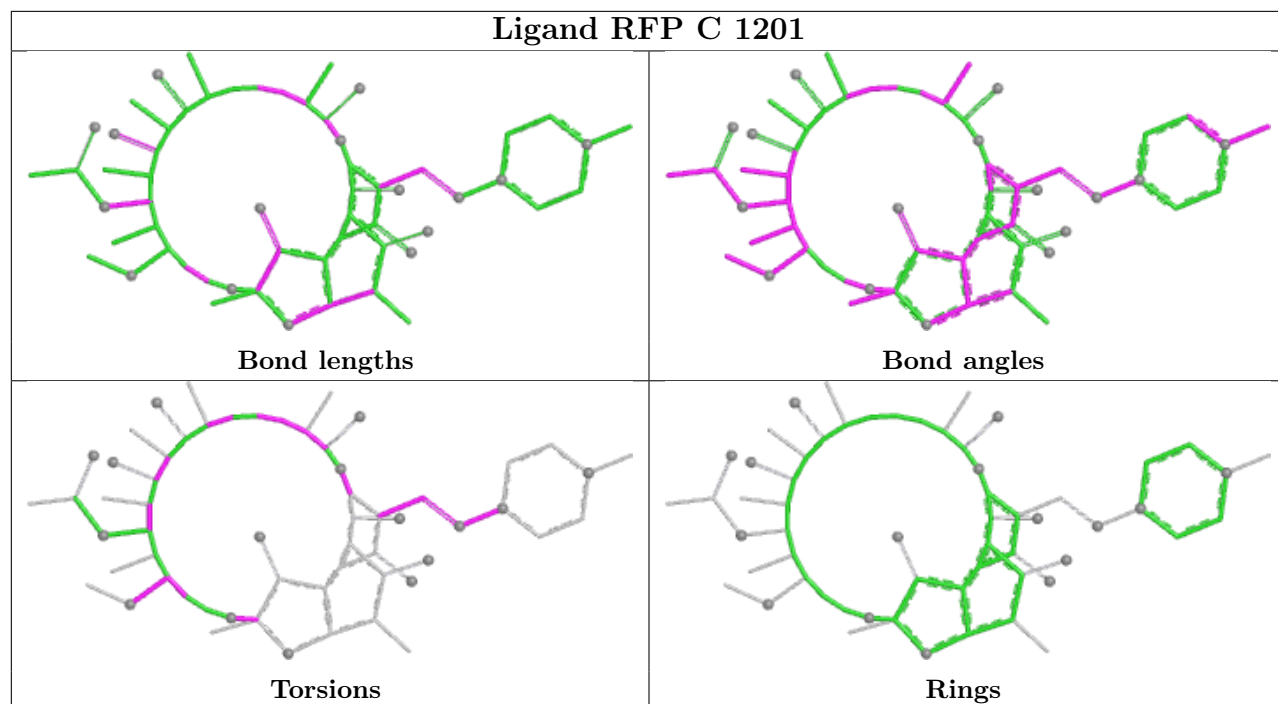
Mol	Chain	Res	Type	Atoms
9	C	1201	RFP	C15-C16-C17-C18
9	C	1201	RFP	C33-C24-C25-C26
9	C	1201	RFP	C32-C22-C23-C24
9	C	1201	RFP	C32-C22-C23-O9
9	C	1201	RFP	N1-C15-C16-C17
9	C	1201	RFP	O11-C15-C16-C17
9	C	1201	RFP	C21-C22-C23-C24
9	C	1201	RFP	C26-C27-O6-C37
9	C	1201	RFP	C23-C24-C25-O7
9	C	1201	RFP	C23-C24-C25-C26
9	C	1201	RFP	C18-C19-C20-C21
9	C	1201	RFP	C2-C3-C43-N2
9	C	1201	RFP	C11-C12-O5-C29
9	C	1201	RFP	O3-C12-O5-C29
9	C	1201	RFP	C33-C24-C25-O7
9	C	1201	RFP	C3-C2-N1-C15

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	C	1201	RFP	4	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 [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	224/347 (64%)	0.38	7 (3%) 51 35	18, 62, 126, 153	0
1	B	225/347 (64%)	0.88	11 (4%) 35 27	57, 100, 147, 171	0
2	C	1126/1178 (95%)	0.17	19 (1%) 69 48	6, 43, 126, 146	0
3	D	1265/1316 (96%)	0.10	11 (0%) 81 61	7, 42, 111, 148	0
4	E	81/110 (73%)	0.17	1 (1%) 76 55	24, 50, 89, 111	0
5	F	322/528 (60%)	0.60	25 (7%) 19 18	11, 69, 170, 191	0
6	H	23/23 (100%)	1.04	4 (17%) 4 6	30, 93, 174, 245	0
7	G	15/16 (93%)	1.22	3 (20%) 3 5	27, 64, 188, 197	0
8	I	2/2 (100%)	0.05	0 100 100	40, 40, 40, 51	0
All	All	3283/3867 (84%)	0.26	81 (2%) 58 40	6, 50, 130, 245	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	F	503	ILE	5.4
1	B	154	ALA	4.9
7	G	6	DA	4.1
2	C	402	GLU	3.9
7	G	5	DC	3.8
1	B	150	VAL	3.7
5	F	474	VAL	3.6
5	F	475	VAL	3.6
1	A	152	ASN	3.6
5	F	389	ASP	3.4
1	A	90	ASP	3.4
5	F	481	LEU	3.4
1	B	207	ALA	3.2
3	D	903	GLU	3.1
1	B	140	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
3	D	464	ASN	3.1
5	F	464	LEU	3.0
5	F	489	LEU	3.0
3	D	610	GLY	3.0
5	F	275	ALA	3.0
3	D	4	VAL	2.9
1	A	222	ALA	2.9
5	F	477	LEU	2.9
2	C	235	THR	2.9
2	C	304	LYS	2.8
6	H	19	DG	2.8
2	C	820	LEU	2.8
5	F	465	ASP	2.8
2	C	284	GLY	2.8
1	B	159	ILE	2.8
5	F	427	ILE	2.7
3	D	1078	ASP	2.7
1	B	51	VAL	2.7
5	F	309	ARG	2.6
1	B	151	GLN	2.6
2	C	1152	ASP	2.6
2	C	406	THR	2.6
3	D	1281	ALA	2.6
6	H	23	DG	2.6
2	C	252	PHE	2.5
7	G	19	DG	2.5
5	F	258	TYR	2.5
2	C	409	VAL	2.5
5	F	405	ILE	2.5
3	D	1280	ALA	2.4
5	F	222	THR	2.4
2	C	268	VAL	2.4
5	F	428	GLY	2.3
1	B	62	GLU	2.3
2	C	217	ASP	2.3
3	D	204	GLU	2.3
5	F	210	GLU	2.3
2	C	287	PRO	2.2
3	D	1102	GLY	2.2
1	A	151	GLN	2.2
2	C	237	LEU	2.2
1	A	3	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
5	F	382	ILE	2.2
5	F	472	ALA	2.2
2	C	824	ILE	2.2
1	A	183	VAL	2.2
5	F	308	LYS	2.2
2	C	296	LEU	2.2
3	D	663	MET	2.1
5	F	429	ASP	2.1
3	D	184	LEU	2.1
1	B	58	GLY	2.1
2	C	219	ARG	2.1
1	B	136	VAL	2.1
2	C	961	ASP	2.1
5	F	207	ASP	2.1
5	F	460	LEU	2.1
1	A	220	GLY	2.1
5	F	404	ASP	2.1
1	B	227	VAL	2.1
4	E	76	LEU	2.1
5	F	514	LEU	2.0
6	H	12	DC	2.0
6	H	18	DC	2.0
2	C	193	LYS	2.0
2	C	31	SER	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](#)

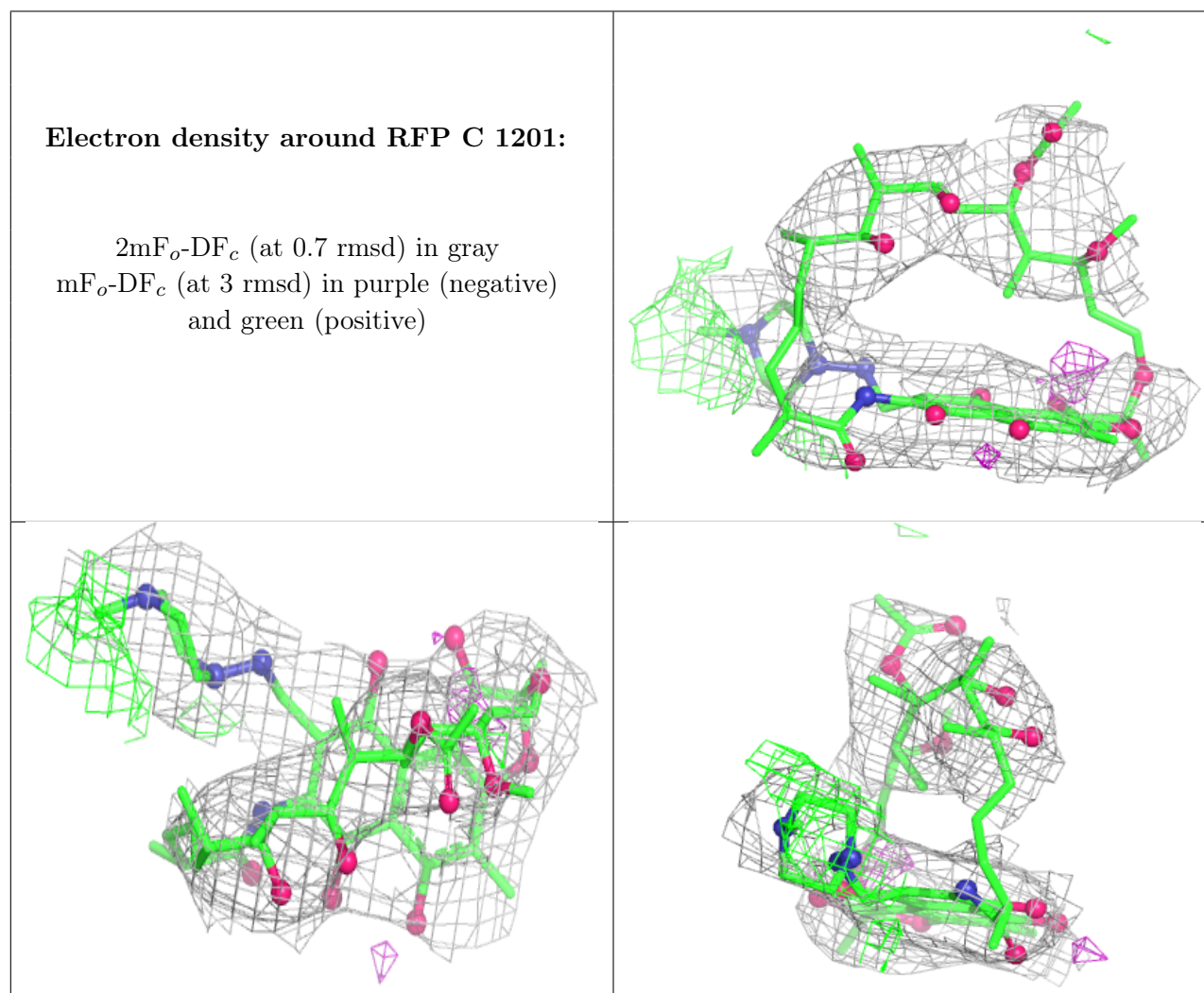
There are no oligosaccharides in this entry.

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($\text{\AA}^2$)	Q<0.9
9	RFP	C	1201	59/59	0.92	0.14	11,25,44,48	0
10	ZN	D	1401	1/1	0.98	0.06	48,48,48,48	0
10	ZN	D	1402	1/1	1.00	0.04	34,34,34,34	0
11	MG	D	1403	1/1	1.00	0.04	18,18,18,18	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 ⓘ

There are no such residues in this entry.