



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 13, 2017 – 11:13 PM EST

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 : unknown
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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

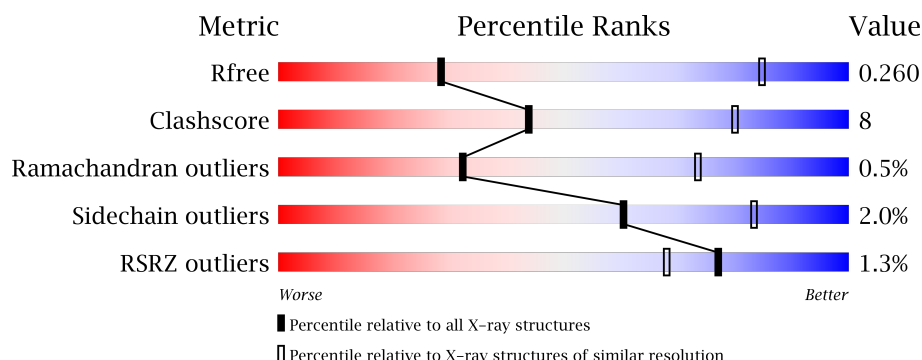
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.97 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}	100719	1066 (4.36-3.60)
Clashscore	112137	1163 (4.36-3.60)
Ramachandran outliers	110173	1119 (4.36-3.60)
Sidechain outliers	110143	1108 (4.36-3.60)
RSRZ outliers	101464	1078 (4.36-3.60)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>0.5%</div> <div>55%</div> <div>9%</div> <div>35%</div> </div>
1	B	347	<div> <div>3%</div> <div>52%</div> <div>14%</div> <div>35%</div> </div>
2	C	1178	<div> <div>77%</div> <div>18%</div> <div>5%</div> </div>
3	D	1316	<div> <div>75%</div> <div>20%</div> <div>5%</div> </div>
4	E	110	<div> <div>57%</div> <div>15%</div> <div>26%</div> </div>

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Mol	Chain	Length	Quality of chain
5	F	528	
6	H	23	
7	G	16	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	88G	D	1404	-	-	-	X

2 Entry composition

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
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	321	Total	C	N	O	S	0	0	0
			2541	1582	457	493	9			

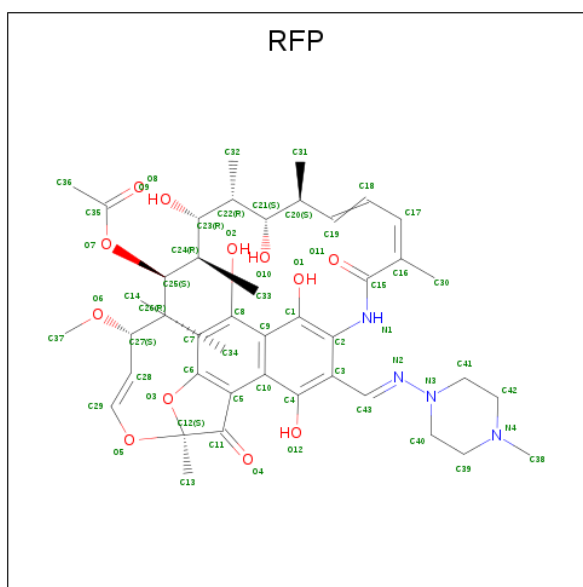
- Molecule 6 is a DNA chain called DNA (5'-D(*TP*AP*TP*AP*AP*TP*GP*GP*GP*AP*GP*CP*TP*GP*TP*CP*AP*CP*GP*GP*AP*TP*G)-3').

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

- Molecule 8 is RIFAMPICIN (three-letter code: RFP) (formula: C₄₃H₅₈N₄O₁₂).



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

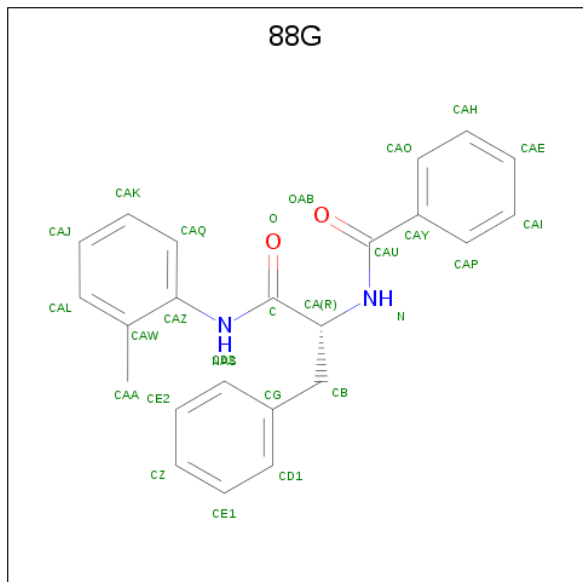
- Molecule 9 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

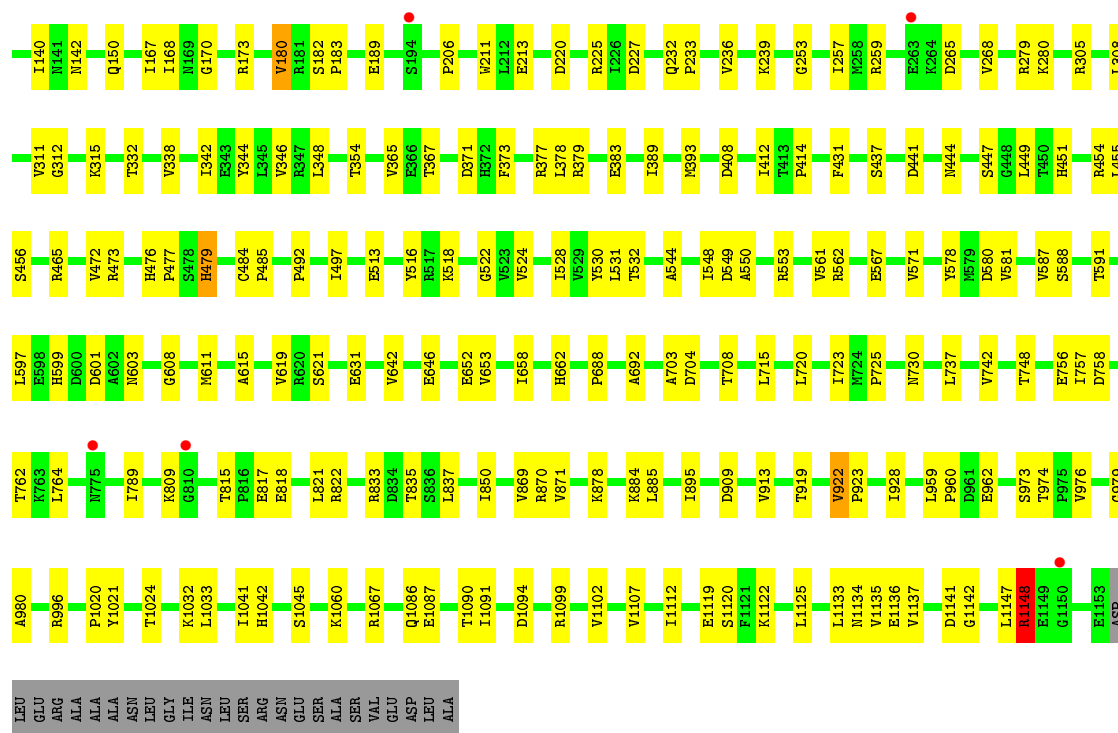
- Molecule 10 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

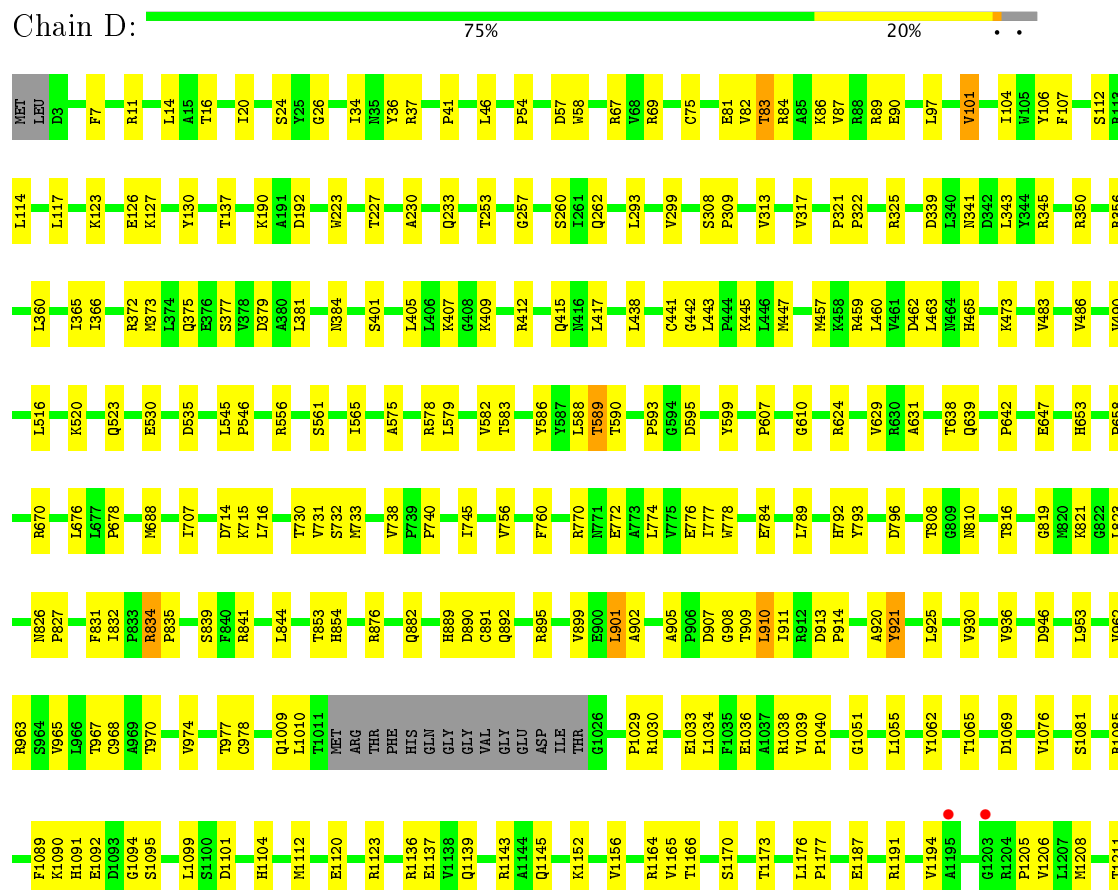
- Molecule 11 is Nalpha-(benzenecarbonyl)-N-(2-methylphenyl)-D-phenylalaninamide (three-letter code: 88G) (formula: C₂₃H₂₂N₂O₂).



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



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





4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	2.85 (at 4.00Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.223 , 0.260 0.232 , 0.260	Depositor DCC
R_{free} test set	2016 reflections (5.39%)	DCC
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	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	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.*

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: ZN, RFP, 88G, MG

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(°)	Ideal(°)
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:O	3:D:910:LEU:HD12	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:658:ILE:HD11	2:C:688:PRO:HB3	1.75	0.69
2:C:279:ARG:HD3	5:F:215:ALA:HB1	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:343:LEU:HD13	3:D:381:LEU:HA	1.84	0.59
3:D:46:LEU:O	3:D:325:ARG:NH2	2.29	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:C18	8:C:1201:RFP:HN1	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:1170:SER:O	3:D:1173:THR:OG1	2.27	0.51
3:D:463:LEU:HB2	3:D:465:HIS:HD2	1.75	0.51
8:C:1201:RFP:O12	8:C:1201:RFP:O4	2.27	0.51
2:C:46:GLU:N	2:C:47:PRO:HD3	2.26	0.51
3:D:417:LEU:HD22	3:D:1253:ILE:HG23	1.92	0.51
2:C:1119:GLU:OE2	3:D:89:ARG:NH2	2.44	0.51
5:F:345:THR:HB	6:H:4:DA:H8	1.74	0.51
4:E:33:LEU:H	4:E:33:LEU:HD23	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:1220:TRP:NE1	3:D:1243:ASP:HB2	2.26	0.50
3:D:778:TRP:CD2	3:D:835:PRO:HG3	2.46	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:1148:ARG:NH1	3:D:86:LYS:HG3	2.28	0.49
2:C:909:ASP:N	2:C:909:ASP:OD1	2.45	0.49
3:D:67:ARG:HG2	3:D:69:ARG:H	1.77	0.49
5:F:489:LEU:HD23	5:F:489:LEU:H	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:N	1:A:120:ASN:OD1	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:HE2	3:D:457:MET:HB2	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:1020:PRO:HB2	2:C:1021:TYR:CD2	2.51	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:454:ARG:HH22	8:C:1201:RFP:C19	2.29	0.46
3:D:586:TYR:O	3:D:590:THR:OG1	2.33	0.46
2:C:821:LEU:HD22	5:F:456:LEU:HD11	1.98	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:1120:GLU:HA	3:D:1123:ARG:HG2	1.99	0.45
3:D:473:LYS:HD2	5:F:448:VAL:HG21	1.98	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:676:LEU:HD23	3:D:716:LEU:HD23	1.99	0.45
3:D:556:ARG:HG3	4:E:35:ILE:HG12	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
3:D:223:TRP:O	3:D:227:THR:OG1	2.28	0.44
2:C:1107:VAL:HG21	5:F:451:VAL:HG11	1.99	0.44
1:A:100:GLN:HG2	1:A:101:GLY:H	1.82	0.44
8:C:1201:RFP:H342	8:C:1201:RFP:H24C	1.70	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
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
8:C:1201:RFP:H18C	8:C:1201:RFP:N1	2.25	0.44
2:C:454:ARG:HH22	8:C:1201:RFP:H19C	1.83	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:CD1	3:D:901:LEU:C	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:1166:THR:HB	3:D:1206:VAL:HG21	1.99	0.43
3:D:230:ALA:N	3:D:233:GLN:OE1	2.51	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:HE2	5:F:342:LYS:HB3	1.77	0.43
2:C:484:CYS:HB2	2:C:588:SER:HB3	2.00	0.43
3:D:1062:TYR:CD2	3:D:1081:SER:HA	2.53	0.43
3:D:101:VAL:HG23	3:D:375:GLN:CD	2.38	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:1139:GLN:O	3:D:1143:ARG:HG2	2.17	0.43
3:D:889:HIS:O	3:D:977:THR:OG1	2.27	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:HD2	3:D:123:LYS:HA	1.72	0.42
3:D:676:LEU:HG	3:D:715:LYS:HB3	2.00	0.42
3:D:321:PRO:HA	3:D:322:PRO:HD3	1.79	0.42
3:D:57:ASP:HB3	3:D:58:TRP:CE3	2.54	0.42
2:C:723:ILE:O	3:D:730:THR:HG23	2.18	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:92:PRO:HB3	1:B:141:GLU:HG2	2.02	0.42
1:B:39:ARG:HH21	1:B:173:LYS:NZ	2.18	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:1187:GLU:O	3:D:1191:ARG:HB2	2.20	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
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:384:ASN:HB2	3:D:401:SER:HB3	2.02	0.41
3:D:54:PRO:HG3	3:D:81:GLU:O	2.20	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:1086:GLN:O	2:C:1090:THR:OG1	2.32	0.41
2:C:513:GLU:HG2	2:C:532:THR:HG22	2.01	0.41
4:E:102:ASP:N	4:E:102:ASP:OD1	2.53	0.41
8:C:1201:RFP:H28C	8:C:1201:RFP:H341	1.75	0.41
2:C:642:VAL:HB	2:C:703:ALA:HB3	2.02	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:1133:LEU:O	2:C:1135:VAL:N	2.54	0.41
2:C:974:THR:HG23	2:C:980:ALA:H	1.86	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:130:TYR:O	3:D:372:ARG:HD3	2.21	0.41
3:D:87:VAL:O	3:D:90:GLU:HG2	2.20	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:1141:ASP:OD1	2:C:1142:GLY:N	2.54	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
3:D:1176:LEU:H	3:D:1176:LEU:HD12	1.86	0.41
3:D:350:ARG:HD2	3:D:377:SER:OG	2.20	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:CD	2:C:631:GLU:H	2.24	0.40
2:C:817:GLU:OE1	2:C:817:GLU:N	2.53	0.40
2:C:850:ILE:HG13	2:C:871:VAL:HG22	2.03	0.40
2:C:1094:ASP:OD1	2:C:1119:GLU:N	2.55	0.40
2:C:213:GLU:HG3	2:C:225:ARG:HB2	2.02	0.40
2:C:1137:VAL:HG21	2:C:1147:LEU:HD11	2.03	0.40
2:C:516:TYR:HD2	2:C:531:LEU:HD13	1.86	0.40
2:C:70:TRP:CH2	2:C:82:PRO:HB2	2.56	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:1152:LYS:O	3:D:1156:VAL:HG23	2.22	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

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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%)	32	73
1	B	225/347 (65%)	207 (92%)	15 (7%)	3 (1%)	14	57
2	C	1124/1178 (95%)	1055 (94%)	63 (6%)	6 (0%)	32	73
3	D	1261/1316 (96%)	1200 (95%)	56 (4%)	5 (0%)	38	77
4	E	79/110 (72%)	77 (98%)	2 (2%)	0	100	100
5	F	317/528 (60%)	300 (95%)	16 (5%)	1 (0%)	44	80
All	All	3228/3826 (84%)	3049 (94%)	163 (5%)	16 (0%)	32	73

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 ⓘ

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%)	80	91
1	B	192/297 (65%)	191 (100%)	1 (0%)	91	96
2	C	948/998 (95%)	935 (99%)	13 (1%)	71	88
3	D	1048/1095 (96%)	1020 (97%)	28 (3%)	50	77
4	E	68/90 (76%)	66 (97%)	2 (3%)	48	75
5	F	269/427 (63%)	261 (97%)	8 (3%)	46	75
All	All	2717/3204 (85%)	2663 (98%)	54 (2%)	60	83

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

Some 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 carbohydrates 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	$\# Z > 2$
8	RFP	C	1201	-	62,63,63	2.61	10 (16%)	91,94,94	1.92	14 (15%)
11	88G	D	1404	-	29,29,29	1.80	4 (13%)	38,38,38	0.93	2 (5%)

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	-	-	0/60/85/85	0/1/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	88G	D	1404	-	-	0/20/20/20	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	D	1404	88G	CAA-CAW	-5.54	1.40	1.51
8	C	1201	RFP	O7-C25	-4.89	1.37	1.44
11	D	1404	88G	CAY-CAU	-4.72	1.40	1.50
11	D	1404	88G	CB-CG	-4.58	1.40	1.51
11	D	1404	88G	CAZ-NAS	-3.50	1.34	1.41
8	C	1201	RFP	C12-C11	-2.96	1.40	1.54
8	C	1201	RFP	O9-C23	-2.20	1.37	1.43
8	C	1201	RFP	C6-C7	2.88	1.44	1.39
8	C	1201	RFP	C18-C17	3.57	1.54	1.43
8	C	1201	RFP	C15-N1	4.72	1.46	1.35
8	C	1201	RFP	C3-C43	5.69	1.56	1.46
8	C	1201	RFP	C17-C16	6.44	1.55	1.34
8	C	1201	RFP	C43-N2	10.44	1.50	1.27
8	C	1201	RFP	O4-C11	10.50	1.40	1.21

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	1201	RFP	C30-C16-C17	-6.09	107.40	123.44
8	C	1201	RFP	C43-N2-N3	-6.05	109.61	120.40
8	C	1201	RFP	C2-C3-C43	-4.81	116.48	123.29
8	C	1201	RFP	O4-C11-C5	-3.95	122.79	131.84
11	D	1404	88G	CAZ-NAS-C	-2.85	119.35	126.92
8	C	1201	RFP	C33-C24-C25	-2.51	106.80	111.43
8	C	1201	RFP	C5-C10-C4	-2.28	121.15	124.21
8	C	1201	RFP	C25-O7-C35	2.18	121.14	117.72
8	C	1201	RFP	C42-N4-C39	2.25	112.46	109.47
8	C	1201	RFP	C12-O5-C29	2.32	124.81	118.10
8	C	1201	RFP	C37-O6-C27	2.52	119.55	112.98
11	D	1404	88G	CAL-CAW-CAZ	2.68	119.59	117.42
8	C	1201	RFP	C23-C24-C25	3.55	118.19	110.88
8	C	1201	RFP	O7-C35-C36	4.10	118.80	111.10
8	C	1201	RFP	O3-C6-C7	4.37	130.26	121.31
8	C	1201	RFP	C38-N4-C42	8.15	122.95	110.67

There are no chirality outliers.

There are no torsion outliers.

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

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%)	-0.23	3 (1%) 77 68	12, 52, 117, 140	0
1	B	227/347 (65%)	0.24	11 (4%) 31 24	45, 88, 136, 159	0
2	C	1126/1178 (95%)	-0.31	5 (0%) 92 88	3, 34, 116, 141	0
3	D	1265/1316 (96%)	-0.40	2 (0%) 94 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%) 27 21	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 1	134, 224, 283, 283	0
All	All	3279/3865 (84%)	-0.26	42 (1%) 77 68	3, 43, 123, 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	3.7
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	A	3	ILE	2.6
1	B	130	ASP	2.6
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	275	ALA	2.2
5	F	509	LYS	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
11	88G	D	1404	27/27	0.97	0.35	2.16	27,35,40,43	0
8	RFP	C	1201	59/59	0.95	0.27	0.35	22,26,50,66	0
9	ZN	D	1402	1/1	0.99	0.10	-1.16	52,52,52,52	0
9	ZN	D	1401	1/1	0.98	0.07	-1.69	34,34,34,34	0
10	MG	D	1403	1/1	0.96	0.13	-	5,5,5,5	0

6.5 Other polymers [i](#)

There are no such residues in this entry.