Full wwPDB X-ray Structure Validation Report (i)

Sep 24, 2023 – 06:53 PM EDT

PDB ID	:	5UHE
Title	:	Crystal structure of Mycobacterium tuberculosis transcription initiation complex in complex with D-AAP1
Authors	:	Lin, W.; Das, K.; Feng, Y.; Ebright, R.H.
Deposited on	:	2017-01-11
Resolution	:	4.04 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:

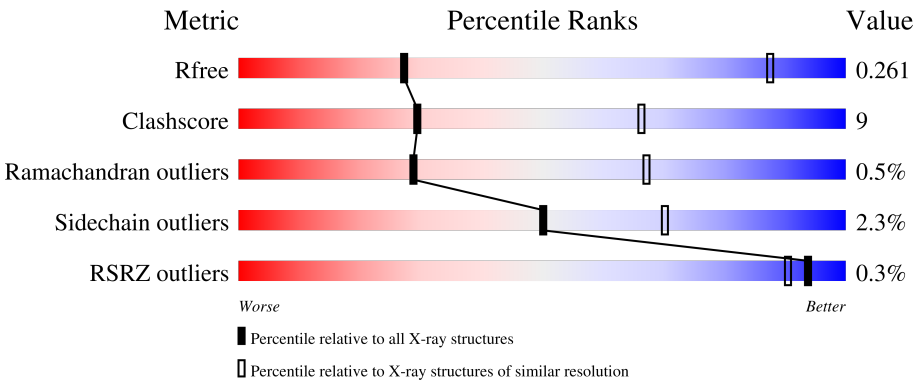
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 4.04 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	1105 (4.38-3.70)
Clashscore	141614	1005 (4.36-3.72)
Ramachandran outliers	138981	1125 (4.38-3.70)
Sidechain outliers	138945	1115 (4.38-3.70)
RSRZ outliers	127900	1003 (4.40-3.68)

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	51% 14% 35%
1	B	347	52% 12% 35%
2	C	1178	73% 22% • •
3	D	1316	69% 26% • •
4	E	110	55% 17% • 26%

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Mol	Chain	Length	Quality of chain
5	F	528	46% 14% 39%
6	H	23	57% 43%
7	G	16	31% 62% 19% 19%

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 25966 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	224	1700	1072	288	338	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	322	2555	1589	461	496	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	13	263	126	48	77	12	0	0	0

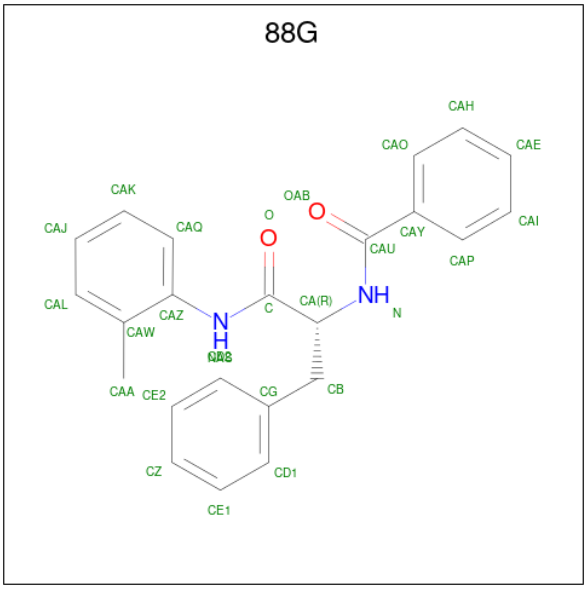
- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 10 is Nalpha-(benzenecarbonyl)-N-(2-methylphenyl)-D-phenylalaninamide (three-letter code: 88G) (formula: $C_{23}H_{22}N_2O_2$).



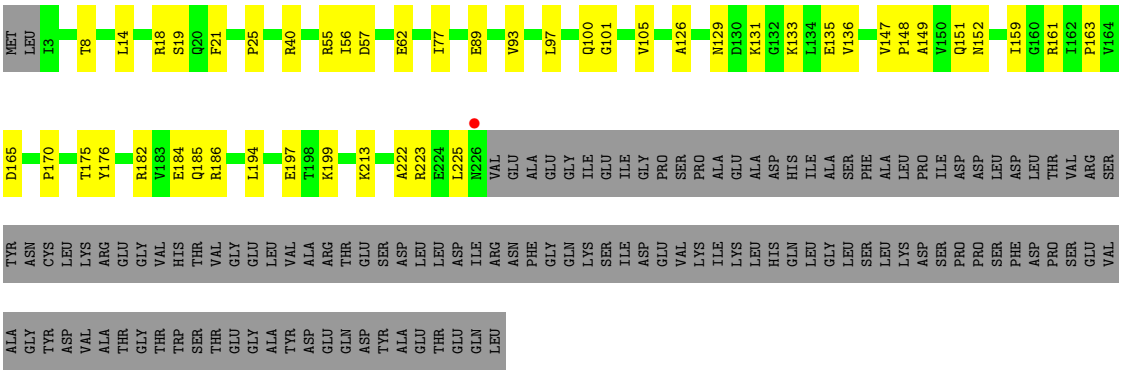
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
10	D	1	27	23	2	2	0	0

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.

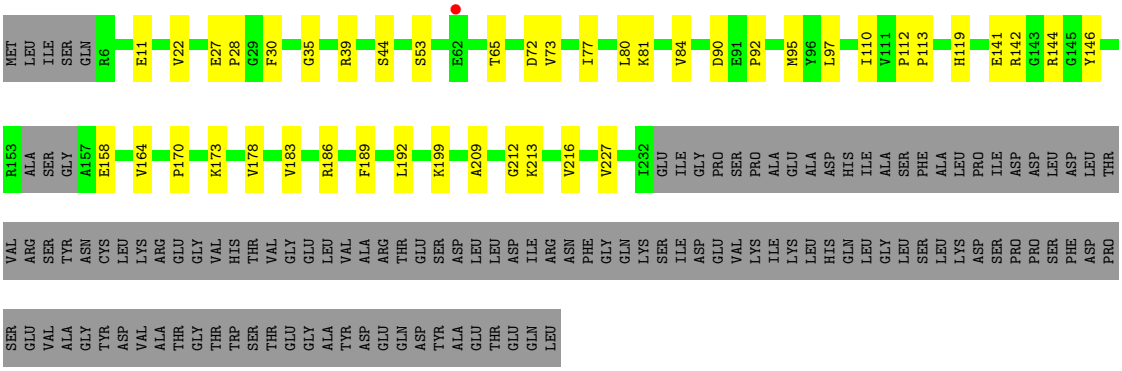
• Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain A:



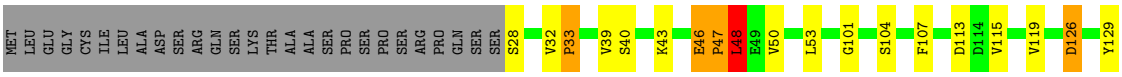
• Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain B:



• Molecule 2: DNA-directed RNA polymerase subunit beta

Chain C:



P132 I140 N141 N142 I167 I168 N169 G170 R173 V180 P183 G184 V185 Y186 F187 D188 E189 H200 P206 W211 D217 K218 R219 D220 I226 D227 R228 K229 Q232 P233 V236 K239 G253 I257 M258 R259 D265 R279 K280 T288 K289

E290 T294 L295 L296 F300 R305 L308 V311 G312 R313 S330 D337 V338 I342 E343 Y344 L348 T354 V365 E366 T367 D368 D369 I370 D371 R377 L378 R379 E383 N387 Q388 I389 R390 V391 G392 M393 M396 R401 M404 D408 I412

I418 N419 I420 V424 I427 F430 F431 S437 Q438 F439 M440 D441 N444 S447 H451 R454 L455 S464 R467 V472 R473 H476 H479 Y480 G481 C484 G495 E513 Y516 R517 K518 G522 V523 V524 I528 V529 Y530 L531 A544

I548 D549 A550 R553 V559 R562 R563 K564 E569 Y578 M579 D580 V581 Q585 S588 V589 A590 M593 L597 E598 H599 G608 M611 Q612 R613 V616 V619 R620 S621 L632 R633 D637 V642 E652 I658 F675 S678 T682

N685 P688 D691 A703 D704 T708 D709 D710 L720 I723 D733 V742 L747 T748 E756 I757 D758 T762 K763 S777 V780 R797 G810 E811 T812 T815 P816 E817 E818 L821 R822 A829 T835 S836 I850 F853 E858

L868 V869 R870 V871 Q875 K876 R877 K878 I879 L885 G893 V894 I895 G896 L899 M904 V913 T919 V922 P923 R924 R925 M926 N927 I928 G929 Q930 W938 W944 L959 P960 D961 E962 L963 S973 T974 P975 V976 G979 A980 Q981 E982 C991 R996

V1002 A1008 G1013 F1019 P1020 Y1021 T1024 V1025 G1026 Y1027 I1030 M1031 K1032 L1036 I1041 S1045 Y1049 I1052 T1053 Q1054 R1067 F1068 M1076 Q1077 A1078 Y1079 E1087 I1091 R1099 V1102 Y1103 E1104 N1111 I1112 I1117 P1118 E1119 K1122 V1123 L1124

L1125 K1126 L1133 N1134 V1135 E1136 D1141 G1142 E1146 L1147 R1148 E1149 G1150 E1153 ASP LEU GLU ARG ALA ALA ALA ASN LEU GLY ILE ASN LEU SER ARG ASN GLU SER ALA SER VAL GLU ASP LEU ALA

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

Chain D: 69% 26%

MET LEU D3 F7 L10 R11 I12 G13 L14 A15 T16 A17 E18 D19 I20 S24 K30 I34 K43 D44 G45 L46 F47 K50 C60 Y65 K66 R67 V68 R69 G72 C75 E76 V82 T83 R84 A85 K86 R89 H94 L97 V101 T102 H103

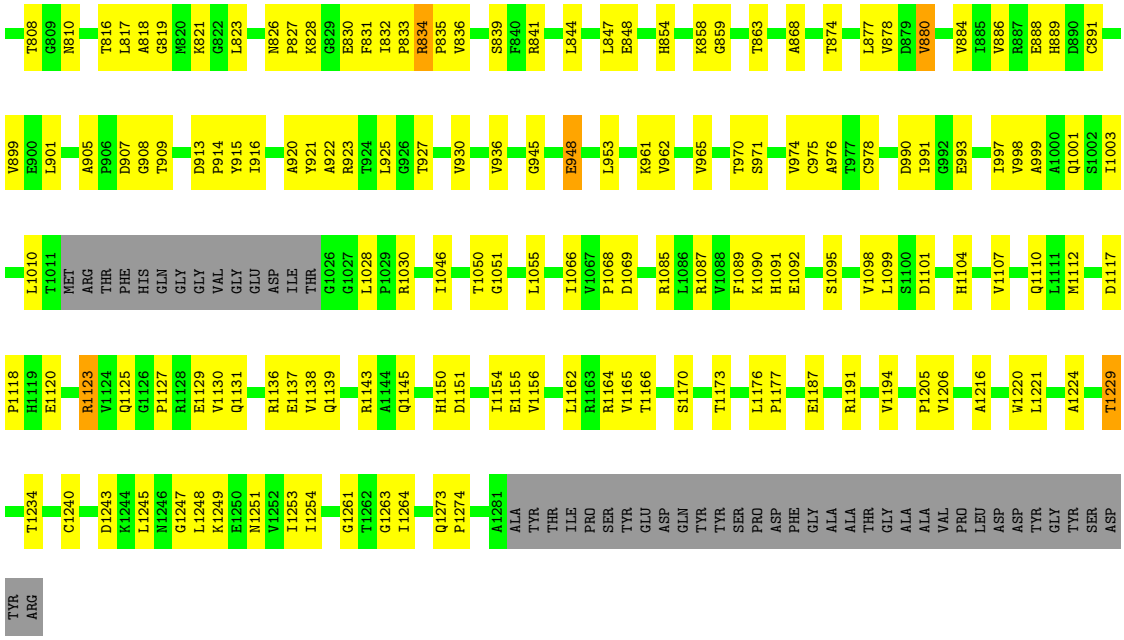
I104 W105 Y106 F107 S112 R113 L114 G115 Y116 L120 A121 P122 K123 D124 L125 E126 K127 I128 I129 Y130 F131 A132 A133 V139 M143 A153 V157 L184 E185 K190 A191 D192 A193 R194 V197 R218 I222 P231 I235 V236 D237 Y241 Y251 G257

S260 I261 Q262 E266 R278 R282 L293 K294 F302 N307 M310 V313 V317 P321 P322 R325 A336 N341 D342 L343 Y344 R345 R350 R356 P363 I366 V367 N368 N369 M373 L374 Q375 E376 S377 V378 D379 A380 L381 N384

K400 S401 K409 Q415 N416 L417 L418 D423 V431 L438 H439 Q440 C441 G442 K445 L446 M447 E450 M457 K458 R459 L460 V461 D462 L463 Q479 R480 V483 V486 V490 I491 A492 L497 R506 M515 L516 Q523 L524 H525 P526 E530 F536

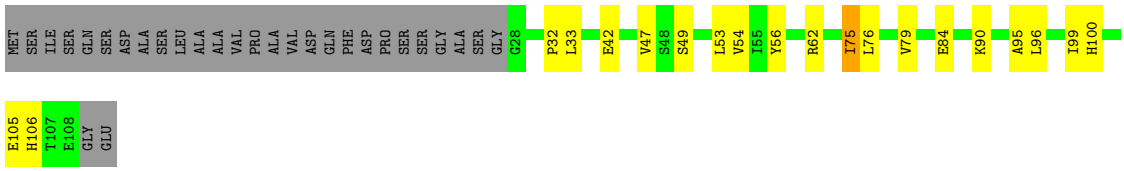
D537 V543 H544 L545 P546 E554 M559 L560 S561 I565 L566 S567 P573 L574 A575 M576 P577 R578 L579 D580 M581 V582 T583 L588 T589 P593 G594 D595 T596 G597 E598 Y599 Q600 P607 E608 T609 G610 R624 L627 A631 K634 T638 Q639 H653 P658

E665 R670 L676 L677 P678 M688 H689 Q693 I707 A710 V713 K717 W723 T730 V731 L737 V738 P739 P740 Y749 V756 F760 R770 N771 E772 A773 L774 V775 E776 I777 W778 E784 L789 H792 Y793 D796 N797 P798 T801



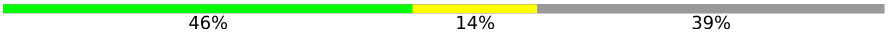
- Molecule 4: DNA-directed RNA polymerase subunit omega

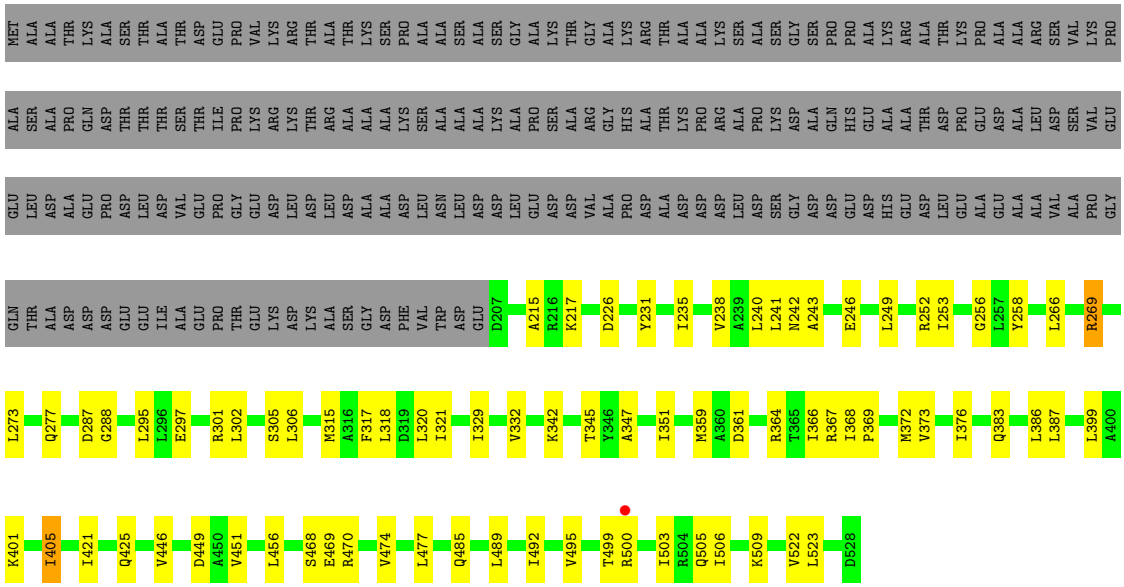
Chain E:



- Molecule 5: RNA polymerase sigma factor SigA

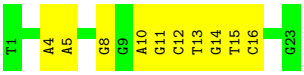
Chain F:





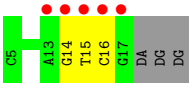
• Molecule 6: DNA (5'-D(*TP*AP*TP*AP*AP*TP*GP*GP*GP*AP*GP*CP*TP*GP*TP*CP*AP*CP*GP*GP*AP*TP*G)-3')

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	151.53Å 162.16Å 195.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.27 – 4.04 49.27 – 4.04	Depositor EDS
% Data completeness (in resolution range)	86.1 (49.27-4.04) 86.1 (49.27-4.04)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.97 (at 4.00Å)	Xtriage
Refinement program	REFMAC, PHENIX	Depositor
R, R_{free}	0.210 , 0.259 0.214 , 0.261	Depositor DCC
R_{free} test set	2009 reflections (5.80%)	wwPDB-VP
Wilson B-factor (Å^2)	23.0	Xtriage
Anisotropy	0.742	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , -6.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.82	EDS
Total number of atoms	25966	wwPDB-VP
Average B, all atoms (Å^2)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.82% 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: 88G, 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	0.25	0/1730	0.47	0/2354
1	B	0.25	0/1725	0.46	0/2348
2	C	0.27	0/8873	0.46	1/12031 (0.0%)
3	D	0.27	0/10052	0.45	0/13591
4	E	0.31	0/650	0.46	0/886
5	F	0.27	0/2585	0.44	0/3485
6	H	0.57	0/535	0.90	0/826
7	G	0.65	0/294	0.89	0/452
All	All	0.29	0/26444	0.48	1/35973 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	48	LEU	CA-CB-CG	5.71	128.44	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	28	0
1	B	1700	0	1725	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	8714	0	8636	163	0
3	D	9887	0	9943	235	0
4	E	637	0	635	16	0
5	F	2555	0	2579	54	0
6	H	476	0	261	9	0
7	G	263	0	148	4	0
8	D	2	0	0	0	0
9	D	1	0	0	0	0
10	D	27	0	0	2	0
All	All	25966	0	25668	484	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 (484) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:913:ASP:OD1	3:D:914:PRO:HD2	1.54	1.06
3:D:913:ASP:OD1	3:D:914:PRO:CD	2.17	0.92
3:D:908:GLY:O	3:D:909:THR:OG1	1.91	0.87
3:D:899:VAL:HG11	3:D:920:ALA:HB2	1.63	0.80
3:D:1090:LYS:HB3	3:D:1092:GLU:HG2	1.65	0.78
2:C:279:ARG:HD3	5:F:215:ALA:HB1	1.66	0.77
3:D:1165:VAL:HG12	3:D:1205:PRO:HA	1.67	0.75
1:A:152:ASN:HB3	1:A:163:PRO:HB3	1.67	0.74
3:D:826:ASN:HD22	3:D:832:ILE:HD11	1.54	0.73
2:C:168:ILE:HG12	2:C:431:PHE:HB3	1.71	0.72
3:D:595:ASP:HB3	3:D:631:ALA:HB2	1.71	0.72
3:D:1030:ARG:HH21	3:D:1137:GLU:HG2	1.53	0.72
3:D:107:PHE:HZ	3:D:126:GLU:HG2	1.51	0.72
2:C:48:LEU:HD12	2:C:528:ILE:HD13	1.71	0.72
3:D:554:GLU:HG3	4:E:54:VAL:HG11	1.72	0.72
3:D:907:ASP:OD1	3:D:908:GLY:N	2.21	0.72
2:C:441:ASP:HB2	2:C:451:HIS:HD2	1.53	0.71
2:C:101:GLY:O	2:C:142:ASN:ND2	2.24	0.71
2:C:658:ILE:HD11	2:C:688:PRO:HB3	1.73	0.71
2:C:464:SER:HB3	2:C:467:ARG:HG3	1.73	0.70
2:C:189:GLU:HB2	2:C:367:THR:HG21	1.74	0.70
2:C:1024:THR:H	3:D:730:THR:HG21	1.55	0.70
5:F:446:VAL:HB	5:F:449:ASP:HB2	1.75	0.69
5:F:470:ARG:HB3	5:F:506:ILE:HD13	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:901:LEU:HD11	3:D:953:LEU:HD13	1.74	0.68
3:D:891:CYS:SG	3:D:970:THR:OG1	2.51	0.68
3:D:46:LEU:O	3:D:325:ARG:NH2	2.23	0.67
3:D:409:LYS:NZ	7:G:14:DG:OP1	2.24	0.67
3:D:901:LEU:HD13	3:D:901:LEU:C	2.14	0.67
3:D:1247:GLY:O	3:D:1251:ASN:ND2	2.26	0.66
3:D:350:ARG:HD3	3:D:373:MET:HE3	1.77	0.66
3:D:530:GLU:HB2	3:D:578:ARG:HD2	1.77	0.65
3:D:638:THR:HG23	3:D:639:GLN:HG2	1.77	0.65
2:C:371:ASP:OD1	6:H:14:DG:N1	2.30	0.65
2:C:113:ASP:HB2	2:C:132:PRO:HG2	1.79	0.64
3:D:123:LYS:HE3	3:D:127:LYS:HE2	1.79	0.64
3:D:418:LEU:HD11	3:D:1249:LYS:HE3	1.80	0.64
2:C:815:THR:HG22	2:C:817:GLU:H	1.62	0.63
3:D:266:GLU:HA	3:D:310:MET:HE1	1.80	0.63
3:D:530:GLU:OE1	3:D:578:ARG:NH1	2.32	0.63
3:D:749:TYR:OH	3:D:784:GLU:OE1	2.15	0.63
5:F:477:LEU:HD13	5:F:492:ILE:HG23	1.80	0.63
3:D:445:LYS:HA	3:D:516:LEU:HD22	1.80	0.63
2:C:1122:LYS:HE2	2:C:1148:ARG:HG2	1.80	0.62
5:F:256:GLY:HA3	5:F:288:GLY:HA3	1.81	0.62
3:D:600:GLN:HB2	3:D:609:THR:HB	1.82	0.62
3:D:190:LYS:HE3	3:D:192:ASP:HB3	1.81	0.62
3:D:104:ILE:HD12	3:D:379:ASP:HB3	1.82	0.62
5:F:401:LYS:HA	5:F:405:ILE:HA	1.82	0.62
1:B:97:LEU:HD22	1:B:110:ILE:HG12	1.82	0.61
3:D:930:VAL:HG22	3:D:936:VAL:HG12	1.82	0.61
3:D:836:VAL:HG13	3:D:848:GLU:HG2	1.81	0.61
4:E:42:GLU:OE1	4:E:100:HIS:NE2	2.32	0.61
5:F:522:VAL:HG23	5:F:523:LEU:HD12	1.81	0.60
1:B:90:ASP:HA	1:B:142:ARG:HD3	1.83	0.60
1:A:55:ARG:HG3	1:A:161:ARG:HA	1.83	0.60
3:D:1089:PHE:HA	3:D:1095:SER:HA	1.84	0.60
3:D:1055:LEU:HB2	3:D:1101:ASP:HB3	1.83	0.60
1:A:56:ILE:HG12	1:A:136:VAL:HG13	1.82	0.60
1:A:197:GLU:OE1	2:C:996:ARG:NH1	2.32	0.59
5:F:242:ASN:OD1	5:F:243:ALA:N	2.35	0.59
3:D:343:LEU:HD13	3:D:381:LEU:HA	1.84	0.59
3:D:130:TYR:OH	3:D:379:ASP:OD2	2.19	0.59
1:A:40:ARG:NH1	2:C:1013:GLY:O	2.32	0.59
1:B:72:ASP:OD1	1:B:73:VAL:N	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:965:VAL:HG13	3:D:974:VAL:HG11	1.83	0.59
3:D:384:ASN:HB2	3:D:401:SER:HB3	1.83	0.59
1:B:27:GLU:HG3	1:B:28:PRO:HD2	1.85	0.58
2:C:47:PRO:HB2	2:C:581:VAL:HG13	1.85	0.58
3:D:43:LYS:HE3	3:D:50:LYS:NZ	2.18	0.58
2:C:239:LYS:NZ	2:C:265:ASP:OD2	2.35	0.58
2:C:885:LEU:HD13	2:C:1030:ILE:HG21	1.85	0.58
3:D:913:ASP:OD1	3:D:914:PRO:N	2.36	0.58
5:F:364:ARG:HG3	5:F:368:ILE:HG12	1.85	0.58
1:A:57:ASP:HB2	1:A:135:GLU:HB3	1.85	0.58
2:C:944:TRP:NE1	2:C:963:LEU:O	2.37	0.58
2:C:608:GLY:HA2	2:C:611:MET:HE2	1.86	0.57
3:D:923:ARG:NH2	3:D:1155:GLU:OE2	2.35	0.57
2:C:853:PHE:HD2	2:C:868:LEU:HD23	1.68	0.57
3:D:588:LEU:HD12	3:D:589:THR:HG23	1.87	0.57
2:C:206:PRO:HA	2:C:308:LEU:HD23	1.86	0.57
2:C:473:ARG:HB3	2:C:495:GLY:HA3	1.85	0.57
2:C:441:ASP:H	2:C:451:HIS:CD2	2.22	0.56
3:D:565:ILE:HG23	3:D:575:ALA:HB3	1.87	0.56
2:C:982:GLU:HG3	3:D:841:ARG:HH12	1.69	0.56
1:A:89:GLU:HG3	1:A:93:VAL:HG11	1.87	0.56
1:B:27:GLU:HB3	1:B:30:PHE:HD2	1.69	0.56
2:C:348:LEU:HD13	2:C:365:VAL:HG12	1.86	0.56
3:D:1051:GLY:HA2	3:D:1069:ASP:HB2	1.87	0.56
1:A:213:LYS:HD3	1:B:227:VAL:HG23	1.87	0.56
2:C:1125:LEU:HD22	2:C:1135:VAL:HG11	1.87	0.56
5:F:506:ILE:HA	5:F:509:LYS:HD2	1.86	0.56
6:H:15:DT:H2"	6:H:16:DC:H5'	1.86	0.56
3:D:460:LEU:HD11	3:D:483:VAL:HG12	1.87	0.56
3:D:905:ALA:HB3	3:D:908:GLY:O	2.06	0.56
3:D:823:LEU:HD13	3:D:831:PHE:HB3	1.88	0.55
1:A:62:GLU:HG3	1:A:77:ILE:HD12	1.89	0.55
2:C:472:VAL:HG22	6:H:14:DG:C2	2.42	0.55
2:C:516:TYR:HD2	2:C:531:LEU:HD13	1.71	0.55
3:D:827:PRO:HD3	3:D:854:HIS:NE2	2.22	0.55
3:D:1273:GLN:O	4:E:105:GLU:N	2.36	0.55
3:D:1069:ASP:OD2	3:D:1104:HIS:NE2	2.40	0.55
2:C:893:GLY:HA2	3:D:537:ASP:HA	1.88	0.55
3:D:914:PRO:HG2	3:D:915:TYR:HD1	1.72	0.55
4:E:33:LEU:HD23	4:E:33:LEU:H	1.72	0.55
2:C:733:ASP:OD2	2:C:925:ARG:NH2	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1148:ARG:NH1	3:D:86:LYS:O	2.40	0.55
1:A:148:PRO:HD2	1:A:151:GLN:NE2	2.21	0.54
1:A:223:ARG:HD3	1:B:213:LYS:HB2	1.89	0.54
2:C:959:LEU:HD12	2:C:960:PRO:HD2	1.90	0.54
5:F:231:TYR:CE2	5:F:235:ILE:HD11	2.43	0.54
2:C:616:VAL:N	2:C:1032:LYS:O	2.40	0.54
1:A:170:PRO:HA	1:A:199:LYS:HD2	1.90	0.54
3:D:1170:SER:O	3:D:1173:THR:OG1	2.25	0.54
3:D:740:PRO:HD3	3:D:792:HIS:ND1	2.22	0.54
3:D:756:VAL:HG21	3:D:777:ILE:HD11	1.90	0.53
2:C:377:ARG:NH2	2:C:383:GLU:OE1	2.41	0.53
2:C:1020:PRO:HB2	2:C:1021:TYR:CD2	2.43	0.53
1:B:84:VAL:HG12	1:B:199:LYS:HD3	1.90	0.53
2:C:549:ASP:HB3	2:C:553:ARG:H	1.73	0.53
1:B:77:ILE:HG22	1:B:81:LYS:HE3	1.89	0.53
2:C:173:ARG:NH1	2:C:437:SER:O	2.41	0.53
3:D:834:ARG:NH2	10:D:1404:88G:OAB	2.24	0.53
2:C:1049:TYR:OH	3:D:423:ASP:OD2	2.25	0.53
3:D:442:GLY:HA3	3:D:523:GLN:HB2	1.91	0.53
1:A:175:THR:OG1	1:A:176:TYR:N	2.42	0.53
2:C:46:GLU:N	2:C:47:PRO:HD3	2.24	0.53
2:C:119:VAL:HG13	2:C:167:ILE:HD11	1.91	0.53
2:C:919:THR:HG23	3:D:731:VAL:HG23	1.91	0.53
5:F:252:ARG:NH1	5:F:287:ASP:OD1	2.42	0.53
2:C:1133:LEU:HD13	3:D:12:ILE:HD11	1.91	0.52
4:E:56:TYR:HE2	4:E:99:ILE:HG12	1.73	0.52
2:C:1078:ALA:HB1	3:D:998:VAL:HG22	1.91	0.52
2:C:723:ILE:O	3:D:730:THR:HG23	2.10	0.52
3:D:235:ILE:HD12	3:D:241:TYR:HD1	1.73	0.52
3:D:901:LEU:HD13	3:D:901:LEU:O	2.09	0.52
3:D:1010:LEU:HD12	3:D:1028:LEU:HB2	1.91	0.52
5:F:499:THR:OG1	5:F:500:ARG:N	2.41	0.52
3:D:143:MET:HG2	3:D:251:TYR:CE2	2.45	0.52
2:C:183:PRO:HB2	2:C:312:GLY:HA2	1.92	0.52
3:D:83:THR:HG22	3:D:84:ARG:H	1.72	0.52
1:B:53:SER:HA	1:B:164:VAL:HG23	1.92	0.52
2:C:40:SER:HB2	2:C:973:SER:HB2	1.91	0.52
3:D:184:LEU:HD12	3:D:197:VAL:HG21	1.91	0.52
3:D:369:ASN:O	3:D:373:MET:HG3	2.10	0.52
2:C:126:ASP:HA	2:C:170:GLY:HA3	1.92	0.51
2:C:378:LEU:HD21	2:C:455:LEU:HD22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:908:GLY:C	3:D:909:THR:HG1	2.00	0.51
2:C:1104:GLU:HB2	5:F:451:VAL:HG22	1.93	0.51
5:F:492:ILE:HG22	5:F:503:ILE:HG21	1.91	0.51
1:A:100:GLN:HG3	1:A:133:LYS:HB2	1.92	0.51
3:D:915:TYR:HA	3:D:1143:ARG:HH12	1.76	0.51
2:C:619:VAL:HG23	2:C:748:THR:O	2.10	0.51
3:D:363:PRO:HD2	3:D:366:ILE:HD12	1.93	0.51
3:D:891:CYS:SG	3:D:975:CYS:HB3	2.49	0.51
5:F:317:PHE:O	5:F:321:ILE:HG13	2.10	0.51
2:C:28:SER:N	2:C:962:GLU:OE1	2.44	0.51
5:F:499:THR:HG23	5:F:500:ARG:HD2	1.93	0.51
2:C:678:SER:HG	2:C:682:THR:H	1.58	0.51
3:D:69:ARG:HE	5:F:485:GLN:HB2	1.76	0.50
3:D:925:LEU:HD12	3:D:962:VAL:HG12	1.93	0.50
1:A:129:ASN:ND2	2:C:652:GLU:HG3	2.26	0.50
3:D:218:ARG:O	3:D:222:ILE:HG13	2.11	0.50
4:E:75:ILE:HG22	4:E:76:LEU:H	1.76	0.50
3:D:772:GLU:O	3:D:776:GLU:HG2	2.12	0.50
3:D:1176:LEU:H	3:D:1176:LEU:HD12	1.77	0.50
1:B:170:PRO:HA	1:B:199:LYS:HD2	1.93	0.50
2:C:821:LEU:HD22	5:F:456:LEU:HD11	1.94	0.50
1:A:100:GLN:HG2	1:A:101:GLY:H	1.78	0.49
1:B:84:VAL:HG23	1:B:119:HIS:HB2	1.93	0.49
2:C:187:PHE:O	2:C:368:ASP:N	2.40	0.49
2:C:974:THR:HG23	2:C:979:GLY:HA3	1.95	0.49
3:D:774:LEU:HD23	3:D:777:ILE:HD12	1.94	0.49
6:H:11:DG:H5"	6:H:12:DC:C4	2.47	0.49
3:D:738:VAL:HG13	3:D:841:ARG:HD3	1.94	0.49
3:D:844:LEU:HB3	3:D:848:GLU:HB3	1.94	0.49
5:F:505:GLN:HG3	5:F:509:LYS:HE3	1.93	0.49
2:C:408:ASP:OD1	2:C:408:ASP:N	2.42	0.49
3:D:30:LYS:HB2	3:D:45:GLY:HA2	1.94	0.49
2:C:313:ARG:HH22	2:C:337:ASP:CG	2.16	0.49
3:D:1139:GLN:O	3:D:1143:ARG:HG2	2.13	0.49
5:F:240:LEU:HD21	5:F:301:ARG:HD2	1.94	0.49
5:F:302:LEU:O	5:F:305:SER:OG	2.19	0.49
2:C:756:GLU:HG3	2:C:870:ARG:HG2	1.95	0.49
3:D:816:THR:HG23	3:D:821:LYS:HA	1.94	0.49
2:C:522:GLY:O	2:C:553:ARG:HA	2.13	0.48
2:C:1102:VAL:HG13	2:C:1112:ILE:HD12	1.95	0.48
2:C:544:ALA:HB2	2:C:580:ASP:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:815:THR:HB	2:C:818:GLU:HB2	1.95	0.48
2:C:1054:GLN:OE1	2:C:1099:ARG:NH2	2.42	0.48
3:D:877:LEU:O	3:D:880:VAL:HG12	2.13	0.48
6:H:12:DC:H1'	6:H:13:DT:C2	2.47	0.48
2:C:1136:GLU:OE1	3:D:11:ARG:NH1	2.45	0.48
3:D:689:HIS:O	3:D:693:GLN:HG3	2.14	0.48
3:D:798:PRO:HA	3:D:801:THR:HB	1.94	0.48
2:C:742:VAL:O	2:C:878:LYS:HE3	2.13	0.48
2:C:1052:ILE:O	3:D:89:ARG:NH1	2.45	0.48
2:C:1087:GLU:HG3	2:C:1091:ILE:HD11	1.96	0.48
3:D:589:THR:HG21	3:D:688:MET:HG2	1.95	0.48
3:D:1120:GLU:HA	3:D:1123:ARG:HG2	1.95	0.48
4:E:96:LEU:HA	4:E:99:ILE:HD12	1.95	0.48
5:F:369:PRO:O	5:F:373:VAL:HG23	2.13	0.48
3:D:293:LEU:HD21	3:D:1177:PRO:HG2	1.95	0.48
5:F:372:MET:O	5:F:376:ILE:HG13	2.13	0.48
2:C:211:TRP:HB2	2:C:227:ASP:HA	1.94	0.48
2:C:344:TYR:OH	2:C:365:VAL:HA	2.14	0.48
3:D:438:LEU:O	3:D:561:SER:OG	2.24	0.48
3:D:67:ARG:HD2	3:D:69:ARG:NE	2.29	0.48
3:D:901:LEU:HD22	3:D:916:ILE:HG12	1.95	0.48
2:C:817:GLU:N	2:C:817:GLU:OE1	2.47	0.48
1:B:183:VAL:HB	1:B:189:PHE:CD1	2.48	0.47
2:C:822:ARG:NE	2:C:829:ALA:HB2	2.29	0.47
3:D:1274:PRO:HG3	4:E:79:VAL:HG21	1.96	0.47
5:F:345:THR:HB	6:H:4:DA:H8	1.79	0.47
5:F:345:THR:HA	6:H:5:DA:N7	2.29	0.47
2:C:1068:PHE:HZ	2:C:1076:MET:HG2	1.80	0.47
3:D:336:ALA:HA	5:F:421:ILE:O	2.13	0.47
2:C:389:ILE:O	2:C:393:MET:HG2	2.15	0.47
3:D:1087:ARG:HG2	3:D:1098:VAL:HG22	1.95	0.47
2:C:444:ASN:H	2:C:447:SER:HB3	1.80	0.47
2:C:549:ASP:OD2	2:C:550:ALA:N	2.47	0.47
3:D:492:ALA:HB3	4:E:90:LYS:HE2	1.97	0.47
4:E:95:ALA:O	4:E:99:ILE:HG13	2.14	0.47
3:D:114:LEU:HA	3:D:114:LEU:HD23	1.77	0.47
3:D:579:LEU:HD22	3:D:808:THR:HB	1.97	0.47
3:D:1085:ARG:HA	3:D:1112:MET:HA	1.97	0.47
3:D:102:THR:HG22	3:D:313:VAL:HG22	1.96	0.47
3:D:278:ARG:O	3:D:282:ARG:HG2	2.14	0.47
5:F:226:ASP:OD1	6:H:8:DG:N1	2.41	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:599:HIS:HB3	2:C:928:ILE:HD12	1.97	0.47
3:D:127:LYS:HA	3:D:132:ALA:HB3	1.96	0.47
2:C:938:TRP:HB2	2:C:1026:GLY:HA2	1.97	0.47
3:D:1221:LEU:HG	3:D:1253:ILE:HD12	1.97	0.47
2:C:518:LYS:HA	2:C:578:TYR:HD1	1.79	0.46
2:C:704:ASP:HB2	2:C:708:THR:HB	1.96	0.46
3:D:153:ALA:O	3:D:157:VAL:HG23	2.15	0.46
3:D:321:PRO:HA	3:D:322:PRO:HD3	1.82	0.46
3:D:431:VAL:O	3:D:523:GLN:HA	2.15	0.46
3:D:1220:TRP:CD1	3:D:1243:ASP:HB2	2.50	0.46
3:D:1220:TRP:NE1	3:D:1243:ASP:HB2	2.31	0.46
2:C:43:LYS:NZ	2:C:544:ALA:O	2.49	0.46
2:C:904:MET:HG2	2:C:913:VAL:O	2.16	0.46
4:E:84:GLU:CD	4:E:84:GLU:H	2.18	0.46
1:B:178:VAL:HG22	1:B:192:LEU:HD13	1.97	0.46
3:D:373:MET:SD	5:F:318:LEU:HB3	2.56	0.46
5:F:474:VAL:HA	5:F:477:LEU:HB2	1.98	0.46
2:C:590:ALA:HA	2:C:593:MET:HE2	1.98	0.46
3:D:325:ARG:NH1	3:D:341:ASN:OD1	2.46	0.46
5:F:320:LEU:HD21	5:F:359:MET:HE3	1.98	0.46
3:D:107:PHE:CZ	3:D:126:GLU:HG2	2.40	0.46
3:D:486:VAL:O	3:D:490:VAL:HG23	2.16	0.46
2:C:524:VAL:HG21	2:C:548:ILE:HD13	1.97	0.46
3:D:459:ARG:HA	3:D:462:ASP:HB2	1.98	0.46
2:C:747:LEU:HD13	2:C:879:ILE:HD13	1.98	0.46
3:D:237:ASP:OD2	5:F:217:LYS:NZ	2.44	0.46
3:D:16:THR:O	3:D:20:ILE:HG12	2.16	0.45
3:D:400:LYS:HD3	3:D:400:LYS:HA	1.72	0.45
3:D:1138:VAL:HG11	3:D:1154:ILE:HD12	1.98	0.45
3:D:789:LEU:HD22	3:D:793:TYR:CE2	2.51	0.45
1:A:185:GLN:HG2	1:A:186:ARG:H	1.81	0.45
3:D:778:TRP:CD2	3:D:835:PRO:HG3	2.51	0.45
3:D:545:LEU:HD12	3:D:546:PRO:HD2	1.99	0.45
3:D:573:PRO:HB2	3:D:576:MET:HE3	1.98	0.45
3:D:886:VAL:HG12	3:D:991:ILE:HA	1.98	0.45
2:C:642:VAL:HB	2:C:703:ALA:HB3	1.98	0.45
3:D:859:GLY:O	3:D:863:THR:OG1	2.27	0.45
5:F:474:VAL:HA	5:F:477:LEU:HD12	1.99	0.45
2:C:107:PHE:HE1	2:C:418:ILE:HD11	1.82	0.45
2:C:233:PRO:HB2	2:C:236:VAL:HG23	1.98	0.45
3:D:47:PHE:CD2	3:D:322:PRO:HB3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:868:ALA:HA	7:G:14:DG:O4'	2.16	0.45
3:D:1046:ILE:HG22	3:D:1110:GLN:HA	1.97	0.45
3:D:1125:GLN:HB3	3:D:1129:GLU:HG2	1.99	0.45
2:C:481:GLY:HA2	2:C:585:GLN:O	2.17	0.45
2:C:720:LEU:HD23	2:C:913:VAL:HA	1.98	0.45
2:C:305:ARG:HH12	6:H:10:DA:H62	1.65	0.45
2:C:922:VAL:H	2:C:923:PRO:HD2	1.82	0.45
2:C:974:THR:HG23	2:C:980:ALA:H	1.82	0.45
3:D:34:ILE:HD11	5:F:366:ILE:HD13	1.98	0.45
3:D:457:MET:HB2	3:D:457:MET:HE3	1.67	0.45
3:D:1117:ASP:HA	3:D:1118:PRO:HD3	1.84	0.45
2:C:220:ASP:HB3	2:C:257:ILE:HG22	1.97	0.45
2:C:758:ASP:N	2:C:758:ASP:OD1	2.50	0.45
2:C:1141:ASP:OD1	2:C:1142:GLY:N	2.50	0.45
3:D:760:PHE:CG	3:D:770:ARG:HD2	2.51	0.45
3:D:922:ALA:HB3	3:D:1150:HIS:CE1	2.52	0.45
4:E:47:VAL:HG23	4:E:106:HIS:NE2	2.31	0.45
1:B:28:PRO:HG3	1:B:186:ARG:NH1	2.32	0.44
2:C:53:LEU:HD12	2:C:637:ASP:HB2	1.99	0.44
2:C:253:GLY:HA2	2:C:259:ARG:HE	1.81	0.44
2:C:563:ARG:NE	2:C:569:GLU:OE2	2.50	0.44
2:C:1117:ILE:HA	2:C:1118:PRO:HD3	1.80	0.44
3:D:105:TRP:HB3	3:D:1234:THR:HG22	1.99	0.44
5:F:231:TYR:O	5:F:235:ILE:HG13	2.16	0.44
2:C:513:GLU:HB3	2:C:530:TYR:HB3	1.98	0.44
3:D:116:TYR:HE1	3:D:294:LYS:HB3	1.82	0.44
3:D:139:VAL:HG12	3:D:231:PRO:HD3	1.99	0.44
3:D:945:GLY:H	3:D:948:GLU:HG3	1.83	0.44
2:C:1133:LEU:HD11	3:D:105:TRP:HZ3	1.81	0.44
3:D:257:GLY:O	3:D:260:SER:OG	2.31	0.44
3:D:848:GLU:HG3	10:D:1404:88G:CAH	2.48	0.44
5:F:329:ILE:O	5:F:332:VAL:HG12	2.17	0.44
1:A:14:LEU:HD23	1:A:19:SER:CB	2.47	0.44
2:C:401:ARG:HA	2:C:404:MET:HE2	1.99	0.44
2:C:420:ILE:O	2:C:424:VAL:HG23	2.18	0.44
3:D:440:GLN:HB3	3:D:515:MET:HE2	1.98	0.44
3:D:901:LEU:C	3:D:901:LEU:CD1	2.85	0.44
3:D:1127:PRO:O	3:D:1130:VAL:HG12	2.17	0.44
5:F:266:LEU:HA	5:F:269:ARG:HG2	1.99	0.44
5:F:273:LEU:HD13	5:F:277:GLN:HB3	1.98	0.44
1:B:110:ILE:O	1:B:112:PRO:HD3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:232:GLN:OE1	2:C:280:LYS:HG3	2.15	0.44
2:C:850:ILE:HG13	2:C:871:VAL:HG22	1.99	0.44
2:C:944:TRP:HB2	2:C:991:CYS:HB2	2.00	0.44
3:D:120:LEU:HD23	3:D:120:LEU:HA	1.85	0.44
5:F:342:LYS:HE2	5:F:342:LYS:HB3	1.75	0.44
5:F:468:SER:OG	5:F:469:GLU:N	2.50	0.44
1:A:8:THR:HG22	1:A:25:PRO:O	2.18	0.44
1:A:186:ARG:H	1:A:186:ARG:HG2	1.67	0.44
2:C:47:PRO:HG2	2:C:581:VAL:O	2.17	0.44
3:D:1131:GLN:HG3	3:D:1162:LEU:HD12	1.98	0.44
5:F:249:LEU:O	5:F:253:ILE:HG13	2.18	0.44
2:C:810:GLY:O	2:C:812:THR:N	2.49	0.44
2:C:1067:ARG:HD3	7:G:16:DC:OP1	2.17	0.44
3:D:16:THR:HG22	3:D:18:GLU:H	1.83	0.44
5:F:347:ALA:O	5:F:351:ILE:HG13	2.18	0.44
2:C:344:TYR:CE2	2:C:365:VAL:HG13	2.52	0.44
2:C:1045:SER:HB3	3:D:450:GLU:O	2.18	0.44
2:C:1148:ARG:HH11	3:D:86:LYS:HG3	1.83	0.44
3:D:121:ALA:HB3	3:D:124:ASP:HB2	1.99	0.44
3:D:579:LEU:O	3:D:582:VAL:HG13	2.18	0.44
3:D:1010:LEU:HA	3:D:1145:GLN:HG3	2.00	0.44
2:C:104:SER:HB3	2:C:140:ILE:HB	2.00	0.43
2:C:338:VAL:O	2:C:342:ILE:HG13	2.18	0.43
2:C:926:MET:HE1	3:D:817:LEU:HA	2.00	0.43
2:C:927:ASN:O	2:C:930:GLN:HG2	2.17	0.43
2:C:1146:GLU:HB2	2:C:1149:GLU:O	2.18	0.43
3:D:72:GLY:H	3:D:82:VAL:HG23	1.83	0.43
3:D:409:LYS:O	3:D:415:GLN:HB2	2.18	0.43
2:C:484:CYS:HB2	2:C:588:SER:HB3	2.00	0.43
2:C:896:GLY:HA2	3:D:431:VAL:HG13	2.00	0.43
3:D:43:LYS:HE3	3:D:50:LYS:HZ1	1.81	0.43
3:D:341:ASN:O	3:D:345:ARG:HB2	2.17	0.43
3:D:1164:ARG:NH2	3:D:1216:ALA:O	2.51	0.43
2:C:295:LEU:HD12	2:C:296:LEU:HD12	2.00	0.43
3:D:114:LEU:HB3	3:D:125:LEU:HD21	1.99	0.43
2:C:50:VAL:O	2:C:633:ARG:NH2	2.51	0.43
3:D:773:ALA:O	3:D:777:ILE:HG13	2.18	0.43
5:F:315:MET:HE2	5:F:359:MET:HA	2.00	0.43
1:A:21:PHE:O	1:A:194:LEU:N	2.49	0.43
4:E:47:VAL:HG11	4:E:53:LEU:HB2	2.00	0.43
5:F:383:GLN:O	5:F:387:LEU:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:288:THR:HG22	2:C:290:GLU:H	1.82	0.43
3:D:97:LEU:HD11	3:D:317:VAL:HG13	2.01	0.43
3:D:350:ARG:NH1	3:D:373:MET:HB3	2.34	0.43
2:C:33:PRO:HG2	2:C:632:LEU:HD21	2.01	0.43
3:D:914:PRO:HG2	3:D:915:TYR:CD1	2.52	0.43
5:F:317:PHE:O	5:F:320:LEU:HB2	2.18	0.43
1:B:39:ARG:HH21	1:B:173:LYS:NZ	2.17	0.43
3:D:599:TYR:HA	3:D:610:GLY:HA3	2.01	0.43
3:D:737:LEU:O	3:D:818:ALA:HB1	2.19	0.43
3:D:990:ASP:OD2	4:E:49:SER:HB2	2.19	0.43
5:F:249:LEU:HD12	5:F:295:LEU:HD13	1.99	0.43
2:C:408:ASP:O	2:C:412:ILE:HG13	2.19	0.43
1:A:147:VAL:HA	1:A:148:PRO:HD3	1.83	0.43
3:D:480:ARG:O	3:D:483:VAL:HG22	2.18	0.43
3:D:597:GLY:HA3	3:D:627:LEU:HA	1.99	0.43
3:D:1166:THR:HB	3:D:1206:VAL:HG21	1.99	0.43
5:F:242:ASN:O	5:F:246:GLU:HG3	2.18	0.43
2:C:217:ASP:HB3	2:C:219:ARG:H	1.83	0.42
2:C:762:THR:OG1	2:C:763:LYS:N	2.52	0.42
2:C:1119:GLU:O	2:C:1123:VAL:HG23	2.18	0.42
3:D:185:GLU:HA	3:D:194:ARG:NH2	2.34	0.42
3:D:884:VAL:HG11	3:D:1156:VAL:HG13	2.01	0.42
2:C:899:LEU:HB2	2:C:904:MET:HE1	2.01	0.42
3:D:107:PHE:O	3:D:112:SER:HB2	2.19	0.42
3:D:827:PRO:HA	3:D:858:LYS:HD2	2.01	0.42
3:D:1261:GLY:O	3:D:1264:ILE:HG12	2.19	0.42
3:D:997:ILE:HD11	3:D:1248:LEU:HD13	2.01	0.42
2:C:1041:ILE:HD11	3:D:447:MET:HG3	2.01	0.42
3:D:16:THR:HB	3:D:19:ASP:H	1.84	0.42
3:D:1245:LEU:HD13	3:D:1254:ILE:HD13	2.01	0.42
5:F:470:ARG:HH11	5:F:506:ILE:HD11	1.85	0.42
1:A:131:LYS:HE2	1:A:131:LYS:HB3	1.93	0.42
2:C:115:VAL:HG11	2:C:129:TYR:CE1	2.55	0.42
3:D:124:ASP:O	3:D:128:ILE:HG13	2.18	0.42
3:D:127:LYS:O	3:D:133:ALA:N	2.48	0.42
3:D:927:THR:OG1	3:D:961:LYS:HD3	2.20	0.42
3:D:1050:THR:HB	3:D:1107:VAL:N	2.34	0.42
3:D:1151:ASP:O	3:D:1155:GLU:HG3	2.19	0.42
2:C:562:ARG:HD3	3:D:847:LEU:HD11	2.02	0.42
3:D:677:LEU:N	3:D:678:PRO:HA	2.35	0.42
3:D:913:ASP:HB3	3:D:916:ILE:HG13	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:212:GLY:O	1:B:216:VAL:HG23	2.19	0.42
3:D:889:HIS:HB2	3:D:991:ILE:HD11	2.02	0.42
3:D:1224:ALA:O	3:D:1229:THR:HG23	2.20	0.42
1:A:97:LEU:HD21	1:A:105:VAL:HG21	2.02	0.42
3:D:634:LYS:HE2	3:D:665:GLU:HG2	2.02	0.42
3:D:999:ALA:O	3:D:1003:ILE:HG13	2.20	0.42
1:A:105:VAL:HG12	1:A:126:ALA:O	2.20	0.42
1:B:92:PRO:HB3	1:B:141:GLU:HG2	2.00	0.42
1:B:95:MET:HB3	1:B:113:PRO:HD3	2.02	0.42
3:D:262:GLN:HB2	3:D:313:VAL:HG11	2.02	0.42
3:D:819:GLY:O	3:D:839:SER:HB3	2.19	0.42
1:A:149:ALA:HB2	1:A:165:ASP:N	2.34	0.42
2:C:675:PHE:N	2:C:685:ASN:OD1	2.48	0.42
3:D:588:LEU:HD23	3:D:723:TRP:CG	2.55	0.42
3:D:567:SER:HB2	3:D:574:LEU:HG	2.02	0.41
1:A:14:LEU:HD23	1:A:19:SER:HB2	2.01	0.41
1:B:27:GLU:HB3	1:B:30:PHE:CD2	2.53	0.41
1:B:146:TYR:O	3:D:624:ARG:NE	2.53	0.41
2:C:1111:ASN:HB3	4:E:62:ARG:HH12	1.85	0.41
2:C:1148:ARG:NH1	3:D:86:LYS:HG3	2.34	0.41
2:C:1019:PHE:HA	2:C:1020:PRO:HD3	1.83	0.41
3:D:101:VAL:HG23	3:D:375:GLN:NE2	2.36	0.41
3:D:302:PHE:HD1	3:D:307:ASN:O	2.03	0.41
5:F:342:LYS:O	5:F:345:THR:HG22	2.20	0.41
1:B:80:LEU:HD23	1:B:80:LEU:HA	1.87	0.41
2:C:678:SER:OG	2:C:682:THR:N	2.50	0.41
3:D:459:ARG:NH1	3:D:463:LEU:HD11	2.35	0.41
3:D:580:ASP:N	3:D:580:ASP:OD1	2.54	0.41
3:D:707:ILE:HD11	4:E:32:PRO:HB3	2.02	0.41
3:D:1187:GLU:O	3:D:1191:ARG:HB2	2.20	0.41
5:F:238:VAL:HG21	5:F:297:GLU:HB3	2.03	0.41
1:B:44:SER:O	1:B:144:ARG:HB3	2.19	0.41
2:C:226:ILE:O	2:C:229:LYS:HG2	2.21	0.41
2:C:387:ASN:O	2:C:391:VAL:HG23	2.20	0.41
2:C:982:GLU:HG3	3:D:841:ARG:NH1	2.34	0.41
3:D:497:LEU:O	3:D:543:VAL:HA	2.20	0.41
3:D:1090:LYS:HG2	3:D:1091:HIS:H	1.85	0.41
7:G:15:DT:H2'	7:G:16:DC:C6	2.55	0.41
2:C:549:ASP:HB3	2:C:553:ARG:N	2.34	0.41
3:D:14:LEU:HD13	3:D:106:TYR:OH	2.19	0.41
3:D:374:LEU:O	3:D:378:VAL:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:828:LYS:HE3	3:D:830:GLU:HB2	2.02	0.41
1:B:11:GLU:HB2	1:B:22:VAL:HB	2.02	0.41
2:C:290:GLU:O	2:C:294:THR:OG1	2.29	0.41
2:C:313:ARG:HD3	2:C:330:SER:HB3	2.02	0.41
2:C:597:LEU:HD23	2:C:976:VAL:HG11	2.03	0.41
2:C:720:LEU:HD13	2:C:1027:TYR:CE2	2.55	0.41
3:D:589:THR:HG22	3:D:670:ARG:HG2	2.02	0.41
3:D:874:THR:O	3:D:878:VAL:HG23	2.21	0.41
2:C:597:LEU:HB3	2:C:976:VAL:HG13	2.03	0.41
3:D:525:HIS:HA	3:D:526:PRO:HD3	1.92	0.41
3:D:710:ALA:O	3:D:713:VAL:HG12	2.21	0.41
5:F:252:ARG:HD2	5:F:287:ASP:OD2	2.20	0.41
5:F:489:LEU:H	5:F:489:LEU:HD23	1.84	0.41
1:B:65:THR:HG22	1:B:72:ASP:HA	2.03	0.41
2:C:200:HIS:CE1	2:C:348:LEU:HG	2.56	0.41
2:C:226:ILE:HG23	2:C:300:PHE:HZ	1.85	0.41
2:C:388:GLN:HG3	2:C:430:PHE:CD1	2.56	0.41
2:C:447:SER:HA	2:C:613:ARG:HB3	2.03	0.41
3:D:356:ARG:HD2	3:D:356:ARG:HA	1.88	0.41
3:D:506:ARG:N	3:D:1001:GLN:OE1	2.54	0.41
3:D:888:GLU:O	3:D:976:ALA:N	2.53	0.41
2:C:180:VAL:HG21	2:C:379:ARG:HE	1.84	0.41
2:C:516:TYR:HE1	2:C:580:ASP:OD1	2.04	0.41
2:C:777:SER:OG	2:C:780:VAL:HG23	2.20	0.41
2:C:894:VAL:HG22	3:D:536:PHE:O	2.20	0.41
2:C:1126:LYS:HD3	2:C:1126:LYS:HA	1.82	0.41
3:D:102:THR:H	3:D:375:GLN:HE22	1.69	0.41
3:D:125:LEU:O	3:D:129:ILE:HG13	2.21	0.41
3:D:717:LYS:HE2	3:D:717:LYS:HB3	1.82	0.41
3:D:1066:ILE:O	3:D:1068:PRO:HD3	2.21	0.41
1:B:84:VAL:CG2	1:B:119:HIS:HB2	2.51	0.40
3:D:1261:GLY:C	3:D:1263:GLY:H	2.25	0.40
5:F:386:LEU:HD12	5:F:399:LEU:HD23	2.03	0.40
5:F:492:ILE:HA	5:F:495:VAL:HG12	2.03	0.40
2:C:476:HIS:HB3	2:C:479:HIS:CE1	2.56	0.40
2:C:797:ARG:HH22	3:D:479:GLN:CD	2.24	0.40
3:D:60:CYS:HB3	3:D:65:TYR:HB2	2.03	0.40
3:D:350:ARG:HD2	3:D:377:SER:OG	2.21	0.40
2:C:388:GLN:HG3	2:C:430:PHE:HB2	2.03	0.40
3:D:24:SER:HB2	3:D:94:HIS:HB3	2.03	0.40
3:D:417:LEU:HD13	3:D:1253:ILE:HG23	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:ALA:O	1:B:209:ALA:HA	2.22	0.40
2:C:928:ILE:H	2:C:928:ILE:HG13	1.56	0.40
3:D:363:PRO:O	3:D:367:VAL:HG23	2.21	0.40
3:D:832:ILE:HA	3:D:833:PRO:HD2	1.93	0.40
1:B:97:LEU:HD13	1:B:110:ILE:HA	2.04	0.40
2:C:877:ARG:HH11	2:C:1036:LEU:HD12	1.85	0.40
2:C:1002:VAL:HG12	2:C:1008:ALA:HB2	2.04	0.40
2:C:1079:TYR:CD2	3:D:559:MET:HG2	2.56	0.40
3:D:10:LEU:HB3	3:D:1245:LEU:HD21	2.03	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%)	209 (94%)	12 (5%)	1 (0%)	29	67
1	B	220/347 (63%)	203 (92%)	15 (7%)	2 (1%)	17	55
2	C	1124/1178 (95%)	1047 (93%)	69 (6%)	8 (1%)	22	61
3	D	1261/1316 (96%)	1190 (94%)	66 (5%)	5 (0%)	34	71
4	E	79/110 (72%)	76 (96%)	3 (4%)	0	100	100
5	F	320/528 (61%)	305 (95%)	14 (4%)	1 (0%)	41	75
All	All	3226/3826 (84%)	3030 (94%)	179 (6%)	17 (0%)	29	67

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	678	PRO
3	D	593	PRO
5	F	405	ILE

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Mol	Chain	Res	Type
1	A	184	GLU
2	C	1148	ARG
3	D	971	SER
2	C	33	PRO
2	C	564	LYS
2	C	922	VAL
1	B	158	GLU
2	C	858	GLU
1	B	35	GLY
3	D	607	PRO
3	D	658	PRO
2	C	32	VAL
2	C	47	PRO
2	C	46	GLU

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%)	188 (98%)	4 (2%)	53	72
1	B	191/297 (64%)	191 (100%)	0	100	100
2	C	948/998 (95%)	926 (98%)	22 (2%)	50	70
3	D	1048/1095 (96%)	1019 (97%)	29 (3%)	43	65
4	E	68/90 (76%)	67 (98%)	1 (2%)	65	80
5	F	271/427 (64%)	264 (97%)	7 (3%)	46	67
All	All	2718/3204 (85%)	2655 (98%)	63 (2%)	50	70

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ARG
1	A	159	ILE
1	A	182	ARG
1	A	225	LEU

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Mol	Chain	Res	Type
2	C	39	VAL
2	C	48	LEU
2	C	126	ASP
2	C	185	VAL
2	C	311	VAL
2	C	354	THR
2	C	370	ILE
2	C	396	MET
2	C	427	ILE
2	C	439	PHE
2	C	454	ARG
2	C	479	HIS
2	C	559	VAL
2	C	621	SER
2	C	691	ASP
2	C	710	ASP
2	C	797	ARG
2	C	835	THR
2	C	836	SER
2	C	875	GLN
2	C	1099	ARG
2	C	1148	ARG
3	D	7	PHE
3	D	60	CYS
3	D	75	CYS
3	D	76	GLU
3	D	97	LEU
3	D	101	VAL
3	D	261	ILE
3	D	440	GLN
3	D	580	ASP
3	D	582	VAL
3	D	583	THR
3	D	653	HIS
3	D	676	LEU
3	D	677	LEU
3	D	793	TYR
3	D	796	ASP
3	D	810	ASN
3	D	834	ARG
3	D	880	VAL
3	D	921	TYR

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Mol	Chain	Res	Type
3	D	948	GLU
3	D	978	CYS
3	D	993	GLU
3	D	1099	LEU
3	D	1123	ARG
3	D	1136	ARG
3	D	1194	VAL
3	D	1229	THR
3	D	1240	CYS
4	E	75	ILE
5	F	241	LEU
5	F	258	TYR
5	F	269	ARG
5	F	306	LEU
5	F	361	ASP
5	F	367	ARG
5	F	425	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	451	HIS
2	C	1034	HIS
2	C	1129	GLN
3	D	375	GLN
3	D	826	ASN

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 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	88G	D	1404	-	29,29,29	1.80	4 (13%)	38,38,38	1.17	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	88G	D	1404	-	-	0/20/20/20	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	88G	CAA-CAW	-5.70	1.39	1.51
10	D	1404	88G	CAY-CAU	-4.22	1.41	1.50
10	D	1404	88G	CB-CG	-4.21	1.41	1.51
10	D	1404	88G	CAZ-NAS	-2.87	1.36	1.41

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	D	1404	88G	CAL-CAW-CAZ	5.06	122.21	117.44
10	D	1404	88G	CAZ-NAS-C	-2.20	120.87	126.92

There are no chirality outliers.

There are no torsion outliers.

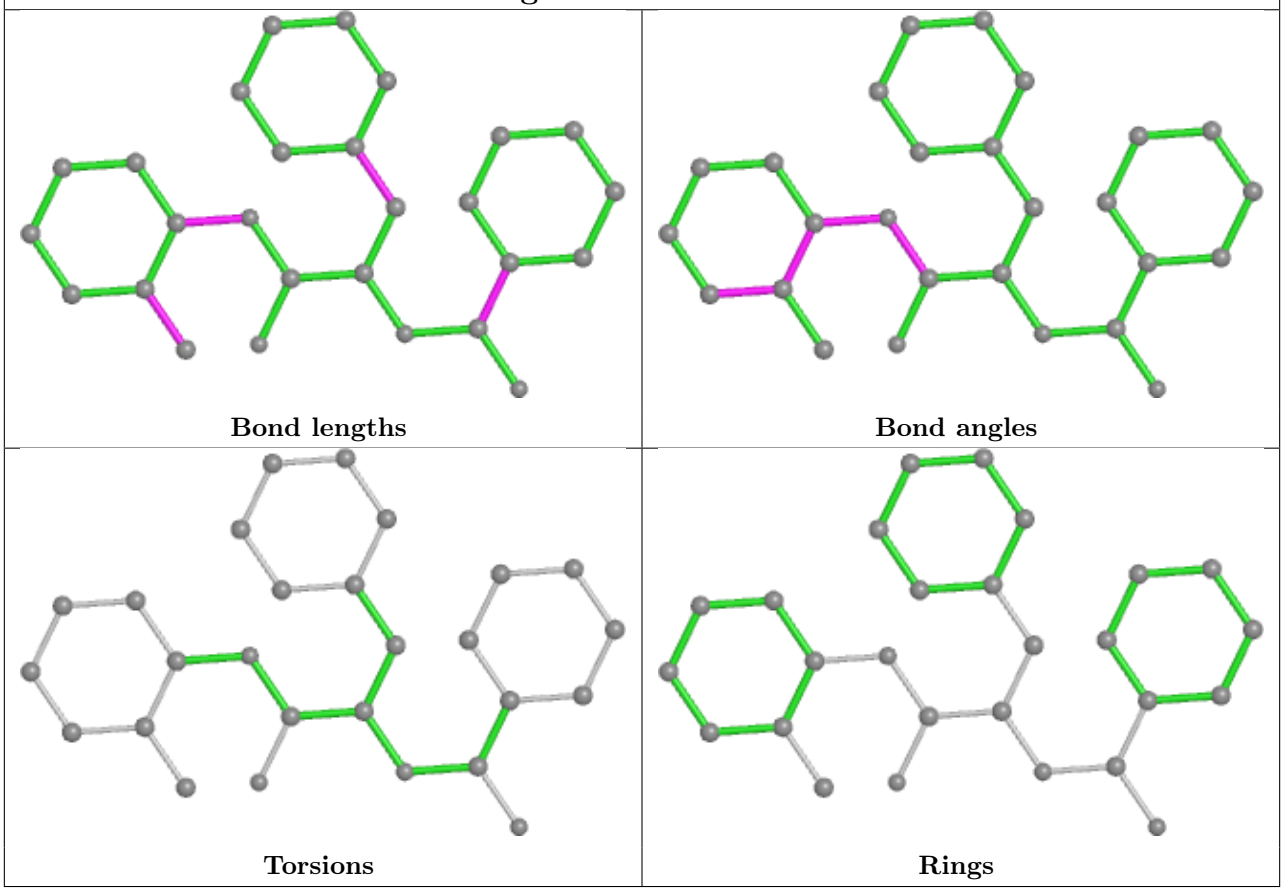
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	D	1404	88G	2	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%)	-0.50	1 (0%)	92	87	32, 65, 126, 153	0
1	B	224/347 (64%)	-0.15	1 (0%)	92	87	56, 106, 148, 173	0
2	C	1126/1178 (95%)	-0.54	1 (0%)	95	95	23, 51, 132, 169	0
3	D	1265/1316 (96%)	-0.61	0	100	100	20, 52, 117, 150	0
4	E	81/110 (73%)	-0.57	0	100	100	36, 66, 101, 148	0
5	F	322/528 (60%)	-0.36	1 (0%)	94	90	24, 77, 157, 181	0
6	H	23/23 (100%)	-0.12	0	100	100	38, 152, 199, 208	0
7	G	13/16 (81%)	1.20	5 (38%)	0	0	174, 190, 357, 357	0
All	All	3278/3865 (84%)	-0.51	9 (0%)	94	90	20, 59, 137, 357	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	F	500	ARG	3.7
2	C	1150	GLY	3.1
7	G	15	DT	3.0
7	G	14	DG	2.9
7	G	17	DG	2.8
7	G	16	DC	2.7
7	G	13	DA	2.3
1	A	226	ASN	2.1
1	B	62	GLU	2.1

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)

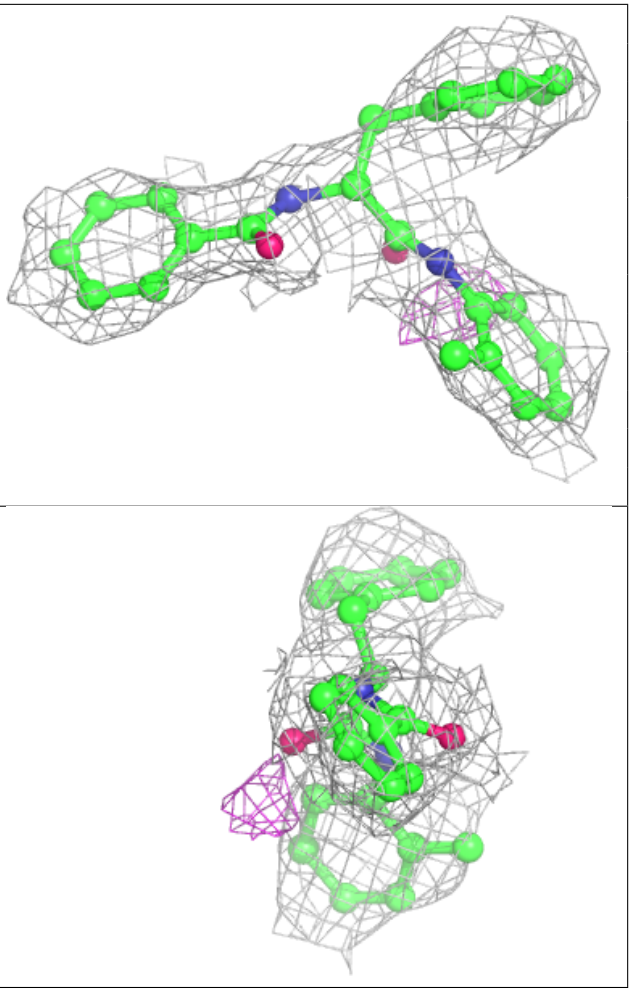
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
10	88G	D	1404	27/27	0.96	0.37	50,60,70,80	0
9	MG	D	1403	1/1	0.97	0.12	18,18,18,18	0
8	ZN	D	1402	1/1	0.98	0.09	45,45,45,45	0
8	ZN	D	1401	1/1	0.99	0.05	51,51,51,51	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 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.