



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:26 PM UTC

PDB ID : 5UHF / pdb_00005uhf
Title : Crystal structure of Mycobacterium tuberculosis transcription initiation complex in complex with D-IX336
Authors : Lin, W.; Das, K.; Feng, Y.; Ebright, R.H.
Deposited on : 2017-01-11
Resolution : 4.34 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

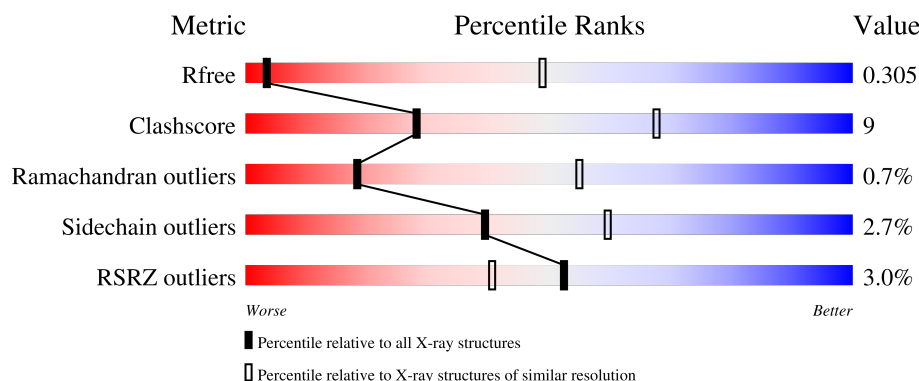
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.34 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	1059 (4.76-3.90)
Clashscore	190562	1105 (4.76-3.90)
Ramachandran outliers	187476	1007 (4.76-3.90)
Sidechain outliers	187428	1022 (4.80-3.88)
RSRZ outliers	180081	1056 (4.76-3.90)

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

Mol	Chain	Length	Quality of chain
1	A	347	2% 51% 13% 35%
1	B	347	5% 51% 13% 35%
2	C	1178	3% 73% 21% . .
3	D	1316	2% 74% 22% . .
4	E	110	3% 56% 17% 26%

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Mol	Chain	Length	Quality of chain
5	F	528	2% 44% 16% 39%
6	H	23	9% 61% 39%
7	G	16	25% 44% 31% 25%

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 25949 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
			1706	1075	289	340	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	12	Total	C	N	O	P	0	0	0
			241	116	43	71	11			

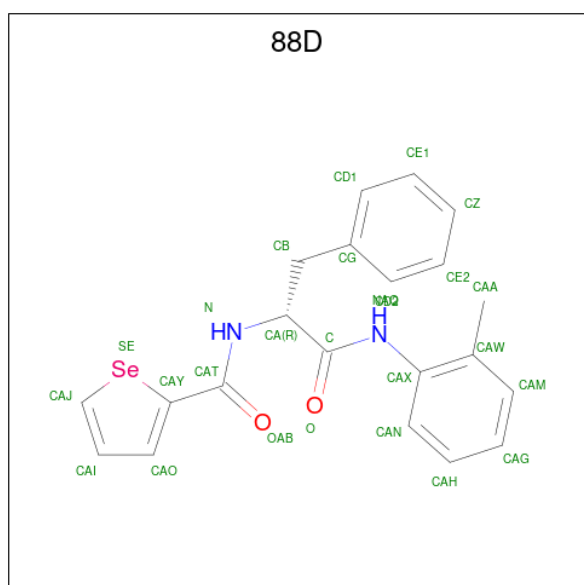
- Molecule 8 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

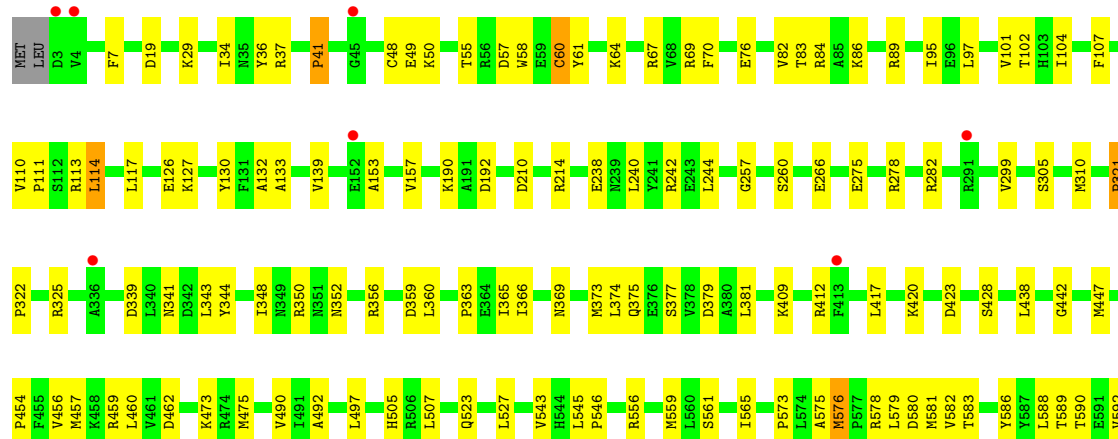
- Molecule 9 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

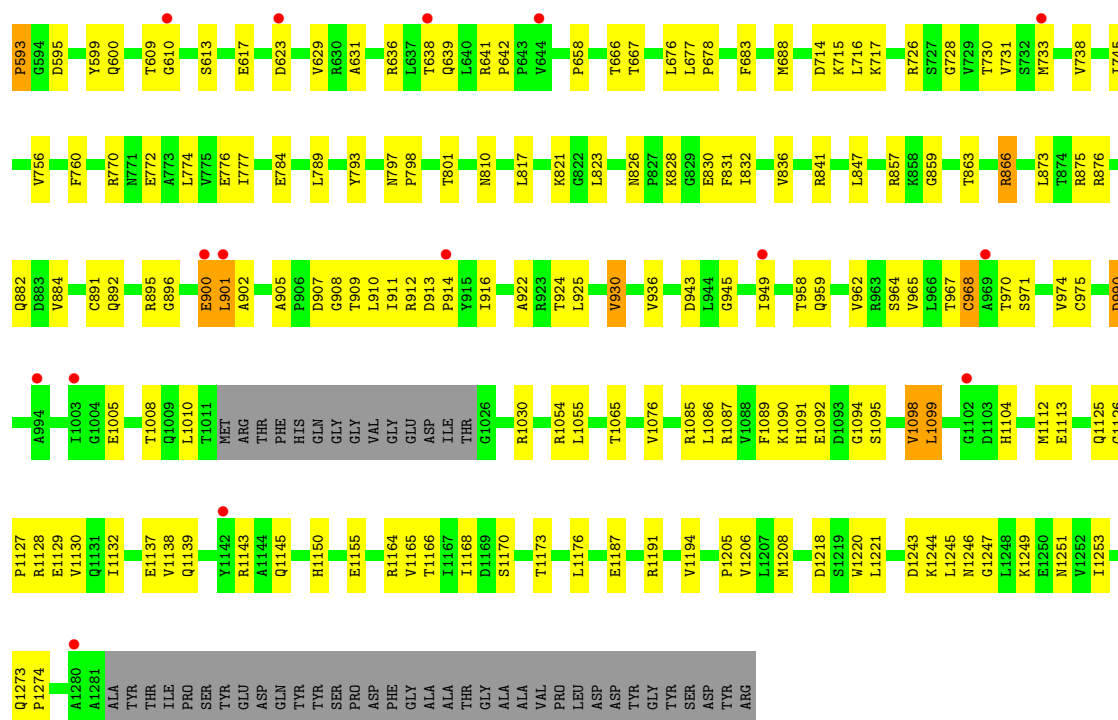
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	D	1	Total	Mg	0	0
			1	1		

- Molecule 10 is N-(2-methylphenyl)-Nalpha-(selenophene-2-carbonyl)-D-phenylalaninamide (CCD ID: 88D) (formula: C₂₁H₂₀N₂O₂Se).

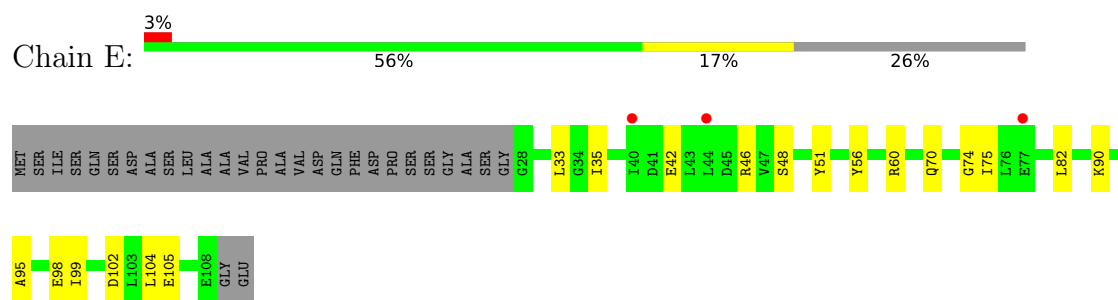


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	D	1	Total	C	N	O	Se	0	0
			26	21	2	2	1		

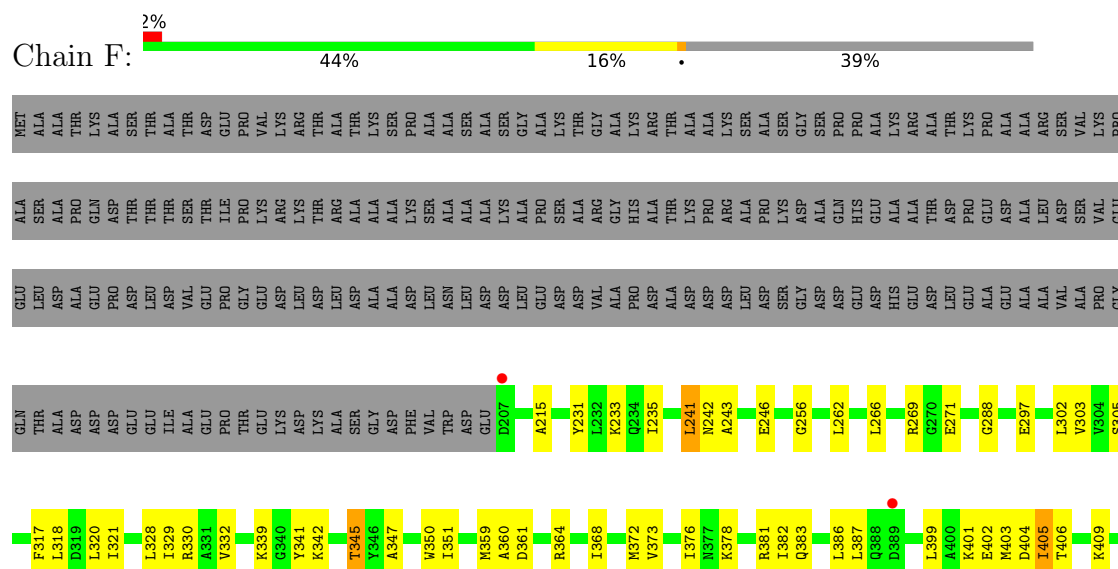


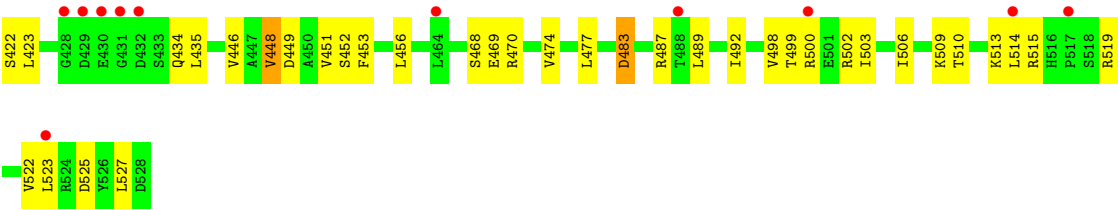


• Molecule 4: DNA-directed RNA polymerase subunit omega

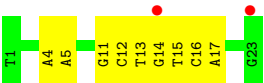


• Molecule 5: RNA polymerase sigma factor SigA

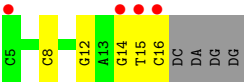




● Molecule 6: DNA (5'-D(*TP*AP*TP*AP*AP*TP*GP*GP*GP*AP*GP*CP*TP*GP*TP*CP*AP*CP*GP*GP*AP*TP*G)-3')



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	152.37Å 163.46Å 197.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.50 – 4.34 48.50 – 4.34	Depositor EDS
% Data completeness (in resolution range)	71.6 (48.50-4.34) 86.2 (48.50-4.34)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.58 (at 4.29Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.198 , 0.267 (Not available) , 0.305	Depositor DCC
R_{free} test set	2005 reflections (7.01%)	wwPDB-VP
Wilson B-factor (Å ²)	52.4	Xtriage
Anisotropy	0.747	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 46.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	25949	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.34% 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: 88D, ZN, 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	0.32	0/1730	0.80	4/2354 (0.2%)
1	B	0.31	0/1731	0.79	1/2356 (0.0%)
2	C	0.31	0/8873	0.76	8/12031 (0.1%)
3	D	0.32	0/10052	0.78	6/13591 (0.0%)
4	E	0.31	0/650	0.76	0/886
5	F	0.31	0/2585	0.77	0/3485
6	H	0.21	0/535	0.37	0/826
7	G	0.22	0/269	0.34	0/413
All	All	0.31	0/26425	0.76	19/35942 (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	6.46	126.69	119.32
3	D	1126	GLY	C-N-CA	6.46	126.69	119.32
2	C	46	GLU	CA-C-N	-6.25	112.02	119.84
2	C	46	GLU	C-N-CA	-6.25	112.02	119.84
3	D	797	ASN	CA-C-N	5.89	125.59	119.05
3	D	797	ASN	C-N-CA	5.89	125.59	119.05
2	C	1019	PHE	CA-C-N	5.66	125.51	119.28
2	C	1019	PHE	C-N-CA	5.66	125.51	119.28
3	D	321	PRO	CA-C-N	5.63	125.30	119.05
3	D	321	PRO	C-N-CA	5.63	125.30	119.05
2	C	687	CYS	CA-C-N	5.52	125.44	119.76
2	C	687	CYS	C-N-CA	5.52	125.44	119.76
1	A	120	ASN	CA-C-N	5.39	124.91	119.19
1	A	120	ASN	C-N-CA	5.39	124.91	119.19
2	C	773	ILE	CA-C-N	5.18	125.47	119.93
2	C	773	ILE	C-N-CA	5.18	125.47	119.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	14	LEU	N-CA-C	5.16	118.09	110.46
1	A	147	VAL	CA-C-N	5.07	125.00	119.78
1	A	147	VAL	C-N-CA	5.07	125.00	119.78

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	26	0
1	B	1706	0	1730	29	0
2	C	8714	0	8636	171	0
3	D	9887	0	9943	195	0
4	E	637	0	635	14	0
5	F	2555	0	2579	60	0
6	H	476	0	261	14	0
7	G	241	0	137	4	0
8	D	2	0	0	0	0
9	D	1	0	0	0	0
10	D	26	0	0	1	0
All	All	25949	0	25662	457	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 9.

All (457) 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:891:CYS:SG	3:D:975:CYS:HB3	2.07	0.95
3:D:902:ALA:HB3	3:D:958:THR:HG22	1.53	0.90
6:H:16:DC:O2	7:G:12:DG:N2	2.06	0.89
3:D:900:GLU:OE1	3:D:959:GLN:NE2	2.06	0.87
3:D:901:LEU:HD22	3:D:901:LEU:O	1.85	0.77
5:F:470:ARG:HB3	5:F:506:ILE:HD13	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:910:LEU:HD12	3:D:910:LEU:O	1.86	0.75
3:D:1090:LYS:HB3	3:D:1092:GLU:HG2	1.69	0.75
3:D:965:VAL:HG13	3:D:974:VAL:HG11	1.68	0.75
3:D:901:LEU:HD13	3:D:901:LEU:C	2.14	0.72
2:C:211:TRP:HB2	2:C:227:ASP:HA	1.73	0.71
3:D:913:ASP:OD1	3:D:914:PRO:HD2	1.90	0.70
3:D:409:LYS:NZ	7:G:14:DG:OP1	2.22	0.70
2:C:483:MET:HE3	2:C:498:GLY:HA3	1.72	0.70
5:F:477:LEU:HD13	5:F:492:ILE:HG23	1.72	0.70
2:C:113:ASP:HB2	2:C:132:PRO:HG2	1.75	0.68
2:C:279:ARG:HD3	5:F:215:ALA:HB1	1.74	0.68
1:A:40:ARG:NH1	2:C:1013:GLY:O	2.27	0.68
3:D:107:PHE:HZ	3:D:126:GLU:HG2	1.59	0.67
2:C:1119:GLU:OE2	3:D:89:ARG:NH2	2.27	0.67
1:A:87:SER:O	1:A:142:ARG:NH1	2.27	0.66
2:C:396:MET:HE1	2:C:418:ILE:HG23	1.77	0.66
2:C:954:ASP:O	2:C:958:ARG:NH1	2.28	0.66
3:D:1165:VAL:HG12	3:D:1205:PRO:HA	1.79	0.66
5:F:522:VAL:HG23	5:F:523:LEU:HD12	1.78	0.65
1:A:107:ALA:HB2	1:A:123:MET:HE2	1.79	0.65
3:D:900:GLU:CD	3:D:959:GLN:HE21	2.04	0.65
3:D:901:LEU:HD13	3:D:902:ALA:HB2	1.78	0.65
2:C:1087:GLU:HG3	2:C:1091:ILE:HD11	1.78	0.64
5:F:256:GLY:HA3	5:F:288:GLY:HA3	1.79	0.64
3:D:130:TYR:OH	3:D:379:ASP:OD2	2.11	0.64
2:C:101:GLY:O	2:C:142:ASN:ND2	2.30	0.64
3:D:1092:GLU:HG3	3:D:1094:GLY:H	1.61	0.64
1:A:197:GLU:OE1	2:C:996:ARG:NH1	2.29	0.64
2:C:104:SER:HB3	2:C:140:ILE:HB	1.79	0.64
3:D:573:PRO:HB2	3:D:576:MET:HE2	1.80	0.64
1:A:152:ASN:HB3	1:A:163:PRO:HB3	1.80	0.64
2:C:182:SER:HB2	2:C:377:ARG:HB2	1.79	0.63
3:D:442:GLY:HA3	3:D:523:GLN:HB2	1.80	0.63
5:F:423:LEU:HA	5:F:435:LEU:HD23	1.80	0.63
3:D:1125:GLN:HB3	3:D:1129:GLU:HG2	1.81	0.63
3:D:545:LEU:HD12	3:D:546:PRO:HD2	1.81	0.63
3:D:638:THR:HG23	3:D:639:GLN:HG2	1.81	0.62
2:C:178:GLN:HG2	2:C:180:VAL:HG13	1.81	0.62
2:C:1148:ARG:NH1	3:D:86:LYS:O	2.33	0.62
2:C:401:ARG:HA	2:C:404:MET:HE2	1.82	0.62
2:C:239:LYS:NZ	2:C:265:ASP:OD2	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:343:LEU:HD13	3:D:381:LEU:HA	1.81	0.62
3:D:738:VAL:HG13	3:D:841:ARG:HD3	1.82	0.61
3:D:882:GLN:HE22	3:D:1249:LYS:HG3	1.65	0.61
4:E:42:GLU:O	4:E:46:ARG:NH1	2.34	0.61
1:B:92:PRO:HB3	1:B:141:GLU:HG2	1.82	0.60
3:D:1065:THR:HG23	3:D:1076:VAL:HB	1.84	0.60
3:D:363:PRO:HD2	3:D:366:ILE:HD12	1.83	0.60
3:D:745:ILE:HD13	3:D:784:GLU:HG2	1.84	0.59
3:D:905:ALA:HB1	3:D:907:ASP:OD1	2.02	0.59
5:F:401:LYS:HA	5:F:405:ILE:HA	1.83	0.59
2:C:168:ILE:HG12	2:C:431:PHE:HB3	1.84	0.59
1:A:214:THR:HA	1:B:230:GLU:HG2	1.85	0.59
5:F:470:ARG:HH11	5:F:506:ILE:HD11	1.67	0.59
3:D:1274:PRO:HB3	4:E:82:LEU:HD11	1.85	0.59
2:C:1045:SER:OG	2:C:1046:THR:N	2.32	0.59
2:C:464:SER:HB3	2:C:467:ARG:HG3	1.85	0.59
2:C:815:THR:HG22	2:C:817:GLU:H	1.67	0.58
3:D:325:ARG:NH1	3:D:341:ASN:OD1	2.32	0.58
2:C:348:LEU:HD13	2:C:365:VAL:HG12	1.84	0.58
3:D:104:ILE:HD12	3:D:379:ASP:HB3	1.86	0.58
3:D:1089:PHE:HA	3:D:1095:SER:HA	1.85	0.58
2:C:899:LEU:HB2	2:C:904:MET:HE1	1.85	0.58
2:C:544:ALA:HB2	2:C:580:ASP:HB2	1.85	0.57
2:C:189:GLU:HB2	2:C:367:THR:HG21	1.85	0.57
2:C:453:ARG:NH1	2:C:500:LEU:O	2.38	0.57
2:C:738:SER:HA	2:C:904:MET:HE3	1.86	0.57
2:C:119:VAL:HG13	2:C:167:ILE:HD11	1.86	0.57
5:F:242:ASN:OD1	5:F:243:ALA:N	2.38	0.57
2:C:487:GLU:OE2	2:C:613:ARG:NH1	2.37	0.57
2:C:549:ASP:HB3	2:C:553:ARG:H	1.68	0.57
2:C:919:THR:HG23	3:D:731:VAL:HG23	1.86	0.57
3:D:990:ASP:OD1	3:D:990:ASP:N	2.36	0.57
3:D:1030:ARG:HH21	3:D:1137:GLU:HG2	1.70	0.57
2:C:934:THR:HG23	2:C:1026:GLY:HA3	1.87	0.56
3:D:600:GLN:HB2	3:D:609:THR:HB	1.86	0.56
3:D:930:VAL:HG22	3:D:936:VAL:HG12	1.86	0.56
4:E:60:ARG:NE	4:E:98:GLU:OE2	2.37	0.56
3:D:556:ARG:HG3	4:E:35:ILE:HG12	1.87	0.56
1:B:183:VAL:HG12	1:B:184:GLU:HG2	1.87	0.56
3:D:891:CYS:HB2	3:D:968:CYS:SG	2.45	0.56
3:D:912:ARG:NH1	3:D:916:ILE:HD12	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:127:LYS:HA	3:D:132:ALA:HB3	1.87	0.56
1:B:39:ARG:NH2	3:D:623:ASP:OD2	2.39	0.55
3:D:578:ARG:H	3:D:581:MET:HE3	1.70	0.55
5:F:470:ARG:HH12	5:F:498:VAL:HG11	1.71	0.55
3:D:1085:ARG:HA	3:D:1112:MET:HA	1.87	0.55
2:C:1012:ASP:OD2	3:D:726:ARG:NH2	2.40	0.55
3:D:905:ALA:HB2	3:D:911:ILE:HG13	1.87	0.55
5:F:302:LEU:O	5:F:305:SER:OG	2.24	0.55
2:C:1080:GLY:HA3	4:E:51:TYR:HE1	1.71	0.55
6:H:15:DT:H2''	6:H:16:DC:H5'	1.88	0.55
3:D:356:ARG:HH21	3:D:360:LEU:HD11	1.71	0.55
2:C:757:ILE:HD12	2:C:837:LEU:HB2	1.89	0.55
2:C:561:VAL:HG21	2:C:571:VAL:HB	1.89	0.55
2:C:1007:LYS:HA	2:C:1024:THR:HA	1.89	0.55
1:A:64:THR:OG1	1:A:65:THR:N	2.40	0.54
3:D:107:PHE:CZ	3:D:126:GLU:HG2	2.42	0.54
2:C:140:ILE:HA	2:C:147:ILE:HG12	1.88	0.54
3:D:190:LYS:HE3	3:D:192:ASP:HB3	1.89	0.54
3:D:459:ARG:HA	3:D:462:ASP:HB2	1.88	0.54
3:D:910:LEU:HD12	3:D:910:LEU:C	2.31	0.54
1:B:90:ASP:HA	1:B:142:ARG:HD3	1.88	0.54
3:D:676:LEU:HG	3:D:715:LYS:HB3	1.89	0.54
5:F:446:VAL:HB	5:F:449:ASP:HB2	1.89	0.54
1:B:77:ILE:HG22	1:B:81:LYS:HE3	1.89	0.54
2:C:1055:GLN:HG2	2:C:1094:ASP:HB3	1.90	0.54
1:A:213:LYS:HD3	1:B:227:VAL:HG23	1.90	0.54
3:D:595:ASP:HB3	3:D:631:ALA:HB2	1.89	0.54
1:B:97:LEU:HD22	1:B:110:ILE:HG12	1.90	0.54
3:D:565:ILE:HG23	3:D:575:ALA:HB3	1.91	0.53
3:D:895:ARG:NH1	3:D:967:THR:O	2.41	0.53
3:D:905:ALA:HB3	3:D:908:GLY:O	2.08	0.53
5:F:510:THR:HA	5:F:513:LYS:HB2	1.90	0.53
2:C:1141:ASP:OD1	2:C:1142:GLY:N	2.38	0.53
5:F:386:LEU:HD12	5:F:399:LEU:HD23	1.90	0.53
3:D:111:PRO:O	3:D:113:ARG:NH1	2.41	0.53
3:D:908:GLY:O	3:D:909:THR:OG1	2.25	0.53
7:G:15:DT:H2'	7:G:16:DC:C6	2.44	0.53
3:D:67:ARG:HD2	3:D:69:ARG:NE	2.24	0.53
2:C:848:ILE:HD13	2:C:874:ALA:HB2	1.91	0.52
5:F:499:THR:OG1	5:F:500:ARG:N	2.29	0.52
4:E:46:ARG:NE	4:E:102:ASP:OD1	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:901:LEU:HD22	3:D:901:LEU:C	2.35	0.52
3:D:1139:GLN:O	3:D:1143:ARG:HG2	2.10	0.52
2:C:513:GLU:HB3	2:C:530:TYR:HB3	1.91	0.52
3:D:438:LEU:O	3:D:561:SER:OG	2.21	0.52
3:D:1010:LEU:HA	3:D:1145:GLN:HG3	1.90	0.52
3:D:901:LEU:HD13	3:D:902:ALA:N	2.24	0.52
2:C:378:LEU:HD21	2:C:455:LEU:HD22	1.91	0.51
3:D:760:PHE:CG	3:D:770:ARG:HD2	2.45	0.51
4:E:56:TYR:HE2	4:E:99:ILE:HG12	1.75	0.51
4:E:70:GLN:O	4:E:74:GLY:N	2.35	0.51
1:B:170:PRO:HA	1:B:199:LYS:HD2	1.92	0.51
1:B:84:VAL:HG12	1:B:199:LYS:HD3	1.91	0.51
3:D:257:GLY:O	3:D:260:SER:OG	2.28	0.51
3:D:676:LEU:HD23	3:D:716:LEU:HD23	1.92	0.51
1:A:62:GLU:HG3	1:A:77:ILE:HD12	1.92	0.51
3:D:350:ARG:HD3	3:D:373:MET:HE3	1.93	0.51
3:D:589:THR:HG21	3:D:688:MET:HG2	1.93	0.51
3:D:599:TYR:HA	3:D:610:GLY:HA3	1.92	0.51
3:D:505:HIS:CE1	3:D:507:LEU:HB2	2.45	0.51
2:C:43:LYS:NZ	2:C:544:ALA:O	2.42	0.51
2:C:587:VAL:HB	2:C:591:THR:HB	1.93	0.51
2:C:1024:THR:H	3:D:730:THR:HG21	1.76	0.51
2:C:1041:ILE:HD11	3:D:447:MET:HG3	1.92	0.51
3:D:60:CYS:SG	3:D:61:TYR:N	2.83	0.51
3:D:1164:ARG:HH11	3:D:1208:MET:HE1	1.76	0.51
5:F:241:LEU:HD23	5:F:246:GLU:HG2	1.92	0.51
2:C:446:LEU:HD13	2:C:593:MET:HE1	1.93	0.51
1:A:18:ARG:NH1	2:C:997:ASP:OD1	2.43	0.50
2:C:1125:LEU:HD22	2:C:1135:VAL:HG11	1.93	0.50
2:C:891:ASN:ND2	2:C:930:GLN:OE1	2.44	0.50
3:D:1166:THR:HB	3:D:1206:VAL:HG21	1.92	0.50
2:C:1049:TYR:OH	3:D:423:ASP:OD2	2.24	0.50
5:F:360:ALA:HB1	5:F:373:VAL:HG21	1.92	0.50
2:C:376:ARG:NE	6:H:14:DG:O6	2.45	0.50
1:A:56:ILE:HB	1:A:59:VAL:HB	1.92	0.50
2:C:1148:ARG:NH1	3:D:86:LYS:HG3	2.27	0.50
3:D:666:THR:OG1	3:D:667:THR:N	2.44	0.50
6:H:12:DC:H1'	6:H:13:DT:C2	2.47	0.50
2:C:473:ARG:HB3	2:C:495:GLY:HA3	1.94	0.50
3:D:1273:GLN:O	4:E:105:GLU:N	2.44	0.50
1:B:27:GLU:HG3	1:B:28:PRO:HD2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:896:GLY:O	3:D:1128:ARG:NH1	2.45	0.49
2:C:344:TYR:OH	2:C:365:VAL:HA	2.12	0.49
1:B:72:ASP:OD1	1:B:73:VAL:N	2.45	0.49
3:D:505:HIS:HD2	3:D:1005:GLU:HG3	1.77	0.49
3:D:826:ASN:HD22	3:D:832:ILE:HD11	1.76	0.49
3:D:873:LEU:HA	3:D:876:ARG:HE	1.78	0.49
1:A:175:THR:OG1	1:A:176:TYR:N	2.46	0.49
3:D:64:LYS:NZ	3:D:76:GLU:OE2	2.33	0.49
3:D:339:ASP:OD1	5:F:422:SER:OG	2.15	0.49
3:D:859:GLY:O	3:D:863:THR:OG1	2.20	0.49
3:D:1090:LYS:HG2	3:D:1091:HIS:H	1.77	0.49
1:B:83:LEU:HD11	1:B:118:VAL:HG13	1.95	0.48
3:D:456:VAL:HG22	3:D:490:VAL:HG21	1.95	0.48
3:D:1128:ARG:O	3:D:1132:ILE:HG13	2.13	0.48
5:F:328:LEU:HD13	5:F:351:ILE:HD11	1.95	0.48
2:C:48:LEU:HD12	2:C:528:ILE:HD13	1.94	0.48
2:C:726:TRP:H	2:C:730:ASN:HD21	1.62	0.48
2:C:1070:GLU:OE1	3:D:875:ARG:NH2	2.42	0.48
3:D:492:ALA:HB3	4:E:90:LYS:HE2	1.95	0.48
2:C:757:ILE:HB	2:C:837:LEU:HD22	1.95	0.48
5:F:262:LEU:O	5:F:266:LEU:HG	2.14	0.48
1:A:185:GLN:HG2	1:A:186:ARG:H	1.79	0.48
2:C:315:LYS:NZ	2:C:374:GLY:O	2.38	0.48
2:C:1102:VAL:HG13	2:C:1112:ILE:HD12	1.96	0.48
4:E:33:LEU:HD23	4:E:33:LEU:H	1.78	0.48
1:A:97:LEU:HD21	1:A:105:VAL:HG21	1.96	0.48
3:D:1170:SER:O	3:D:1173:THR:OG1	2.31	0.48
2:C:141:ASN:ND2	2:C:144:THR:OG1	2.37	0.48
2:C:628:THR:N	2:C:631:GLU:OE2	2.45	0.48
2:C:758:ASP:N	2:C:758:ASP:OD1	2.46	0.48
3:D:127:LYS:O	3:D:133:ALA:N	2.47	0.48
2:C:150:GLN:HG2	2:C:414:PRO:HG2	1.96	0.47
3:D:83:THR:HG22	3:D:84:ARG:H	1.79	0.47
5:F:499:THR:HG1	5:F:500:ARG:H	1.59	0.47
2:C:50:VAL:O	2:C:633:ARG:NH1	2.45	0.47
2:C:1089:LEU:HB3	3:D:420:LYS:NZ	2.29	0.47
1:A:191:LYS:HE2	1:A:193:ILE:HD11	1.96	0.47
3:D:891:CYS:SG	3:D:975:CYS:CB	2.87	0.47
5:F:320:LEU:HD21	5:F:359:MET:HE3	1.96	0.47
1:B:26:LEU:HD12	1:B:31:GLY:HA2	1.95	0.47
2:C:371:ASP:OD1	6:H:14:DG:N2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:467:ARG:NH2	6:H:15:DT:H71	2.30	0.47
3:D:369:ASN:O	3:D:373:MET:HG3	2.14	0.47
2:C:678:SER:OG	2:C:682:THR:N	2.47	0.47
2:C:704:ASP:HB2	2:C:708:THR:HB	1.95	0.47
2:C:822:ARG:NE	2:C:829:ALA:HB2	2.30	0.47
3:D:373:MET:SD	5:F:318:LEU:HB3	2.54	0.47
3:D:774:LEU:HD23	3:D:777:ILE:HD12	1.96	0.47
3:D:828:LYS:HE3	3:D:830:GLU:HB2	1.97	0.47
3:D:945:GLY:O	3:D:949:ILE:HG12	2.15	0.47
5:F:269:ARG:NH1	5:F:271:GLU:OE1	2.47	0.47
5:F:382:ILE:HG21	5:F:402:GLU:HG2	1.97	0.47
3:D:438:LEU:HD13	3:D:527:LEU:HD12	1.97	0.47
6:H:15:DT:H2''	6:H:16:DC:H6	1.79	0.47
1:A:96:TYR:O	1:A:111:VAL:N	2.46	0.47
2:C:726:TRP:N	2:C:730:ASN:HD21	2.14	0.46
2:C:959:LEU:HD12	2:C:960:PRO:HD2	1.97	0.46
2:C:1043:ALA:HB2	3:D:447:MET:HE3	1.97	0.46
5:F:489:LEU:H	5:F:489:LEU:HD23	1.80	0.46
3:D:454:PRO:HA	3:D:457:MET:HE2	1.96	0.46
2:C:658:ILE:HD11	2:C:688:PRO:HB3	1.97	0.46
2:C:762:THR:OG1	2:C:763:LYS:N	2.48	0.46
5:F:329:ILE:O	5:F:332:VAL:HG12	2.15	0.46
5:F:474:VAL:HA	5:F:477:LEU:HB2	1.97	0.46
3:D:910:LEU:C	3:D:910:LEU:CD1	2.88	0.46
5:F:510:THR:HG22	5:F:514:LEU:HG	1.98	0.46
2:C:596:PHE:HB3	2:C:599:HIS:CD2	2.51	0.46
3:D:901:LEU:HD13	3:D:902:ALA:CB	2.43	0.46
3:D:1220:TRP:NE1	3:D:1243:ASP:HB2	2.30	0.46
5:F:345:THR:HA	6:H:5:DA:N7	2.31	0.46
2:C:1122:LYS:HE2	2:C:1148:ARG:HG2	1.98	0.46
2:C:211:TRP:HZ2	6:H:13:DT:H1'	1.81	0.46
2:C:1148:ARG:HH11	3:D:86:LYS:HG3	1.81	0.46
5:F:474:VAL:HA	5:F:477:LEU:HD12	1.97	0.46
2:C:472:VAL:HG22	6:H:14:DG:N2	2.31	0.46
2:C:474:ASP:HA	3:D:857:ARG:HD2	1.96	0.46
3:D:1087:ARG:HG2	3:D:1098:VAL:HG22	1.97	0.46
3:D:924:THR:HG22	3:D:943:ASP:HA	1.98	0.45
2:C:315:LYS:HD2	2:C:315:LYS:HA	1.82	0.45
2:C:1089:LEU:HB3	3:D:420:LYS:HZ2	1.80	0.45
3:D:34:ILE:HG22	3:D:41:PRO:HA	1.97	0.45
3:D:1086:LEU:HA	3:D:1113:GLU:HG2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:67:ARG:HB3	3:D:69:ARG:HG2	1.98	0.45
3:D:373:MET:O	3:D:377:SER:OG	2.29	0.45
5:F:468:SER:OG	5:F:469:GLU:N	2.49	0.45
2:C:41:PHE:HB2	2:C:979:GLY:HA2	1.98	0.45
2:C:200:HIS:CD2	2:C:348:LEU:HG	2.52	0.45
2:C:615:ALA:HB3	2:C:715:LEU:HD22	1.98	0.45
3:D:238:GLU:OE2	3:D:242:ARG:NH1	2.47	0.45
2:C:974:THR:HG23	2:C:980:ALA:H	1.81	0.45
3:D:1218:ASP:OD1	3:D:1218:ASP:N	2.48	0.45
1:A:129:ASN:OD1	1:A:130:ASP:N	2.43	0.45
3:D:1220:TRP:CD1	3:D:1243:ASP:HB2	2.52	0.45
5:F:330:ARG:HH21	5:F:350:TRP:HZ3	1.65	0.45
2:C:400:VAL:O	2:C:404:MET:HG3	2.17	0.45
2:C:821:LEU:HD22	5:F:456:LEU:HD11	1.99	0.45
2:C:1104:GLU:HB2	5:F:451:VAL:HG22	1.98	0.45
2:C:1126:LYS:HA	2:C:1126:LYS:HD3	1.77	0.45
3:D:321:PRO:HA	3:D:322:PRO:HD3	1.74	0.45
3:D:866:ARG:NH1	3:D:1008:THR:O	2.37	0.45
3:D:1176:LEU:H	3:D:1176:LEU:HD12	1.80	0.45
2:C:344:TYR:OH	2:C:364:PRO:O	2.33	0.45
2:C:733:ASP:OD2	2:C:925:ARG:NH2	2.50	0.45
5:F:364:ARG:HG3	5:F:368:ILE:HG12	1.97	0.45
2:C:338:VAL:O	2:C:342:ILE:HG13	2.16	0.44
2:C:372:HIS:CE1	2:C:533:ALA:HB1	2.52	0.44
3:D:586:TYR:O	3:D:590:THR:OG1	2.30	0.44
1:A:149:ALA:N	1:A:165:ASP:OD2	2.46	0.44
1:B:39:ARG:HH21	1:B:173:LYS:NZ	2.15	0.44
3:D:460:LEU:HD23	3:D:460:LEU:HA	1.88	0.44
3:D:666:THR:HG21	3:D:683:PHE:CE2	2.52	0.44
2:C:441:ASP:O	2:C:447:SER:OG	2.35	0.44
2:C:922:VAL:H	2:C:923:PRO:HD2	1.81	0.44
1:A:129:ASN:ND2	2:C:652:GLU:HG3	2.32	0.44
2:C:596:PHE:HB3	2:C:599:HIS:HD2	1.82	0.44
3:D:344:TYR:O	3:D:348:ILE:HG13	2.18	0.44
3:D:1090:LYS:HE3	3:D:1104:HIS:H	1.82	0.44
5:F:383:GLN:O	5:F:387:LEU:HB2	2.16	0.44
2:C:944:TRP:HA	2:C:993:LEU:HG	1.98	0.44
3:D:1054:ARG:HB3	3:D:1065:THR:HB	2.00	0.44
6:H:11:DG:H5"	6:H:12:DC:C4	2.53	0.44
2:C:126:ASP:HA	2:C:170:GLY:HA3	2.00	0.44
2:C:653:VAL:HG23	2:C:658:ILE:HG12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:506:ILE:HA	5:F:509:LYS:HD2	1.99	0.44
2:C:252:PHE:HB3	2:C:258:MET:HG3	2.00	0.44
2:C:313:ARG:HH22	2:C:337:ASP:CG	2.25	0.44
2:C:815:THR:HG21	5:F:453:PHE:CE1	2.53	0.44
3:D:756:VAL:HG21	3:D:777:ILE:HD11	1.99	0.44
2:C:762:THR:HG23	2:C:764:LEU:H	1.83	0.44
1:B:178:VAL:HG22	1:B:192:LEU:HD13	1.99	0.44
3:D:641:ARG:HA	3:D:642:PRO:HD2	1.87	0.44
3:D:1221:LEU:HB2	3:D:1243:ASP:OD2	2.17	0.44
5:F:347:ALA:O	5:F:351:ILE:HG13	2.18	0.44
2:C:46:GLU:N	2:C:47:PRO:HD3	2.33	0.43
2:C:789:ILE:HD12	2:C:869:VAL:HG11	2.00	0.43
2:C:974:THR:HG23	2:C:979:GLY:HA3	1.99	0.43
2:C:28:SER:N	2:C:962:GLU:OE1	2.51	0.43
2:C:1127:GLU:O	2:C:1130:SER:OG	2.33	0.43
1:A:223:ARG:HD3	1:B:213:LYS:HB2	2.00	0.43
1:B:8:THR:HA	1:B:25:PRO:HD2	1.98	0.43
1:B:112:PRO:HA	1:B:113:PRO:HD3	1.86	0.43
2:C:233:PRO:HB2	2:C:236:VAL:HG23	2.01	0.43
2:C:419:ASN:O	2:C:422:PRO:HD2	2.18	0.43
2:C:557:PRO:O	2:C:573:SER:N	2.52	0.43
2:C:1079:TYR:CD2	3:D:559:MET:HG2	2.53	0.43
3:D:266:GLU:HA	3:D:310:MET:HE1	2.01	0.43
4:E:95:ALA:O	4:E:98:GLU:HG2	2.19	0.43
5:F:231:TYR:O	5:F:235:ILE:HG13	2.18	0.43
3:D:901:LEU:C	3:D:901:LEU:CD1	2.85	0.43
1:A:225:LEU:HD13	1:A:225:LEU:H	1.83	0.43
1:B:28:PRO:HD3	1:B:189:PHE:HA	2.01	0.43
2:C:599:HIS:HB3	2:C:928:ILE:HD12	2.01	0.43
3:D:57:ASP:HB3	3:D:58:TRP:CE3	2.54	0.43
3:D:847:LEU:HB3	10:D:1404:88D:CAO	2.48	0.43
2:C:321:GLY:HA3	2:C:363:VAL:HG21	2.01	0.43
2:C:396:MET:HE3	2:C:396:MET:HB2	1.82	0.43
3:D:1099:LEU:HD23	3:D:1099:LEU:HA	1.80	0.43
1:B:110:ILE:O	1:B:112:PRO:HD3	2.18	0.43
3:D:29:LYS:O	3:D:352:ASN:ND2	2.50	0.43
3:D:69:ARG:HD2	3:D:70:PHE:CZ	2.53	0.43
2:C:253:GLY:HA2	2:C:259:ARG:HE	1.83	0.43
3:D:36:TYR:HE1	5:F:372:MET:HE3	1.83	0.43
3:D:95:ILE:HD13	3:D:348:ILE:HG12	2.01	0.43
3:D:365:ILE:HG21	5:F:297:GLU:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:417:LEU:HD13	3:D:1253:ILE:HG23	2.01	0.43
1:B:95:MET:HE3	1:B:140:VAL:HG21	2.01	0.43
2:C:408:ASP:OD1	2:C:408:ASP:N	2.42	0.43
3:D:67:ARG:HD2	3:D:69:ARG:HE	1.84	0.43
3:D:1244:LYS:O	3:D:1246:ASN:N	2.51	0.43
5:F:317:PHE:O	5:F:321:ILE:HG13	2.19	0.43
5:F:503:ILE:HD12	5:F:503:ILE:HA	1.89	0.43
1:A:27:GLU:HB2	1:A:30:PHE:HB2	2.01	0.43
1:A:130:ASP:O	1:A:131:LYS:HG2	2.19	0.43
2:C:691:ASP:N	2:C:694:ASP:OD2	2.49	0.43
3:D:588:LEU:HD12	3:D:589:THR:HG23	2.01	0.43
3:D:1247:GLY:H	3:D:1251:ASN:ND2	2.17	0.43
5:F:345:THR:HB	6:H:4:DA:H8	1.83	0.43
5:F:515:ARG:O	5:F:519:ARG:HG2	2.19	0.43
2:C:232:GLN:OE1	2:C:280:LYS:HG3	2.19	0.42
3:D:240:LEU:O	3:D:244:LEU:N	2.51	0.42
3:D:475:MET:HE2	3:D:475:MET:HB3	1.87	0.42
3:D:1065:THR:HA	3:D:1076:VAL:HA	2.01	0.42
4:E:95:ALA:O	4:E:99:ILE:HG13	2.19	0.42
5:F:231:TYR:CE2	5:F:235:ILE:HD11	2.54	0.42
2:C:840:PRO:HB2	2:C:843:GLU:HG3	2.01	0.42
3:D:772:GLU:O	3:D:776:GLU:HG2	2.19	0.42
3:D:798:PRO:HA	3:D:801:THR:HB	2.00	0.42
3:D:1127:PRO:O	3:D:1130:VAL:HG12	2.19	0.42
1:B:79:ASN:ND2	3:D:636:ARG:HH22	2.17	0.42
2:C:39:VAL:O	2:C:973:SER:N	2.53	0.42
3:D:891:CYS:O	3:D:892:GLN:HB2	2.19	0.42
5:F:372:MET:O	5:F:376:ILE:HG13	2.19	0.42
5:F:499:THR:HG23	5:F:500:ARG:HD2	2.01	0.42
2:C:594:ILE:HA	2:C:595:PRO:HD2	1.93	0.42
3:D:97:LEU:HD23	3:D:374:LEU:HD11	2.01	0.42
3:D:964:SER:OG	3:D:1155:GLU:OE1	2.35	0.42
1:B:11:GLU:HB2	1:B:22:VAL:HB	2.01	0.42
2:C:180:VAL:HG22	2:C:379:ARG:HG2	2.02	0.42
3:D:117:LEU:HD12	3:D:299:VAL:HG22	2.02	0.42
3:D:901:LEU:CD1	3:D:902:ALA:HB2	2.46	0.42
1:A:100:GLN:HG2	1:A:101:GLY:H	1.84	0.42
2:C:308:LEU:HB3	2:C:312:GLY:C	2.45	0.42
2:C:388:GLN:HG3	2:C:430:PHE:CD1	2.55	0.42
2:C:522:GLY:O	2:C:553:ARG:HA	2.19	0.42
3:D:275:GLU:OE2	3:D:278:ARG:NH1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:882:GLN:OE1	3:D:1249:LYS:HB2	2.19	0.42
2:C:731:TYR:HE1	3:D:579:LEU:HB2	1.85	0.42
2:C:1021:TYR:HB2	3:D:728:GLY:HA3	2.02	0.42
3:D:48:CYS:SG	3:D:50:LYS:HB3	2.60	0.42
4:E:60:ARG:HG2	4:E:104:LEU:HD11	2.01	0.42
5:F:303:VAL:HG22	5:F:351:ILE:HD13	2.01	0.42
5:F:502:ARG:O	5:F:506:ILE:HG13	2.20	0.42
2:C:318:LYS:NZ	2:C:534:ASP:OD2	2.51	0.42
2:C:950:LYS:HE3	2:C:950:LYS:HB2	1.92	0.42
3:D:717:LYS:HE2	3:D:717:LYS:HB3	1.79	0.42
1:B:173:LYS:HA	1:B:173:LYS:HD2	1.86	0.42
2:C:579:MET:HE3	2:C:579:MET:HB2	1.92	0.42
2:C:1084:THR:O	2:C:1088:LEU:HG	2.20	0.42
3:D:882:GLN:C	3:D:884:VAL:H	2.26	0.42
5:F:378:LYS:HD3	5:F:381:ARG:HH11	1.85	0.42
2:C:178:GLN:HB3	2:C:379:ARG:HG3	2.02	0.42
2:C:1127:GLU:OE1	3:D:412:ARG:NH2	2.46	0.42
2:C:47:PRO:HG2	2:C:581:VAL:O	2.20	0.41
2:C:190:THR:HG23	2:C:199:LEU:HB2	2.02	0.41
3:D:912:ARG:HG2	3:D:916:ILE:HD12	2.01	0.41
3:D:1187:GLU:O	3:D:1191:ARG:HB2	2.19	0.41
5:F:406:THR:HG22	5:F:409:LYS:H	1.85	0.41
1:B:100:GLN:HG3	1:B:133:LYS:HA	2.01	0.41
2:C:183:PRO:HB2	2:C:312:GLY:HA2	2.02	0.41
3:D:49:GLU:OE2	3:D:55:THR:N	2.43	0.41
3:D:497:LEU:O	3:D:543:VAL:HA	2.21	0.41
3:D:913:ASP:HB3	3:D:916:ILE:HG13	2.02	0.41
2:C:157:PHE:HA	2:C:158:PRO:HD3	1.95	0.41
2:C:658:ILE:HG21	2:C:702:ILE:HD12	2.02	0.41
2:C:885:LEU:HG	2:C:895:ILE:HD11	2.02	0.41
3:D:36:TYR:CE1	3:D:37:ARG:HG3	2.55	0.41
1:A:146:TYR:CG	2:C:743:GLU:HG2	2.56	0.41
2:C:211:TRP:HH2	6:H:14:DG:OP1	2.02	0.41
2:C:597:LEU:HB3	2:C:976:VAL:HG13	2.02	0.41
2:C:809:LYS:HD2	2:C:833:ARG:HB2	2.02	0.41
2:C:1041:ILE:HG13	3:D:428:SER:HB2	2.02	0.41
3:D:102:THR:H	3:D:375:GLN:HE22	1.68	0.41
2:C:298:ASN:O	2:C:305:ARG:HB2	2.21	0.41
2:C:540:VAL:HG13	2:C:561:VAL:HG13	2.01	0.41
3:D:505:HIS:CD2	3:D:1005:GLU:HG3	2.54	0.41
2:C:928:ILE:H	2:C:928:ILE:HG13	1.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:153:ALA:O	3:D:157:VAL:HG23	2.19	0.41
3:D:1221:LEU:HG	3:D:1253:ILE:HD12	2.01	0.41
5:F:483:ASP:OD2	5:F:487:ARG:NE	2.53	0.41
3:D:114:LEU:HD23	3:D:114:LEU:HA	1.77	0.41
1:B:84:VAL:HG23	1:B:119:HIS:HB2	2.02	0.41
2:C:33:PRO:HG2	2:C:632:LEU:HD21	2.02	0.41
2:C:408:ASP:O	2:C:412:ILE:HG13	2.21	0.41
3:D:473:LYS:HD2	5:F:448:VAL:HG21	2.02	0.41
3:D:592:VAL:HA	3:D:593:PRO:HD3	1.89	0.41
2:C:356:THR:HG22	2:C:362:GLU:HA	2.02	0.41
2:C:925:ARG:HB2	2:C:927:ASN:OD1	2.21	0.41
2:C:1019:PHE:HA	2:C:1020:PRO:HD3	1.78	0.41
2:C:1094:ASP:OD1	2:C:1119:GLU:N	2.53	0.41
3:D:210:ASP:O	3:D:214:ARG:HG3	2.21	0.41
3:D:545:LEU:HA	3:D:546:PRO:HD2	1.96	0.41
5:F:403:MET:HG3	5:F:404:ASP:H	1.86	0.41
1:B:45:SER:OG	1:B:214:THR:HG21	2.20	0.41
2:C:115:VAL:HG11	2:C:129:TYR:CE1	2.57	0.40
2:C:604:ARG:CZ	2:C:925:ARG:HD2	2.51	0.40
3:D:613:SER:N	3:D:617:GLU:OE1	2.38	0.40
1:B:212:GLY:O	1:B:216:VAL:HG23	2.20	0.40
2:C:1052:ILE:O	3:D:89:ARG:NH1	2.53	0.40
5:F:339:LYS:C	5:F:341:TYR:H	2.29	0.40
2:C:41:PHE:O	2:C:979:GLY:HA2	2.21	0.40
2:C:230:ARG:HH12	7:G:8:DC:H5"	1.86	0.40
2:C:257:ILE:O	2:C:261:THR:OG1	2.34	0.40
2:C:558:ARG:HB3	2:C:570:TYR:HB3	2.03	0.40
2:C:815:THR:O	2:C:819:ARG:N	2.42	0.40
3:D:922:ALA:HB3	3:D:1150:HIS:CE1	2.57	0.40
1:A:89:GLU:HG3	1:A:93:VAL:HG11	2.03	0.40
2:C:773:ILE:HA	2:C:774:PRO:HD3	1.97	0.40
2:C:928:ILE:HG12	3:D:817:LEU:CD1	2.51	0.40
2:C:1139:SER:OG	2:C:1141:ASP:OD1	2.32	0.40
3:D:733:MET:HE2	3:D:733:MET:HB3	1.90	0.40
3:D:821:LYS:HB3	3:D:836:VAL:HB	2.04	0.40
3:D:823:LEU:HD13	3:D:831:PHE:HB3	2.03	0.40
5:F:449:ASP:O	5:F:452:SER:OG	2.38	0.40
6:H:16:DC:H2"	6:H:17:DA:C8	2.56	0.40
3:D:789:LEU:O	3:D:793:TYR:N	2.43	0.40
3:D:925:LEU:HD12	3:D:962:VAL:HG12	2.02	0.40
5:F:342:LYS:HE2	5:F:342:LYS:HB3	1.87	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%)	205 (92%)	16 (7%)	1 (0%)	24	62
1	B	221/347 (64%)	201 (91%)	17 (8%)	3 (1%)	9	39
2	C	1124/1178 (95%)	1042 (93%)	70 (6%)	12 (1%)	11	45
3	D	1261/1316 (96%)	1187 (94%)	67 (5%)	7 (1%)	21	58
4	E	79/110 (72%)	75 (95%)	4 (5%)	0	100	100
5	F	320/528 (61%)	301 (94%)	18 (6%)	1 (0%)	36	71
All	All	3227/3826 (84%)	3011 (93%)	192 (6%)	24 (1%)	18	55

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	227	VAL
3	D	593	PRO
3	D	678	PRO
3	D	971	SER
5	F	405	ILE
1	A	184	GLU
2	C	47	PRO
2	C	441	ASP
2	C	1134	ASN
3	D	658	PRO
3	D	1245	LEU
2	C	552	GLY
2	C	858	GLU
1	B	35	GLY
2	C	32	VAL
2	C	922	VAL
1	B	28	PRO

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Mol	Chain	Res	Type
2	C	33	PRO
2	C	905	PRO
2	C	109	ASP
2	C	520	VAL
2	C	1113	PRO
3	D	41	PRO
3	D	1168	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	192/297 (65%)	189 (98%)	3 (2%)	55	69
1	B	192/297 (65%)	192 (100%)	0	100	100
2	C	948/998 (95%)	919 (97%)	29 (3%)	35	56
3	D	1048/1095 (96%)	1017 (97%)	31 (3%)	36	57
4	E	68/90 (76%)	66 (97%)	2 (3%)	37	58
5	F	271/427 (64%)	262 (97%)	9 (3%)	33	55
All	All	2719/3204 (85%)	2645 (97%)	74 (3%)	39	59

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	136	VAL
1	A	159	ILE
1	A	225	LEU
2	C	39	VAL
2	C	48	LEU
2	C	80	VAL
2	C	185	VAL
2	C	257	ILE
2	C	322	LEU
2	C	346	VAL
2	C	370	ILE

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Mol	Chain	Res	Type
2	C	380	THR
2	C	396	MET
2	C	427	ILE
2	C	447	SER
2	C	472	VAL
2	C	500	LEU
2	C	589	VAL
2	C	598	GLU
2	C	621	SER
2	C	687	CYS
2	C	691	ASP
2	C	719	LEU
2	C	768	GLU
2	C	928	ILE
2	C	934	THR
2	C	962	GLU
2	C	1002	VAL
2	C	1045	SER
2	C	1052	ILE
2	C	1099	ARG
2	C	1148	ARG
3	D	7	PHE
3	D	19	ASP
3	D	60	CYS
3	D	82	VAL
3	D	101	VAL
3	D	110	VAL
3	D	114	LEU
3	D	139	VAL
3	D	282	ARG
3	D	305	SER
3	D	359	ASP
3	D	576	MET
3	D	580	ASP
3	D	582	VAL
3	D	583	THR
3	D	629	VAL
3	D	677	LEU
3	D	714	ASP
3	D	810	ASN
3	D	866	ARG
3	D	900	GLU

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Mol	Chain	Res	Type
3	D	901	LEU
3	D	930	VAL
3	D	968	CYS
3	D	970	THR
3	D	990	ASP
3	D	1055	LEU
3	D	1098	VAL
3	D	1099	LEU
3	D	1138	VAL
3	D	1194	VAL
4	E	48	SER
4	E	75	ILE
5	F	233	LYS
5	F	241	LEU
5	F	345	THR
5	F	361	ASP
5	F	434	GLN
5	F	448	VAL
5	F	483	ASP
5	F	525	ASP
5	F	527	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	79	ASN
1	B	200	ASN
2	C	349	HIS
2	C	388	GLN
2	C	1066	GLN
2	C	1077	GLN
3	D	303	GLN
3	D	375	GLN
3	D	499	ASN
3	D	1125	GLN
3	D	1131	GLN
4	E	37	ASN
5	F	505	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	$\# Z > 2$
10	88D	D	1404	-	27,28,28	1.86	4 (14%)	36,37,37	1.07	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
10	88D	D	1404	-	-	0/18/20/20	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	D	1404	88D	CAA-CAW	-6.25	1.39	1.51
10	D	1404	88D	CB-CG	-4.77	1.40	1.51
10	D	1404	88D	CAX-NAQ	-3.79	1.34	1.41
10	D	1404	88D	SE-CAY	2.56	1.92	1.87

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	D	1404	88D	SE-CAJ-CAI	-2.71	106.55	112.24
10	D	1404	88D	CAX-NAQ-C	-2.66	119.61	126.98

There are no chirality outliers.

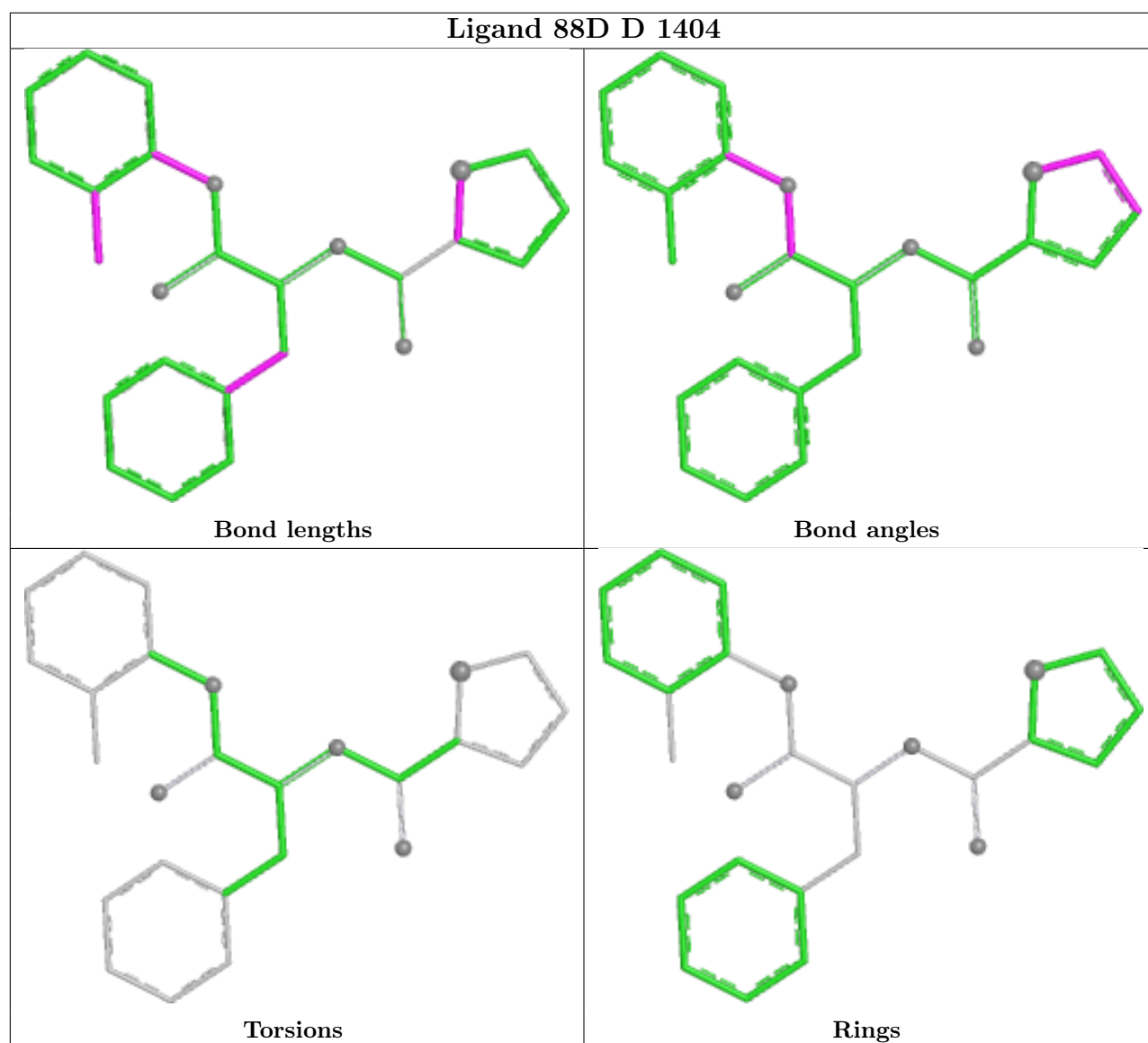
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	D	1404	88D	1	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	224/347 (64%)	0.45	7 (3%) 51 40	31, 66, 148, 176	0
1	B	225/347 (64%)	0.77	16 (7%) 22 24	70, 115, 167, 184	0
2	C	1126/1178 (95%)	0.45	30 (2%) 56 43	24, 47, 139, 169	0
3	D	1265/1316 (96%)	0.38	22 (1%) 69 54	22, 43, 112, 152	0
4	E	81/110 (73%)	0.43	3 (3%) 45 37	29, 49, 84, 105	0
5	F	322/528 (60%)	0.48	13 (4%) 42 36	25, 66, 171, 204	0
6	H	23/23 (100%)	0.95	2 (8%) 16 19	37, 134, 181, 268	0
7	G	12/16 (75%)	1.58	4 (33%) 1 3	128, 176, 352, 369	0
All	All	3278/3865 (84%)	0.46	97 (2%) 52 40	22, 52, 148, 369	0

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	237	LEU	6.2
5	F	389	ASP	5.1
1	B	76	ILE	4.6
1	B	54	ILE	4.6
2	C	722	ALA	4.5
2	C	977	PHE	3.9
3	D	336	ALA	3.8
5	F	431	GLY	3.6
1	B	136	VAL	3.4
3	D	291	ARG	3.4
1	B	162	ILE	3.2
3	D	733	MET	3.2
5	F	523	LEU	3.2
3	D	610	GLY	3.1
3	D	152	GLU	3.1
1	B	154	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	126	ALA	3.0
3	D	623	ASP	3.0
5	F	429	ASP	3.0
5	F	428	GLY	3.0
7	G	5	DC	2.9
1	A	196	VAL	2.9
5	F	207	ASP	2.9
7	G	16	DC	2.9
1	B	78	LEU	2.8
1	B	117	THR	2.8
1	B	80	LEU	2.8
2	C	598	GLU	2.7
2	C	291	SER	2.7
2	C	76	GLU	2.7
7	G	14	DG	2.7
5	F	430	GLU	2.7
5	F	517	PRO	2.7
2	C	252	PHE	2.6
2	C	979	GLY	2.6
1	A	218	LEU	2.6
2	C	820	LEU	2.5
2	C	593	MET	2.5
2	C	288	THR	2.5
5	F	488	THR	2.5
1	A	225	LEU	2.5
2	C	402	GLU	2.5
1	B	159	ILE	2.5
2	C	773	ILE	2.5
2	C	215	ASP	2.5
3	D	4	VAL	2.5
3	D	1102	GLY	2.5
6	H	23	DG	2.4
2	C	28	SER	2.4
2	C	292	ALA	2.4
6	H	14	DG	2.4
1	A	152	ASN	2.4
5	F	432	ASP	2.4
1	B	7	PRO	2.4
3	D	914	PRO	2.3
3	D	994	ALA	2.3
2	C	584	ARG	2.3
3	D	413	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
3	D	901	LEU	2.3
2	C	209	GLY	2.3
1	B	56	ILE	2.3
4	E	40	ILE	2.3
2	C	295	LEU	2.3
2	C	212	LEU	2.3
2	C	268	VAL	2.3
5	F	514	LEU	2.3
2	C	304	LYS	2.2
3	D	3	ASP	2.2
2	C	235	THR	2.2
1	B	155	SER	2.2
3	D	900	GLU	2.2
1	B	167	ILE	2.2
2	C	1025	VAL	2.2
2	C	1152	ASP	2.2
3	D	1142	TYR	2.2
1	A	226	ASN	2.1
4	E	77	GLU	2.1
7	G	15	DT	2.1
5	F	500	ARG	2.1
5	F	464	LEU	2.1
3	D	969	ALA	2.1
1	A	194	LEU	2.1
2	C	256	GLU	2.1
3	D	1003	ILE	2.1
3	D	45	GLY	2.1
4	E	44	LEU	2.1
3	D	949	ILE	2.0
3	D	1280	ALA	2.0
2	C	190	THR	2.0
2	C	464	SER	2.0
1	B	185	GLN	2.0
1	A	183	VAL	2.0
3	D	644	VAL	2.0
1	B	161	ARG	2.0
2	C	204	VAL	2.0
2	C	81	ASN	2.0
3	D	638	THR	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](#)

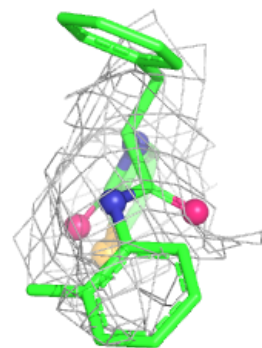
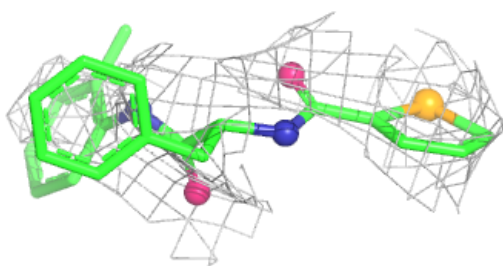
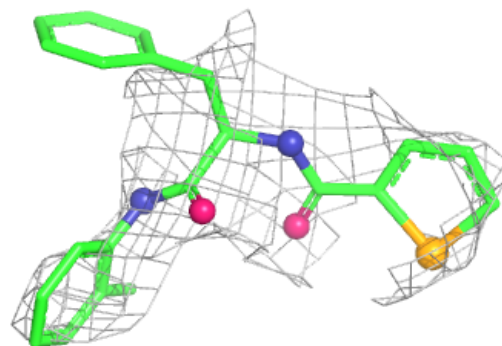
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	MG	D	1403	1/1	0.90	0.11	28,28,28,28	0
10	88D	D	1404	26/26	0.90	0.13	46,64,136,144	0
8	ZN	D	1401	1/1	0.98	0.05	21,21,21,21	0
8	ZN	D	1402	1/1	0.99	0.04	35,35,35,35	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 88D 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.