Full wwPDB X-ray Structure Validation Report (i)

Jun 25, 2024 – 06:39 PM EDT

PDB ID	:	5UHG
Title	:	Crystal structure of Mycobacterium tuberculosis transcription initiation complex in complex with D-AAP1 and Rifampin
Authors	:	Lin, W.; Das, K.; Feng, Y.; Ebright, R.H.
Deposited on	:	2017-01-11
Resolution	:	3.97 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

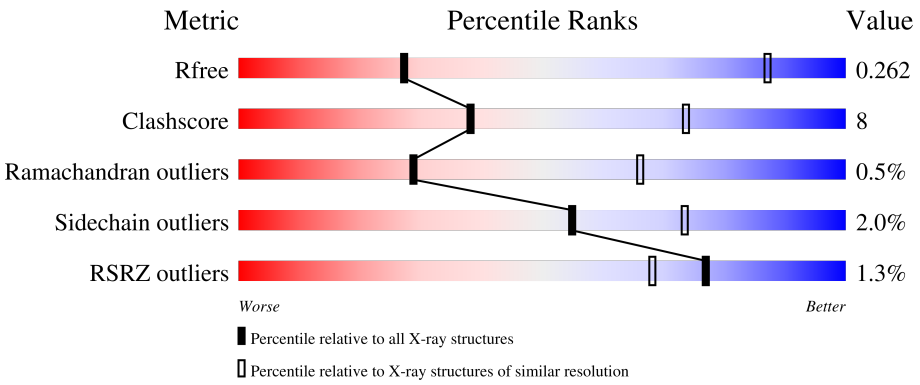
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.97 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	1039 (4.26-3.70)
Clashscore	141614	1099 (4.26-3.70)
Ramachandran outliers	138981	1061 (4.26-3.70)
Sidechain outliers	138945	1053 (4.26-3.70)
RSRZ outliers	127900	1021 (4.30-3.66)

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	% 55% 9% 35%
1	B	347	3% 52% 14% 35%
2	C	1178	77% 18% •
3	D	1316	75% 20% • •
4	E	110	57% 15% • 26%

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Mol	Chain	Length	Quality of chain
5	F	528	3% 48% 13% 39%
6	H	23	35% 61%
7	G	16	25% 50% 25% 25%

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 26004 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
			Total	C	N	O	S			
1	A	224	1704	1072	295	335	2	0	0	0
1	B	227	1715	1080	291	342	2	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	1126	8714	5454	1528	1693	39	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	D	1265	9887	6188	1793	1866	40	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	E	81	637	408	106	123	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	F	321	2541	1582	457	493	9	0	0	0

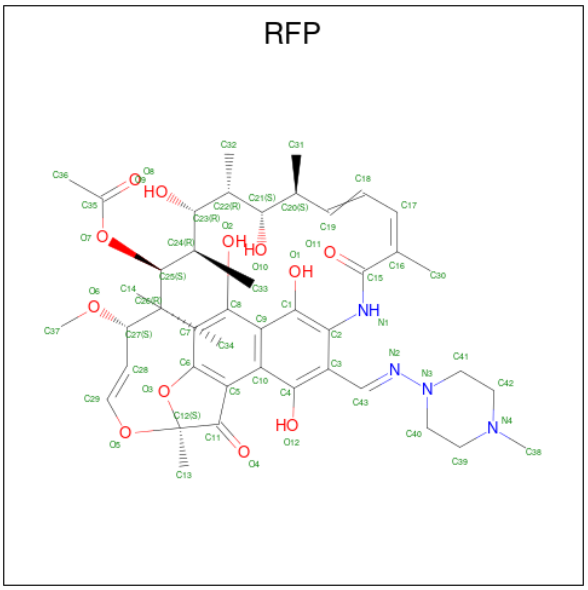
- Molecule 6 is a DNA chain called DNA (5'-D(*TP*AP*TP*AP*AP*TP*GP*GP*GP*AP*GP*CP*TP*GP*TP*CP*AP*CP*GP*GP*AP*TP*G)-3').

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

- 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
			Total	C	N	O	P			
7	G	12	241	116	43	71	11	0	0	0

- Molecule 8 is RIFAMPICIN (three-letter code: RFP) (formula: $C_{43}H_{58}N_4O_{12}$).



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

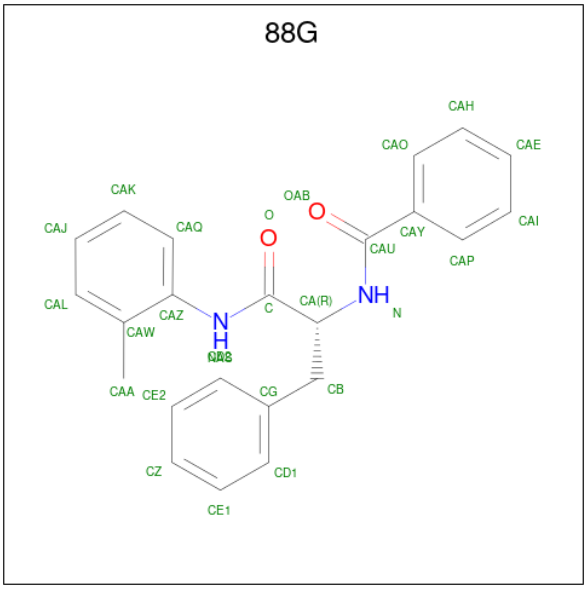
- Molecule 9 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 10 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 11 is Nalpha-(benzenecarbonyl)-N-(2-methylphenyl)-D-phenylalaninamide (three-letter code: 88G) (formula: $C_{23}H_{22}N_2O_2$).



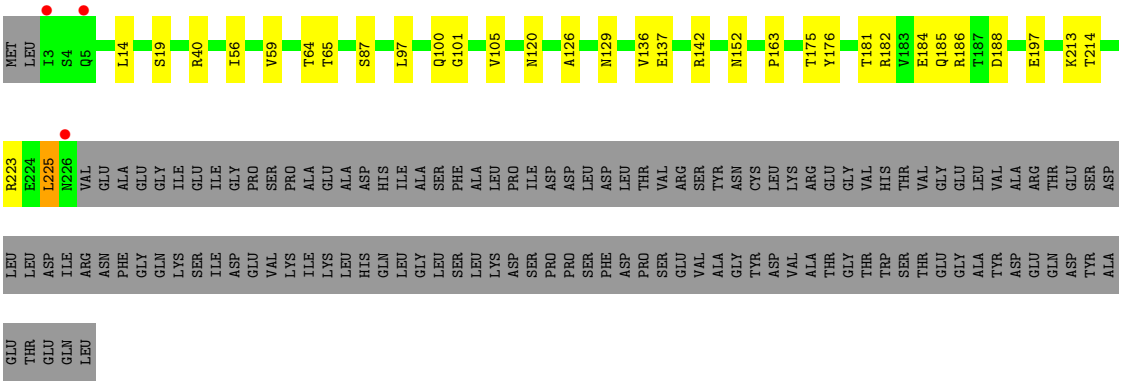
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
11	D	1	27	23	2	2	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

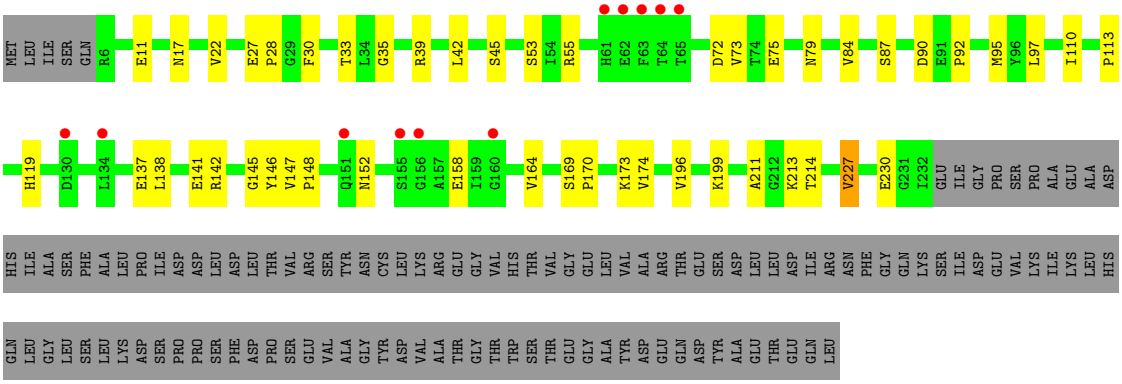
• Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain A:



• Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain B:

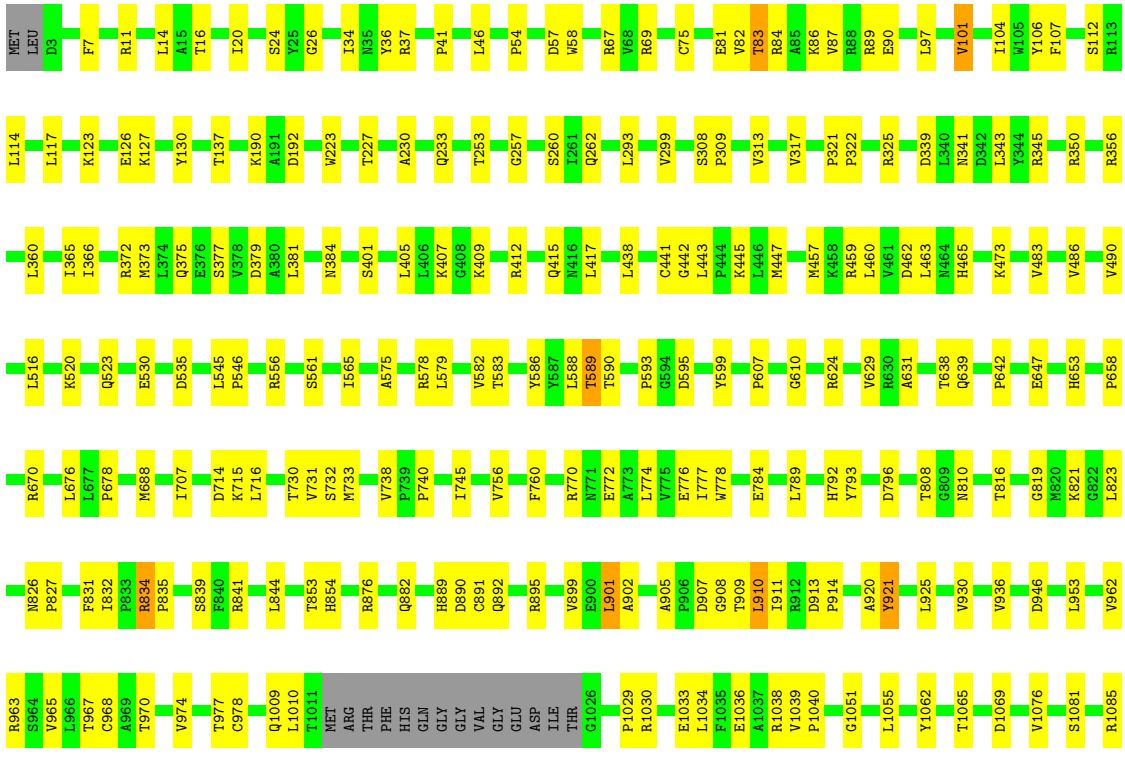


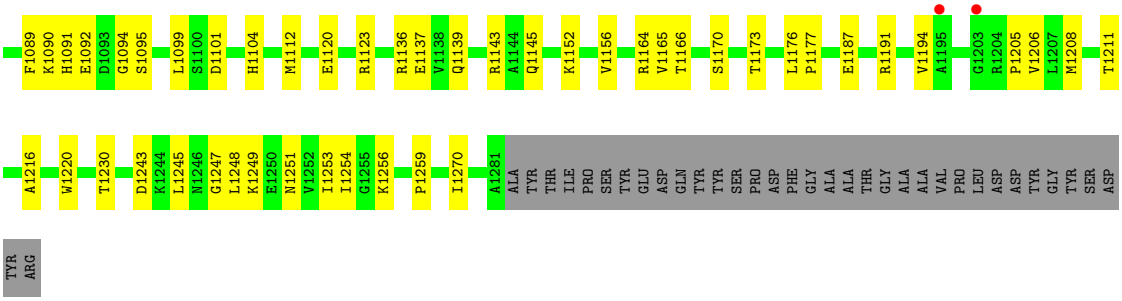
• Molecule 2: DNA-directed RNA polymerase subunit beta

Chain C:

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

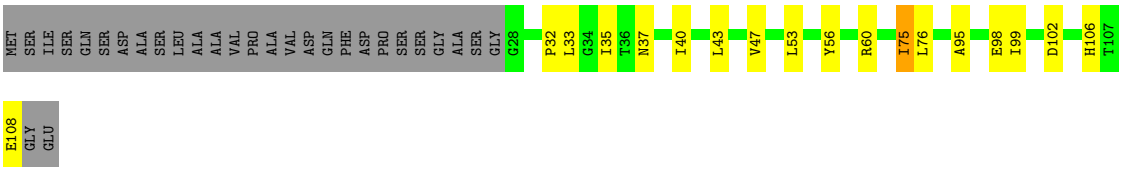
Chain D:





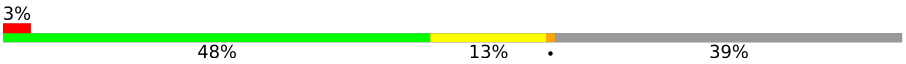
• Molecule 4: DNA-directed RNA polymerase subunit omega

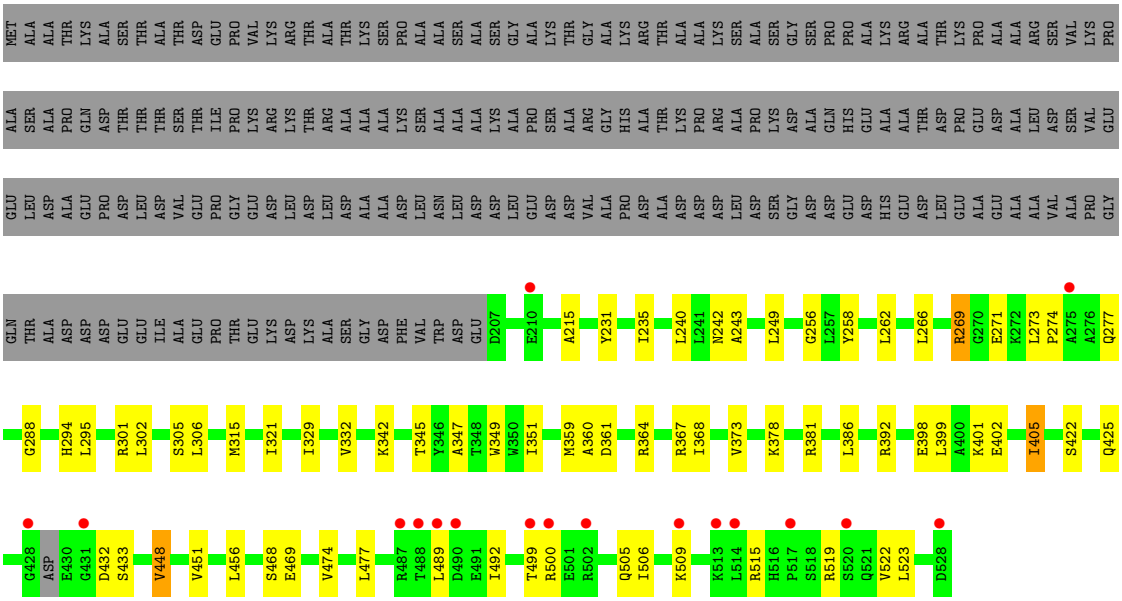
Chain E:



• Molecule 5: RNA polymerase sigma factor SigA

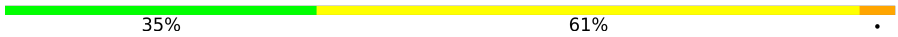
Chain F:

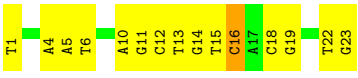




• Molecule 6: DNA (5'-D(*TP*AP*TP*AP*AP*TP*GP*GP*GP*AP*GP*CP*TP*GP*TP*CP *AP*CP*GP*GP*AP*TP*G)-3')

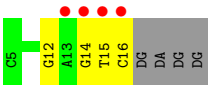
Chain H:





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

Chain G:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	151.43Å 162.15Å 194.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.24 – 3.97 49.24 – 3.97	Depositor EDS
% Data completeness (in resolution range)	93.9 (49.24-3.97) 93.9 (49.24-3.97)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.85 (at 4.00Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.223 , 0.260 0.227 , 0.262	Depositor DCC
R_{free} test set	2016 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å^2)	40.7	Xtriage
Anisotropy	0.301	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , -22.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.82	EDS
Total number of atoms	26004	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.94% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 88G, MG, RFP

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	0.22	0/1730	0.45	0/2354
1	B	0.22	0/1741	0.44	0/2371
2	C	0.24	0/8873	0.42	1/12031 (0.0%)
3	D	0.24	0/10052	0.42	0/13591
4	E	0.31	0/650	0.44	0/886
5	F	0.23	0/2570	0.39	0/3464
6	H	0.52	0/535	0.92	1/826 (0.1%)
7	G	0.48	0/269	0.90	0/413
All	All	0.25	0/26420	0.45	2/35936 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	H	16	DC	P-O3'-C3'	6.80	127.86	119.70
2	C	48	LEU	CA-CB-CG	5.32	127.55	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1704	0	1741	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1715	0	1739	30	0
2	C	8714	0	8636	131	0
3	D	9887	0	9943	161	0
4	E	637	0	635	13	0
5	F	2541	0	2563	46	0
6	H	476	0	261	20	0
7	G	241	0	137	6	0
8	C	59	0	58	10	0
9	D	2	0	0	0	0
10	D	1	0	0	0	0
11	D	27	0	0	0	0
All	All	26004	0	25713	392	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 (392) 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:OD2	3:D:914:PRO:HD2	1.35	1.24
6:H:16:DC:N3	7:G:12:DG:N1	2.17	0.91
3:D:908:GLY:O	3:D:909:THR:OG1	1.91	0.88
6:H:16:DC:O2	7:G:12:DG:N2	2.15	0.79
3:D:905:ALA:HB3	3:D:908:GLY:O	1.83	0.78
3:D:907:ASP:OD1	3:D:908:GLY:N	2.15	0.78
2:C:305:ARG:HH12	6:H:10:DA:H62	1.31	0.77
3:D:913:ASP:OD2	3:D:914:PRO:CD	2.27	0.76
3:D:902:ALA:HB1	3:D:911:ILE:O	1.86	0.75
3:D:530:GLU:HB2	3:D:578:ARG:HD2	1.67	0.75
8:C:1201:RFP:HN1	8:C:1201:RFP:H18C	1.52	0.74
5:F:256:GLY:HA3	5:F:288:GLY:HA3	1.69	0.74
3:D:891:CYS:SG	3:D:970:THR:OG1	2.46	0.73
3:D:910:LEU:HD21	3:D:953:LEU:O	1.89	0.73
3:D:1090:LYS:HB3	3:D:1092:GLU:HG2	1.71	0.72
3:D:901:LEU:HD13	3:D:901:LEU:O	1.90	0.71
3:D:107:PHE:HZ	3:D:126:GLU:HG2	1.56	0.70
2:C:113:ASP:HB2	2:C:132:PRO:HG2	1.74	0.70
3:D:910:LEU:HD12	3:D:910:LEU:O	1.92	0.69
3:D:826:ASN:HD22	3:D:832:ILE:HD11	1.56	0.69
2:C:1024:THR:H	3:D:730:THR:HG21	1.57	0.69
6:H:16:DC:N4	7:G:12:DG:O6	2.20	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:279:ARG:HD3	5:F:215:ALA:HB1	1.75	0.69
2:C:658:ILE:HD11	2:C:688:PRO:HB3	1.75	0.69
2:C:168:ILE:HG12	2:C:431:PHE:HB3	1.73	0.68
2:C:1148:ARG:NH1	3:D:86:LYS:O	2.26	0.68
2:C:101:GLY:O	2:C:142:ASN:ND2	2.28	0.67
2:C:189:GLU:HB2	2:C:367:THR:HG21	1.77	0.67
3:D:1030:ARG:HH21	3:D:1137:GLU:HG2	1.59	0.65
2:C:48:LEU:HD12	2:C:528:ILE:HD13	1.77	0.65
5:F:401:LYS:HA	5:F:405:ILE:HA	1.78	0.65
3:D:899:VAL:HG11	3:D:920:ALA:HB2	1.79	0.65
3:D:638:THR:HG23	3:D:639:GLN:HG2	1.79	0.64
5:F:522:VAL:HG23	5:F:523:LEU:HD12	1.78	0.64
3:D:930:VAL:HG22	3:D:936:VAL:HG12	1.81	0.63
1:B:75:GLU:O	1:B:79:ASN:ND2	2.31	0.62
3:D:1165:VAL:HG12	3:D:1205:PRO:HA	1.82	0.62
5:F:477:LEU:HD13	5:F:492:ILE:HG23	1.81	0.62
2:C:173:ARG:NH1	2:C:437:SER:O	2.32	0.62
1:B:170:PRO:HA	1:B:199:LYS:HD2	1.82	0.62
2:C:40:SER:HB2	2:C:973:SER:HB2	1.81	0.62
2:C:815:THR:HG22	2:C:817:GLU:H	1.64	0.61
3:D:104:ILE:HD12	3:D:379:ASP:HB3	1.82	0.61
1:A:197:GLU:OE1	2:C:996:ARG:NH1	2.31	0.61
3:D:293:LEU:HD21	3:D:1177:PRO:HG2	1.82	0.61
3:D:908:GLY:C	3:D:909:THR:HG1	1.99	0.60
1:A:87:SER:O	1:A:142:ARG:NH1	2.32	0.60
5:F:506:ILE:HA	5:F:509:LYS:HD2	1.83	0.60
2:C:587:VAL:HB	2:C:591:THR:HB	1.81	0.60
5:F:499:THR:OG1	5:F:500:ARG:N	2.34	0.60
3:D:1085:ARG:HA	3:D:1112:MET:HA	1.84	0.60
2:C:1122:LYS:HE2	2:C:1148:ARG:HG2	1.84	0.59
3:D:1092:GLU:HG3	3:D:1094:GLY:H	1.66	0.59
3:D:137:THR:OG1	3:D:253:THR:O	2.18	0.59
3:D:46:LEU:O	3:D:325:ARG:NH2	2.29	0.59
3:D:343:LEU:HD13	3:D:381:LEU:HA	1.84	0.59
3:D:373:MET:O	3:D:377:SER:OG	2.18	0.59
5:F:242:ASN:OD1	5:F:243:ALA:N	2.36	0.58
3:D:1069:ASP:OD2	3:D:1104:HIS:NE2	2.36	0.58
1:B:90:ASP:HA	1:B:142:ARG:HD3	1.86	0.58
1:B:27:GLU:HG3	1:B:28:PRO:HD2	1.85	0.58
6:H:15:DT:H2"	6:H:16:DC:H5'	1.85	0.58
1:B:42:LEU:HD23	1:B:211:ALA:HB2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:485:PRO:HB2	3:D:853:THR:HG21	1.86	0.58
1:B:42:LEU:HD23	1:B:211:ALA:CB	2.34	0.58
3:D:107:PHE:CZ	3:D:126:GLU:HG2	2.39	0.58
2:C:126:ASP:HA	2:C:170:GLY:HA3	1.85	0.58
3:D:262:GLN:HB2	3:D:313:VAL:HG11	1.84	0.58
3:D:190:LYS:HE3	3:D:192:ASP:HB3	1.85	0.57
2:C:919:THR:HG23	3:D:731:VAL:HG23	1.87	0.57
3:D:459:ARG:HA	3:D:462:ASP:HB2	1.85	0.57
3:D:442:GLY:HA3	3:D:523:GLN:HB2	1.86	0.57
4:E:47:VAL:HG11	4:E:53:LEU:HB2	1.87	0.57
3:D:1245:LEU:HD13	3:D:1254:ILE:HD13	1.87	0.57
1:B:27:GLU:HB3	1:B:30:PHE:HD2	1.70	0.56
2:C:239:LYS:NZ	2:C:265:ASP:OD2	2.38	0.56
2:C:211:TRP:NE1	6:H:13:DT:O2	2.39	0.56
1:B:146:TYR:O	3:D:624:ARG:NE	2.39	0.56
3:D:965:VAL:HG13	3:D:974:VAL:HG11	1.87	0.56
3:D:599:TYR:HA	3:D:610:GLY:HA3	1.88	0.56
2:C:959:LEU:HD12	2:C:960:PRO:HD2	1.88	0.55
1:A:152:ASN:HB3	1:A:163:PRO:HB3	1.88	0.55
2:C:441:ASP:HB2	2:C:451:HIS:HD2	1.71	0.55
8:C:1201:RFP:HN1	8:C:1201:RFP:C18	2.14	0.55
1:A:223:ARG:HD3	1:B:213:LYS:HB2	1.89	0.55
1:B:72:ASP:OD1	1:B:73:VAL:N	2.38	0.55
2:C:601:ASP:OD2	2:C:603:ASN:ND2	2.40	0.55
3:D:257:GLY:O	3:D:260:SER:OG	2.20	0.55
2:C:1125:LEU:HD22	2:C:1135:VAL:HG11	1.87	0.55
1:B:97:LEU:HD22	1:B:110:ILE:HG12	1.88	0.55
1:B:148:PRO:O	1:B:152:ASN:ND2	2.40	0.55
3:D:738:VAL:HG13	3:D:841:ARG:HD3	1.88	0.55
3:D:1089:PHE:HA	3:D:1095:SER:HA	1.89	0.55
3:D:901:LEU:HD13	3:D:901:LEU:C	2.28	0.54
2:C:789:ILE:HD12	2:C:869:VAL:HG11	1.90	0.54
1:B:84:VAL:HG12	1:B:199:LYS:HD3	1.89	0.54
2:C:47:PRO:HB2	2:C:581:VAL:HG13	1.89	0.54
2:C:41:PHE:HB2	2:C:979:GLY:HA2	1.90	0.54
3:D:1051:GLY:HA2	3:D:1069:ASP:HB2	1.88	0.54
2:C:756:GLU:HG3	2:C:870:ARG:HG2	1.90	0.54
3:D:1010:LEU:HD23	3:D:1145:GLN:HG3	1.90	0.54
3:D:595:ASP:HB3	3:D:631:ALA:HB2	1.91	0.53
3:D:24:SER:OG	3:D:26:GLY:O	2.25	0.53
2:C:544:ALA:HB2	2:C:580:ASP:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:182:SER:HB2	2:C:377:ARG:HB2	1.89	0.53
2:C:720:LEU:HD23	2:C:913:VAL:HA	1.90	0.53
3:D:745:ILE:HD13	3:D:784:GLU:HG2	1.91	0.53
3:D:123:LYS:HE3	3:D:127:LYS:HE2	1.91	0.53
3:D:1248:LEU:HD23	3:D:1259:PRO:HD2	1.91	0.53
2:C:561:VAL:HG21	2:C:571:VAL:HB	1.90	0.53
2:C:305:ARG:HH12	6:H:10:DA:N6	2.04	0.52
2:C:704:ASP:HB2	2:C:708:THR:HB	1.91	0.52
2:C:1042:HIS:HB2	2:C:1060:LYS:HG3	1.91	0.52
3:D:356:ARG:HH21	3:D:360:LEU:HD11	1.73	0.52
3:D:565:ILE:HG23	3:D:575:ALA:HB3	1.92	0.52
3:D:1055:LEU:HB2	3:D:1101:ASP:HB3	1.91	0.52
2:C:1041:ILE:HD12	3:D:520:LYS:HB3	1.91	0.52
3:D:921:TYR:HE1	3:D:946:ASP:HA	1.75	0.52
5:F:273:LEU:HD13	5:F:277:GLN:HB3	1.91	0.52
5:F:505:GLN:HG3	5:F:509:LYS:HE3	1.91	0.52
3:D:1090:LYS:HG2	3:D:1091:HIS:H	1.74	0.52
3:D:876:ARG:NH1	3:D:1036:GLU:OE2	2.42	0.52
3:D:1247:GLY:O	3:D:1251:ASN:ND2	2.42	0.52
4:E:56:TYR:HE2	4:E:99:ILE:HG12	1.74	0.52
2:C:348:LEU:HD13	2:C:365:VAL:HG12	1.91	0.52
3:D:589:THR:HG22	3:D:670:ARG:HG2	1.91	0.52
2:C:597:LEU:HD23	2:C:976:VAL:HG11	1.91	0.52
3:D:890:ASP:OD1	3:D:963:ARG:NH2	2.43	0.51
2:C:597:LEU:HB3	2:C:976:VAL:HG13	1.93	0.51
3:D:463:LEU:HB2	3:D:465:HIS:HD2	1.75	0.51
3:D:1170:SER:O	3:D:1173:THR:OG1	2.27	0.51
8:C:1201:RFP:O4	8:C:1201:RFP:O12	2.27	0.51
2:C:46:GLU:N	2:C:47:PRO:HD3	2.26	0.51
2:C:1119:GLU:OE2	3:D:89:ARG:NH2	2.44	0.51
3:D:417:LEU:HD22	3:D:1253:ILE:HG23	1.92	0.51
5:F:345:THR:HB	6:H:4:DA:H8	1.74	0.51
4:E:33:LEU:HD23	4:E:33:LEU:H	1.76	0.51
3:D:341:ASN:O	3:D:345:ARG:HB2	2.11	0.51
6:H:11:DG:H5"	6:H:12:DC:C4	2.46	0.51
3:D:1038:ARG:NH1	6:H:18:DC:O3'	2.44	0.50
5:F:360:ALA:HB1	5:F:373:VAL:HG21	1.93	0.50
2:C:211:TRP:HB2	2:C:227:ASP:HA	1.94	0.50
2:C:233:PRO:HB2	2:C:236:VAL:HG23	1.94	0.50
3:D:778:TRP:CD2	3:D:835:PRO:HG3	2.46	0.50
3:D:1220:TRP:NE1	3:D:1243:ASP:HB2	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:ASN:ND2	2:C:652:GLU:HG3	2.26	0.50
6:H:22:DT:H1'	6:H:23:DG:H5'	1.94	0.50
2:C:762:THR:HG23	2:C:764:LEU:H	1.76	0.50
3:D:445:LYS:HA	3:D:516:LEU:HD22	1.93	0.50
2:C:513:GLU:HB3	2:C:530:TYR:HB3	1.94	0.50
2:C:599:HIS:HB3	2:C:928:ILE:HD12	1.94	0.50
5:F:269:ARG:NH1	5:F:271:GLU:OE1	2.44	0.50
3:D:707:ILE:HD11	4:E:32:PRO:HB3	1.93	0.49
3:D:756:VAL:HG21	3:D:777:ILE:HD11	1.93	0.49
1:A:56:ILE:HB	1:A:59:VAL:HB	1.92	0.49
2:C:608:GLY:HA2	2:C:611:MET:HE2	1.94	0.49
2:C:909:ASP:N	2:C:909:ASP:OD1	2.45	0.49
2:C:1148:ARG:NH1	3:D:86:LYS:HG3	2.28	0.49
3:D:67:ARG:HG2	3:D:69:ARG:H	1.77	0.49
5:F:489:LEU:H	5:F:489:LEU:HD23	1.77	0.49
2:C:371:ASP:OD1	6:H:14:DG:N1	2.38	0.49
3:D:67:ARG:HD2	3:D:69:ARG:NE	2.27	0.49
5:F:392:ARG:NH1	5:F:398:GLU:OE2	2.45	0.49
3:D:1164:ARG:HD2	3:D:1208:MET:HE1	1.94	0.48
5:F:345:THR:HA	6:H:5:DA:N7	2.28	0.48
3:D:589:THR:HG21	3:D:688:MET:HG2	1.94	0.48
1:A:175:THR:OG1	1:A:176:TYR:N	2.45	0.48
2:C:150:GLN:HG2	2:C:414:PRO:HG2	1.95	0.48
2:C:444:ASN:H	2:C:447:SER:HB3	1.78	0.48
1:A:213:LYS:HD3	1:B:227:VAL:HG23	1.94	0.48
2:C:119:VAL:HG13	2:C:167:ILE:HD11	1.96	0.48
2:C:28:SER:N	2:C:962:GLU:OE1	2.46	0.48
4:E:60:ARG:NE	4:E:98:GLU:OE2	2.46	0.48
2:C:1136:GLU:OE1	3:D:11:ARG:NH1	2.46	0.48
5:F:499:THR:HG1	5:F:500:ARG:H	1.60	0.48
3:D:409:LYS:NZ	7:G:14:DG:OP1	2.30	0.47
3:D:895:ARG:NH1	3:D:967:THR:O	2.47	0.47
1:B:11:GLU:HB2	1:B:22:VAL:HB	1.96	0.47
5:F:240:LEU:HD21	5:F:301:ARG:HD2	1.96	0.47
1:A:14:LEU:HD23	1:A:19:SER:HB2	1.96	0.47
3:D:1029:PRO:O	3:D:1033:GLU:N	2.44	0.47
3:D:1065:THR:HG23	3:D:1076:VAL:HB	1.96	0.47
5:F:474:VAL:HA	5:F:477:LEU:HD12	1.95	0.47
1:A:136:VAL:HG12	1:A:137:GLU:H	1.79	0.47
1:A:185:GLN:HG2	1:A:186:ARG:H	1.80	0.47
5:F:432:ASP:OD1	5:F:433:SER:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:ASN:OD1	1:A:120:ASN:N	2.48	0.47
2:C:53:LEU:HD13	2:C:449:LEU:HD21	1.95	0.47
3:D:760:PHE:CG	3:D:770:ARG:HD2	2.50	0.47
5:F:231:TYR:CE2	5:F:235:ILE:HD11	2.50	0.47
2:C:758:ASP:N	2:C:758:ASP:OD1	2.48	0.47
5:F:274:PRO:HG2	5:F:277:GLN:HB2	1.97	0.47
1:B:174:VAL:HG22	1:B:196:VAL:HA	1.97	0.46
2:C:476:HIS:CG	2:C:477:PRO:HD2	2.50	0.46
5:F:474:VAL:HA	5:F:477:LEU:HB2	1.96	0.46
3:D:740:PRO:HD3	3:D:792:HIS:ND1	2.31	0.46
2:C:220:ASP:HB3	2:C:257:ILE:HG22	1.98	0.46
2:C:104:SER:HB3	2:C:140:ILE:HB	1.97	0.46
3:D:823:LEU:HD13	3:D:831:PHE:HB3	1.97	0.46
2:C:377:ARG:NH2	2:C:383:GLU:OE1	2.47	0.46
3:D:407:LYS:HE2	3:D:1230:THR:HG21	1.97	0.46
5:F:386:LEU:HD12	5:F:399:LEU:HD23	1.97	0.46
5:F:468:SER:OG	5:F:469:GLU:N	2.48	0.46
1:B:53:SER:HA	1:B:164:VAL:HG23	1.97	0.46
2:C:884:LYS:HE2	2:C:1033:LEU:HD12	1.98	0.46
3:D:457:MET:HB2	3:D:457:MET:HE2	1.66	0.46
3:D:925:LEU:HD12	3:D:962:VAL:HG12	1.98	0.46
7:G:15:DT:H2'	7:G:16:DC:C6	2.51	0.46
1:A:225:LEU:HD13	1:A:225:LEU:H	1.80	0.46
2:C:115:VAL:HG11	2:C:129:TYR:CE1	2.51	0.46
2:C:472:VAL:HG22	6:H:14:DG:C2	2.51	0.46
2:C:1020:PRO:HB2	2:C:1021:TYR:CD2	2.51	0.46
2:C:454:ARG:HH22	8:C:1201:RFP:C19	2.29	0.46
2:C:821:LEU:HD22	5:F:456:LEU:HD11	1.98	0.46
3:D:586:TYR:O	3:D:590:THR:OG1	2.33	0.46
2:C:497:ILE:HD13	8:C:1201:RFP:C1	2.45	0.45
8:C:1201:RFP:H28C	8:C:1201:RFP:C5	2.45	0.45
3:D:473:LYS:HD2	5:F:448:VAL:HG21	1.98	0.45
3:D:1120:GLU:HA	3:D:1123:ARG:HG2	1.99	0.45
2:C:524:VAL:HG21	2:C:548:ILE:HD13	1.97	0.45
2:C:653:VAL:HG12	2:C:692:ALA:HB2	1.97	0.45
3:D:405:LEU:O	3:D:412:ARG:N	2.50	0.45
3:D:774:LEU:HD23	3:D:777:ILE:HD12	1.98	0.45
3:D:816:THR:HG23	3:D:821:LYS:HA	1.98	0.45
4:E:75:ILE:HG22	4:E:76:LEU:H	1.81	0.45
3:D:882:GLN:OE1	3:D:1249:LYS:HB2	2.17	0.45
1:A:181:THR:O	1:A:188:ASP:HA	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:549:ASP:OD2	2:C:550:ALA:N	2.50	0.45
2:C:619:VAL:HG23	2:C:748:THR:O	2.17	0.45
3:D:1039:VAL:HA	3:D:1040:PRO:HD3	1.82	0.45
5:F:315:MET:HE1	5:F:359:MET:HA	1.97	0.45
5:F:249:LEU:HD11	5:F:294:HIS:ND1	2.31	0.45
1:B:45:SER:OG	1:B:214:THR:HG21	2.16	0.45
2:C:183:PRO:HB2	2:C:312:GLY:HA2	1.98	0.45
3:D:556:ARG:HG3	4:E:35:ILE:HG12	1.99	0.45
3:D:676:LEU:HD23	3:D:716:LEU:HD23	1.99	0.45
2:C:1102:VAL:HG13	2:C:1112:ILE:HD12	1.99	0.45
3:D:473:LYS:HZ3	5:F:448:VAL:HG11	1.82	0.45
5:F:477:LEU:HB3	5:F:492:ILE:HD13	1.99	0.45
2:C:818:GLU:OE2	2:C:822:ARG:NH1	2.49	0.45
3:D:789:LEU:HD22	3:D:793:TYR:CE2	2.52	0.45
4:E:95:ALA:O	4:E:99:ILE:HG13	2.17	0.45
5:F:349:TRP:HB3	6:H:1:DT:H4'	1.98	0.45
2:C:1107:VAL:HG21	5:F:451:VAL:HG11	1.99	0.44
3:D:223:TRP:O	3:D:227:THR:OG1	2.28	0.44
1:A:100:GLN:HG2	1:A:101:GLY:H	1.82	0.44
2:C:473:ARG:NH2	2:C:492:PRO:O	2.50	0.44
2:C:922:VAL:H	2:C:923:PRO:HD2	1.82	0.44
8:C:1201:RFP:H24C	8:C:1201:RFP:H342	1.70	0.44
5:F:262:LEU:O	5:F:266:LEU:HG	2.17	0.44
1:B:145:GLY:HA2	1:B:169:SER:HB2	1.98	0.44
2:C:253:GLY:HA2	2:C:259:ARG:HE	1.83	0.44
2:C:344:TYR:OH	2:C:365:VAL:HA	2.17	0.44
2:C:516:TYR:OH	2:C:562:ARG:NH1	2.51	0.44
2:C:1067:ARG:HD3	7:G:16:DC:OP1	2.18	0.44
1:B:27:GLU:HB3	1:B:30:PHE:CD2	2.51	0.44
2:C:454:ARG:HH22	8:C:1201:RFP:H19C	1.83	0.44
8:C:1201:RFP:H18C	8:C:1201:RFP:N1	2.25	0.44
3:D:130:TYR:OH	3:D:379:ASP:OD2	2.22	0.44
2:C:232:GLN:OE1	2:C:280:LYS:HG3	2.18	0.44
2:C:476:HIS:HB3	2:C:479:HIS:CE1	2.52	0.44
3:D:443:LEU:HD11	3:D:447:MET:HE2	1.98	0.44
4:E:32:PRO:HB2	4:E:37:ASN:HB2	2.00	0.44
3:D:1164:ARG:NH2	3:D:1216:ALA:O	2.50	0.44
3:D:1251:ASN:OD1	3:D:1256:LYS:HE2	2.18	0.44
5:F:378:LYS:HD3	5:F:381:ARG:HH11	1.82	0.44
3:D:901:LEU:C	3:D:901:LEU:CD1	2.85	0.43
6:H:12:DC:H1'	6:H:13:DT:C2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:206:PRO:HA	2:C:308:LEU:HD23	2.00	0.43
3:D:1030:ARG:NH2	3:D:1034:LEU:HD21	2.33	0.43
2:C:180:VAL:HG21	2:C:379:ARG:HE	1.82	0.43
2:C:378:LEU:HD21	2:C:455:LEU:HD22	2.00	0.43
2:C:725:PRO:HA	2:C:730:ASN:HD21	1.83	0.43
3:D:114:LEU:HD23	3:D:114:LEU:HA	1.87	0.43
3:D:230:ALA:N	3:D:233:GLN:OE1	2.51	0.43
3:D:1166:THR:HB	3:D:1206:VAL:HG21	1.99	0.43
2:C:522:GLY:O	2:C:553:ARG:HA	2.19	0.43
3:D:438:LEU:O	3:D:561:SER:OG	2.30	0.43
5:F:342:LYS:HB3	5:F:342:LYS:HE2	1.77	0.43
2:C:484:CYS:HB2	2:C:588:SER:HB3	2.00	0.43
3:D:101:VAL:HG23	3:D:375:GLN:CD	2.38	0.43
3:D:1062:TYR:CD2	3:D:1081:SER:HA	2.53	0.43
5:F:329:ILE:O	5:F:332:VAL:HG12	2.19	0.43
3:D:83:THR:HG22	3:D:84:ARG:H	1.84	0.43
1:A:214:THR:HA	1:B:230:GLU:HG2	2.00	0.43
3:D:889:HIS:O	3:D:977:THR:OG1	2.27	0.43
3:D:1139:GLN:O	3:D:1143:ARG:HG2	2.17	0.43
5:F:347:ALA:O	5:F:351:ILE:HG13	2.19	0.43
1:A:64:THR:OG1	1:A:65:THR:N	2.51	0.43
3:D:365:ILE:HG23	3:D:366:ILE:HG13	2.01	0.43
3:D:460:LEU:HD11	3:D:483:VAL:HG12	2.01	0.43
2:C:239:LYS:HZ3	2:C:268:VAL:HG23	1.83	0.42
3:D:123:LYS:HA	3:D:123:LYS:HD2	1.72	0.42
3:D:676:LEU:HG	3:D:715:LYS:HB3	2.00	0.42
2:C:723:ILE:O	3:D:730:THR:HG23	2.18	0.42
3:D:57:ASP:HB3	3:D:58:TRP:CE3	2.54	0.42
3:D:321:PRO:HA	3:D:322:PRO:HD3	1.79	0.42
3:D:733:MET:HE2	3:D:733:MET:HB3	1.84	0.42
5:F:302:LEU:O	5:F:305:SER:OG	2.20	0.42
6:H:18:DC:H2"	6:H:19:DG:C8	2.55	0.42
2:C:408:ASP:O	2:C:412:ILE:HG13	2.19	0.42
2:C:809:LYS:HD2	2:C:833:ARG:HD3	2.01	0.42
3:D:486:VAL:O	3:D:490:VAL:HG23	2.19	0.42
3:D:832:ILE:HG22	3:D:834:ARG:H	1.82	0.42
2:C:41:PHE:O	2:C:979:GLY:HA2	2.20	0.42
1:B:147:VAL:HA	1:B:148:PRO:HD3	1.92	0.42
2:C:646:GLU:HB2	2:C:662:HIS:CE1	2.54	0.42
3:D:117:LEU:HD12	3:D:299:VAL:HG22	2.01	0.42
3:D:732:SER:OG	3:D:733:MET:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:MET:HG3	1:B:138:LEU:HB2	2.01	0.42
2:C:315:LYS:HA	2:C:315:LYS:HD2	1.77	0.42
3:D:827:PRO:HG3	3:D:854:HIS:NE2	2.34	0.42
3:D:460:LEU:HD23	3:D:460:LEU:HA	1.93	0.42
3:D:1270:ILE:HG12	4:E:108:GLU:HA	2.01	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
2:C:567:GLU:HA	3:D:834:ARG:HH12	1.85	0.42
2:C:615:ALA:HB3	2:C:715:LEU:HD22	2.02	0.42
2:C:737:LEU:HG	2:C:895:ILE:HD12	2.01	0.42
3:D:642:PRO:HG2	3:D:647:GLU:HB2	2.01	0.42
3:D:772:GLU:O	3:D:776:GLU:HG2	2.20	0.42
3:D:819:GLY:O	3:D:839:SER:HB3	2.19	0.42
3:D:1187:GLU:O	3:D:1191:ARG:HB2	2.20	0.42
1:A:97:LEU:HD21	1:A:105:VAL:HG21	2.02	0.42
1:B:95:MET:HB3	1:B:113:PRO:HD3	2.01	0.42
2:C:1087:GLU:HG3	2:C:1091:ILE:HD11	2.00	0.42
3:D:54:PRO:HG2	3:D:83:THR:O	2.20	0.42
3:D:844:LEU:HD12	3:D:844:LEU:H	1.85	0.42
1:B:87:SER:O	1:B:142:ARG:NH1	2.52	0.41
3:D:36:TYR:CZ	3:D:37:ARG:HG3	2.54	0.41
3:D:54:PRO:HG3	3:D:81:GLU:O	2.20	0.41
3:D:384:ASN:HB2	3:D:401:SER:HB3	2.02	0.41
2:C:518:LYS:HA	2:C:578:TYR:HD1	1.85	0.41
5:F:515:ARG:O	5:F:519:ARG:N	2.50	0.41
1:A:105:VAL:HG12	1:A:126:ALA:O	2.21	0.41
2:C:742:VAL:HG13	2:C:878:LYS:HD3	2.01	0.41
3:D:16:THR:O	3:D:20:ILE:HG12	2.20	0.41
3:D:459:ARG:NH1	3:D:463:LEU:HD11	2.35	0.41
5:F:231:TYR:HE2	5:F:321:ILE:HG21	1.85	0.41
1:B:84:VAL:HG23	1:B:119:HIS:HB2	2.02	0.41
2:C:513:GLU:HG2	2:C:532:THR:HG22	2.01	0.41
2:C:1086:GLN:O	2:C:1090:THR:OG1	2.32	0.41
4:E:102:ASP:OD1	4:E:102:ASP:N	2.53	0.41
2:C:642:VAL:HB	2:C:703:ALA:HB3	2.02	0.41
8:C:1201:RFP:H28C	8:C:1201:RFP:H341	1.75	0.41
3:D:308:SER:HA	3:D:309:PRO:HD3	1.80	0.41
3:D:409:LYS:O	3:D:415:GLN:HB2	2.19	0.41
3:D:463:LEU:HB2	3:D:465:HIS:CD2	2.53	0.41
2:C:974:THR:HG23	2:C:980:ALA:H	1.86	0.41
2:C:1133:LEU:O	2:C:1135:VAL:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1036:GLU:OE2	3:D:1211:THR:OG1	2.37	0.41
5:F:249:LEU:HD12	5:F:295:LEU:HD13	2.03	0.41
3:D:588:LEU:HD12	3:D:589:THR:N	2.36	0.41
2:C:257:ILE:HD11	2:C:346:VAL:HG23	2.02	0.41
2:C:757:ILE:HB	2:C:837:LEU:HD22	2.03	0.41
3:D:87:VAL:O	3:D:90:GLU:HG2	2.20	0.41
3:D:130:TYR:O	3:D:372:ARG:HD3	2.21	0.41
5:F:231:TYR:O	5:F:235:ILE:HG13	2.20	0.41
6:H:15:DT:C4	6:H:16:DC:N4	2.89	0.41
2:C:389:ILE:O	2:C:393:MET:HG2	2.21	0.41
2:C:885:LEU:HD23	2:C:1032:LYS:HA	2.03	0.41
3:D:14:LEU:HD13	3:D:106:TYR:OH	2.21	0.41
3:D:34:ILE:HG22	3:D:41:PRO:HA	2.01	0.41
5:F:364:ARG:HG3	5:F:368:ILE:HG12	2.03	0.41
1:A:40:ARG:HB2	1:B:33:THR:HG23	2.02	0.41
2:C:465:ARG:HD3	2:C:492:PRO:HB2	2.03	0.41
2:C:549:ASP:HB3	2:C:553:ARG:H	1.85	0.41
2:C:928:ILE:H	2:C:928:ILE:HG13	1.49	0.41
2:C:1141:ASP:OD1	2:C:1142:GLY:N	2.54	0.41
3:D:350:ARG:HD2	3:D:377:SER:OG	2.20	0.41
3:D:1176:LEU:H	3:D:1176:LEU:HD12	1.86	0.41
4:E:56:TYR:CE2	4:E:99:ILE:HG12	2.56	0.41
1:B:55:ARG:HB2	1:B:137:GLU:HB3	2.03	0.40
3:D:339:ASP:OD1	5:F:422:SER:OG	2.27	0.40
3:D:545:LEU:HD12	3:D:546:PRO:HD2	2.03	0.40
2:C:211:TRP:HH2	6:H:14:DG:OP1	2.04	0.40
2:C:338:VAL:O	2:C:342:ILE:HG13	2.21	0.40
2:C:631:GLU:H	2:C:631:GLU:CD	2.24	0.40
2:C:817:GLU:N	2:C:817:GLU:OE1	2.53	0.40
2:C:850:ILE:HG13	2:C:871:VAL:HG22	2.03	0.40
2:C:213:GLU:HG3	2:C:225:ARG:HB2	2.02	0.40
2:C:1094:ASP:OD1	2:C:1119:GLU:N	2.55	0.40
2:C:70:TRP:CH2	2:C:82:PRO:HB2	2.56	0.40
2:C:516:TYR:HD2	2:C:531:LEU:HD13	1.86	0.40
2:C:1137:VAL:HG21	2:C:1147:LEU:HD11	2.03	0.40
4:E:40:ILE:HA	4:E:43:LEU:HB2	2.04	0.40
2:C:311:VAL:HG21	2:C:377:ARG:HD2	2.03	0.40
2:C:974:THR:HG23	2:C:979:GLY:HA3	2.03	0.40
3:D:325:ARG:HD2	3:D:341:ASN:OD1	2.22	0.40
3:D:579:LEU:HD22	3:D:808:THR:HB	2.03	0.40
3:D:1152:LYS:O	3:D:1156:VAL:HG23	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:305:SER:HB3	6:H:6:DT:H4'	2.04	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%)	29	66
1	B	225/347 (65%)	207 (92%)	15 (7%)	3 (1%)	12	47
2	C	1124/1178 (95%)	1055 (94%)	63 (6%)	6 (0%)	29	66
3	D	1261/1316 (96%)	1200 (95%)	56 (4%)	5 (0%)	34	70
4	E	79/110 (72%)	77 (98%)	2 (2%)	0	100	100
5	F	317/528 (60%)	300 (95%)	16 (5%)	1 (0%)	41	74
All	All	3228/3826 (84%)	3049 (94%)	163 (5%)	16 (0%)	29	66

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	678	PRO
1	A	184	GLU
2	C	47	PRO
3	D	593	PRO
3	D	892	GLN
2	C	1045	SER
2	C	1134	ASN
2	C	1148	ARG
1	B	158	GLU
2	C	922	VAL
3	D	658	PRO

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Mol	Chain	Res	Type
5	F	405	ILE
1	B	35	GLY
2	C	33	PRO
3	D	607	PRO
1	B	227	VAL

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	192/297 (65%)	190 (99%)	2 (1%)	76	85
1	B	192/297 (65%)	191 (100%)	1 (0%)	88	93
2	C	948/998 (95%)	935 (99%)	13 (1%)	67	80
3	D	1048/1095 (96%)	1020 (97%)	28 (3%)	44	66
4	E	68/90 (76%)	66 (97%)	2 (3%)	42	64
5	F	269/427 (63%)	261 (97%)	8 (3%)	41	64
All	All	2717/3204 (85%)	2663 (98%)	54 (2%)	55	73

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	182	ARG
1	A	225	LEU
1	B	17	ASN
2	C	39	VAL
2	C	48	LEU
2	C	180	VAL
2	C	332	THR
2	C	354	THR
2	C	373	PHE
2	C	456	SER
2	C	479	HIS
2	C	621	SER
2	C	835	THR

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Mol	Chain	Res	Type
2	C	1099	ARG
2	C	1120	SER
2	C	1148	ARG
3	D	7	PHE
3	D	75	CYS
3	D	82	VAL
3	D	83	THR
3	D	97	LEU
3	D	101	VAL
3	D	112	SER
3	D	317	VAL
3	D	441	CYS
3	D	535	ASP
3	D	582	VAL
3	D	583	THR
3	D	589	THR
3	D	629	VAL
3	D	653	HIS
3	D	714	ASP
3	D	796	ASP
3	D	810	ASN
3	D	834	ARG
3	D	901	LEU
3	D	910	LEU
3	D	921	TYR
3	D	968	CYS
3	D	978	CYS
3	D	1009	GLN
3	D	1099	LEU
3	D	1136	ARG
3	D	1194	VAL
4	E	75	ILE
4	E	106	HIS
5	F	258	TYR
5	F	269	ARG
5	F	306	LEU
5	F	361	ASP
5	F	367	ARG
5	F	402	GLU
5	F	425	GLN
5	F	448	VAL

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	451	HIS
3	D	375	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 3 are monoatomic - leaving 2 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	$\#\|Z\| > 2$
11	88G	D	1404	-	29,29,29	1.80	4 (13%)	38,38,38	0.88	2 (5%)
8	RFP	C	1201	-	63,63,63	2.59	12 (19%)	94,94,94	2.22	18 (19%)

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
11	88G	D	1404	-	-	0/20/20/20	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	RFP	C	1201	-	-	23/60/85/85	0/5/5/5

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	1201	RFP	O4-C11	11.18	1.40	1.21
8	C	1201	RFP	C43-N2	8.15	1.50	1.27
8	C	1201	RFP	C17-C16	7.33	1.55	1.34
11	D	1404	88G	CAA-CAW	-5.46	1.40	1.51
8	C	1201	RFP	C3-C43	5.38	1.56	1.46
8	C	1201	RFP	O7-C25	-4.98	1.37	1.44
8	C	1201	RFP	C15-N1	4.91	1.46	1.35
11	D	1404	88G	CAY-CAU	-4.83	1.40	1.50
11	D	1404	88G	CB-CG	-4.57	1.40	1.51
8	C	1201	RFP	C12-C11	-3.68	1.40	1.54
11	D	1404	88G	CAZ-NAS	-3.59	1.34	1.41
8	C	1201	RFP	C18-C17	3.58	1.54	1.43
8	C	1201	RFP	C6-C7	2.95	1.44	1.39
8	C	1201	RFP	O9-C23	-2.16	1.37	1.43
8	C	1201	RFP	O6-C27	-2.05	1.38	1.43
8	C	1201	RFP	C29-C28	2.01	1.41	1.30

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	C	1201	RFP	C38-N4-C42	8.22	122.95	110.66
8	C	1201	RFP	C43-N2-N3	-7.71	109.61	120.43
8	C	1201	RFP	C2-C3-C43	-7.57	116.48	124.17
8	C	1201	RFP	C30-C16-C17	-6.62	107.40	123.42
8	C	1201	RFP	O3-C6-C7	5.30	130.26	121.14
8	C	1201	RFP	O4-C11-C5	-4.73	122.79	131.81
8	C	1201	RFP	O7-C35-C36	4.19	118.80	111.09
8	C	1201	RFP	C23-C24-C25	3.88	118.19	110.61
8	C	1201	RFP	C3-C2-C1	3.09	122.91	120.70
8	C	1201	RFP	C12-O5-C29	2.82	124.81	117.84
11	D	1404	88G	CAZ-NAS-C	-2.76	119.35	126.92
8	C	1201	RFP	C5-C10-C4	-2.75	121.15	124.03
8	C	1201	RFP	C37-O6-C27	2.73	119.55	113.01
8	C	1201	RFP	C4-C3-C43	2.69	119.73	116.52
8	C	1201	RFP	C33-C24-C25	-2.57	106.80	111.40
8	C	1201	RFP	O5-C12-C13	2.43	113.34	106.99
8	C	1201	RFP	C5-C6-C7	-2.40	119.42	125.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	D	1404	88G	CAL-CAW-CAZ	2.28	119.59	117.44
8	C	1201	RFP	C25-O7-C35	2.21	121.14	117.72
8	C	1201	RFP	C42-N4-C39	2.10	112.46	109.52

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	C	1201	RFP	C4-C3-C43-N2
8	C	1201	RFP	C11-C12-O5-C29
8	C	1201	RFP	O3-C12-O5-C29
8	C	1201	RFP	C26-C27-C28-C29
8	C	1201	RFP	C27-C28-C29-O5
8	C	1201	RFP	C43-N2-N3-C40
8	C	1201	RFP	C36-C35-O7-C25
8	C	1201	RFP	C3-C43-N2-N3
8	C	1201	RFP	C17-C18-C19-C20
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	O6-C27-C28-C29
8	C	1201	RFP	C2-C3-C43-N2
8	C	1201	RFP	C16-C17-C18-C19
8	C	1201	RFP	C15-C16-C17-C18
8	C	1201	RFP	C33-C24-C25-C26
8	C	1201	RFP	C23-C24-C25-O7
8	C	1201	RFP	C23-C24-C25-C26
8	C	1201	RFP	N1-C15-C16-C17
8	C	1201	RFP	O11-C15-C16-C17
8	C	1201	RFP	C33-C24-C25-O7
8	C	1201	RFP	C21-C22-C23-C24

There are no ring outliers.

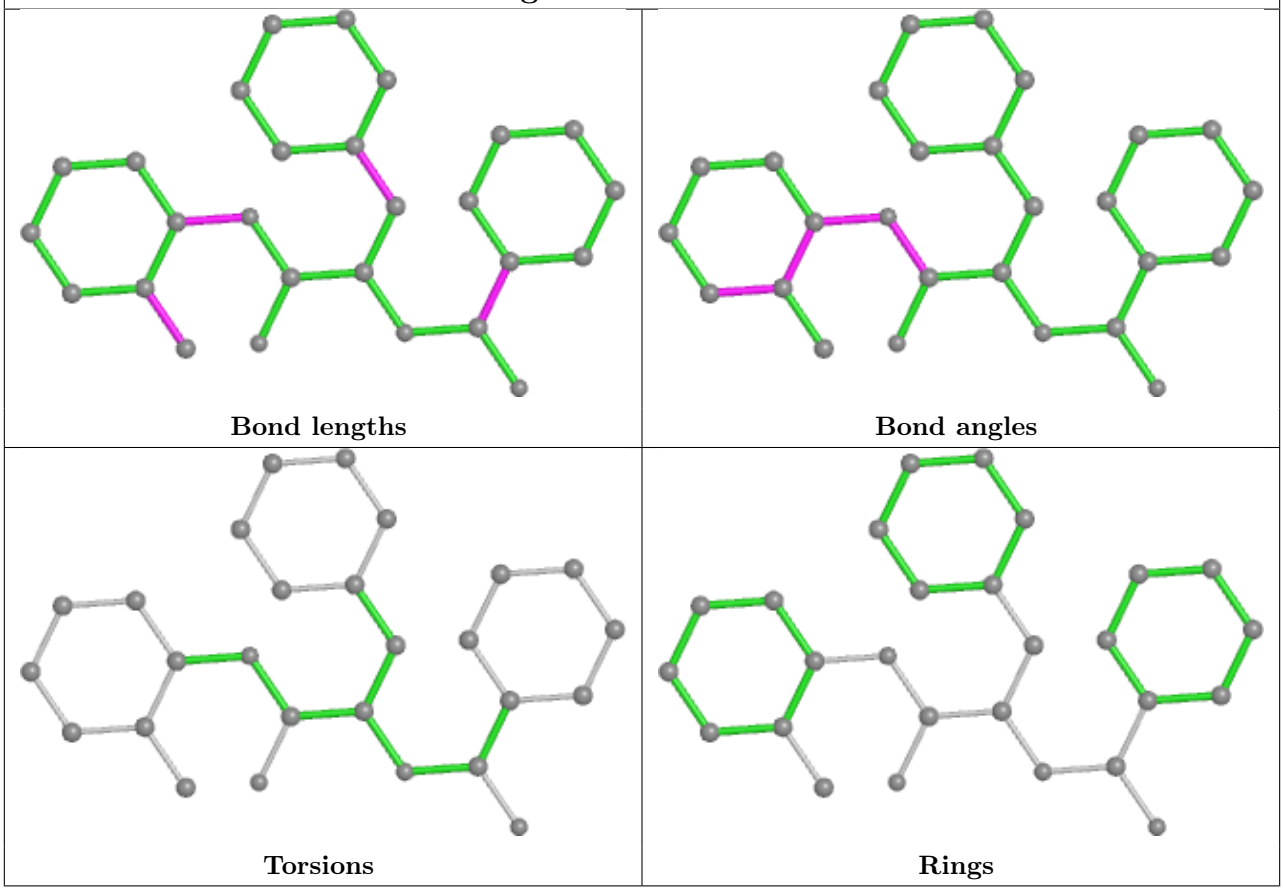
1 monomer is involved in 10 short contacts:

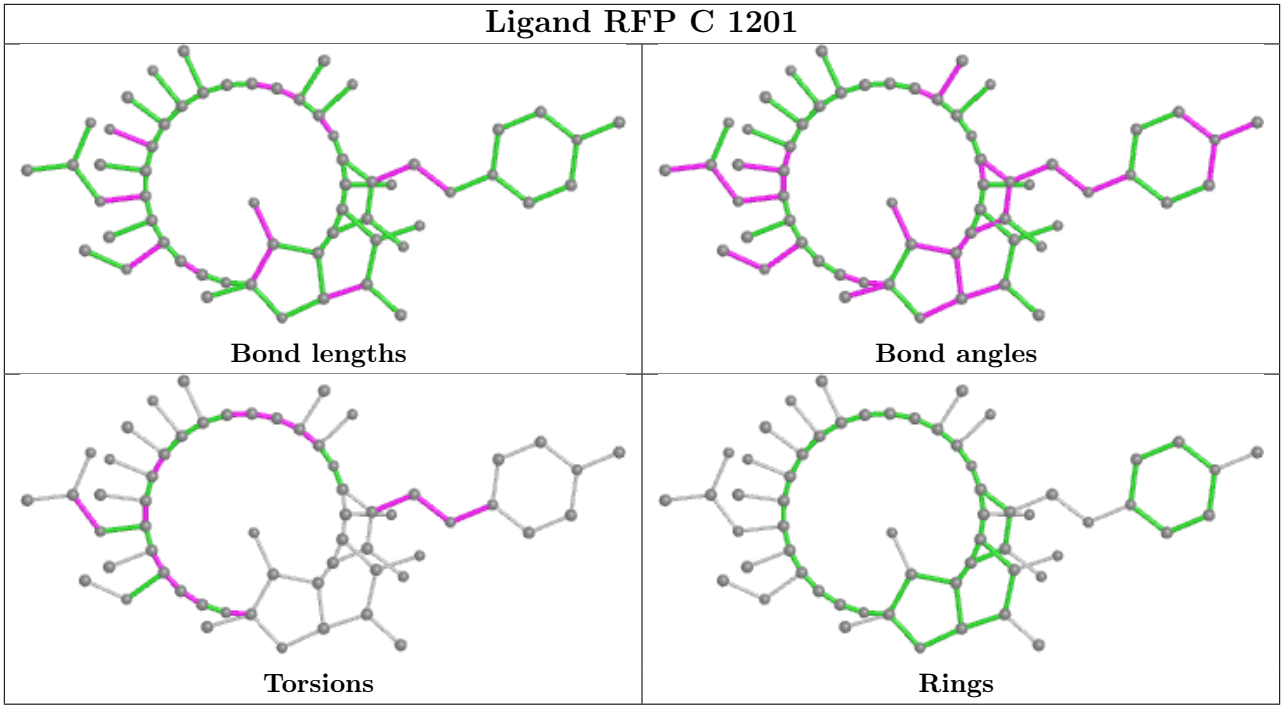
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	1201	RFP	10	0

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.

Ligand 88G D 1404





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%)	-0.23	3 (1%) 77 68	12, 52, 117, 140	0
1	B	227/347 (65%)	0.24	11 (4%) 30 25	45, 88, 136, 159	0
2	C	1126/1178 (95%)	-0.31	5 (0%) 92 87	3, 34, 116, 141	0
3	D	1265/1316 (96%)	-0.40	2 (0%) 95 93	4, 35, 101, 148	0
4	E	81/110 (73%)	-0.47	0 100 100	18, 41, 71, 92	0
5	F	321/528 (60%)	0.06	17 (5%) 26 23	7, 62, 159, 183	0
6	H	23/23 (100%)	0.09	0 100 100	27, 124, 234, 273	0
7	G	12/16 (75%)	1.71	4 (33%) 0 0	134, 224, 283, 283	0
All	All	3279/3865 (84%)	-0.26	42 (1%) 77 68	3, 43, 122, 283	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	G	14	DG	5.3
1	B	156	GLY	4.4
7	G	15	DT	4.0
7	G	16	DC	3.9
5	F	488	THR	3.9
5	F	500	ARG	3.7
1	B	155	SER	3.7
2	C	1150	GLY	3.6
5	F	520	SER	3.6
5	F	514	LEU	3.5
1	B	61	HIS	3.3
5	F	513	LYS	3.2
5	F	428	GLY	3.2
2	C	194	SER	3.1
5	F	210	GLU	3.1
1	B	62	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
2	C	775	ASN	3.1
5	F	490	ASP	3.1
1	A	226	ASN	3.0
7	G	13	DA	2.9
5	F	528	ASP	2.8
5	F	431	GLY	2.8
5	F	487	ARG	2.7
2	C	263	GLU	2.7
1	B	63	PHE	2.6
1	B	130	ASP	2.6
1	A	3	ILE	2.5
1	A	5	GLN	2.5
3	D	1195	ALA	2.5
5	F	517	PRO	2.3
1	B	65	THR	2.2
1	B	151	GLN	2.2
1	B	64	THR	2.2
5	F	509	LYS	2.2
5	F	275	ALA	2.2
1	B	134	LEU	2.2
5	F	502	ARG	2.2
1	B	160	GLY	2.1
3	D	1203	GLY	2.1
5	F	499	THR	2.0
5	F	489	LEU	2.0
2	C	810	GLY	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

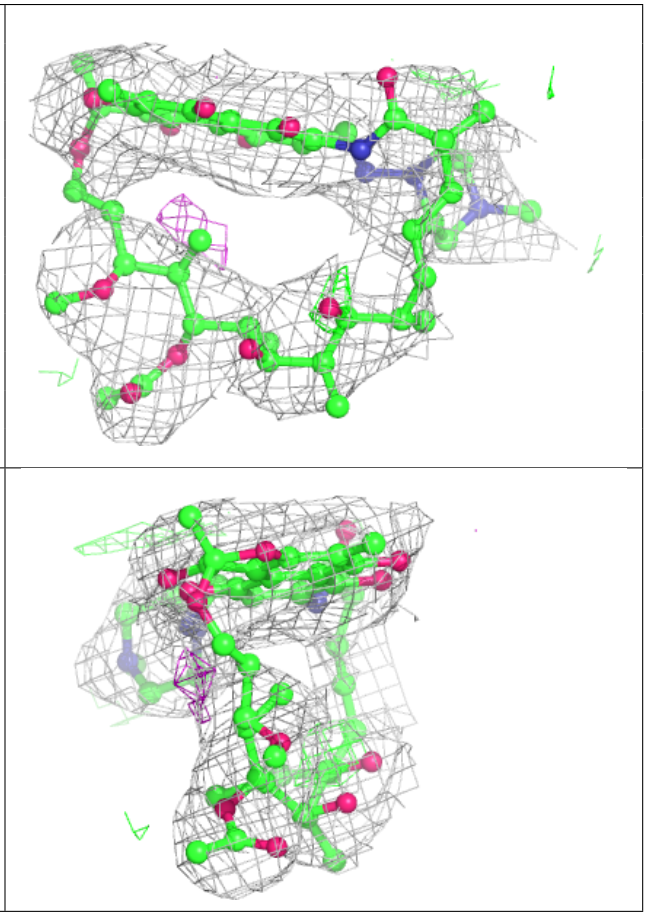
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	RFP	C	1201	59/59	0.95	0.27	22,26,50,66	0
10	MG	D	1403	1/1	0.96	0.13	5,5,5,5	0
11	88G	D	1404	27/27	0.97	0.35	27,35,40,43	0
9	ZN	D	1401	1/1	0.98	0.07	34,34,34,34	0
9	ZN	D	1402	1/1	0.99	0.10	52,52,52,52	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

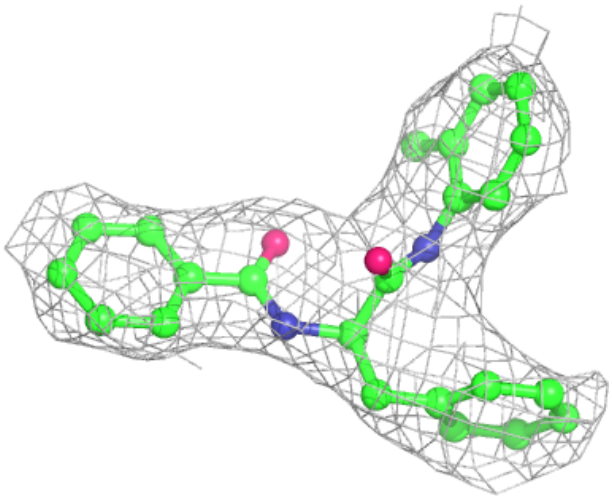
Electron density around RFP C 1201:

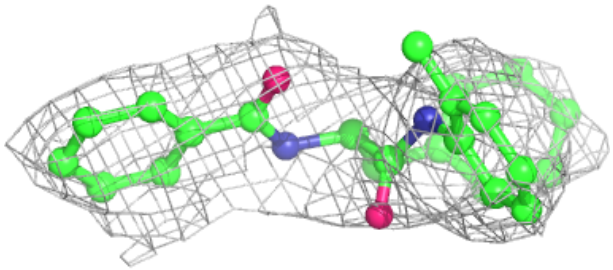
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

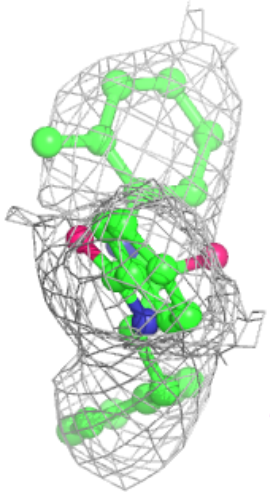


Electron density around 88G D 1404:

$2mF_o$-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.