Full wwPDB X-ray Structure Validation Report ⓘ

Dec 19, 2023 – 02:45 PM EST

PDB ID	:	8U16
Title	:	The ternary complex structure of DDB1-CRBN-SALL4(ZF1,2)-short bound to Pomalidomide
Authors	:	Clifton, M.C.; Ma, X.; Ornelas, E.
Deposited on	:	2023-08-30
Resolution	:	2.90 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:

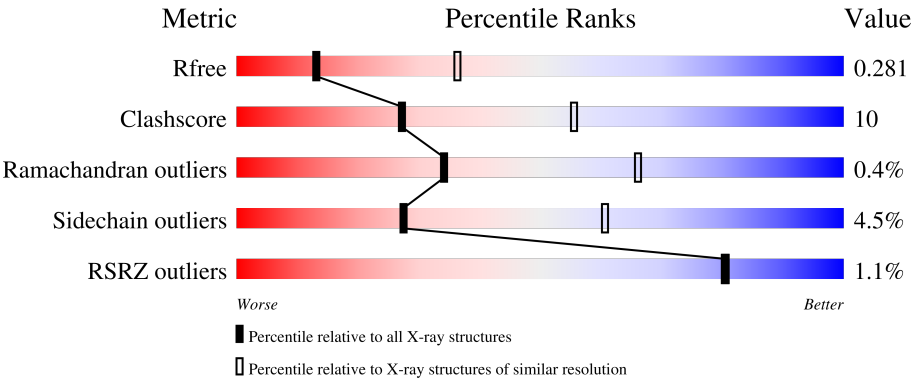
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.90 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.



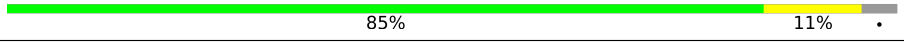
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 <=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	373	71% 21% 7%
1	D	373	2% 72% 19% 7%
2	B	836	74% 22%
2	E	836	71% 23%
3	C	55	67% 27%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	F	55	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 18095 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 Protein cereblon.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	346	Total	C	N	O	S	0	0	0
			2600	1675	438	467	20			
1	D	346	Total	C	N	O	S	0	0	0
			2627	1696	441	469	21			

- Molecule 2 is a protein called DNA damage-binding protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	809	Total	C	N	O	S	0	1	0
			6027	3848	1008	1137	34			
2	E	804	Total	C	N	O	S	0	0	0
			5973	3822	999	1119	33			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	700	GLY	-	linker	UNP Q16531
B	701	ASN	-	linker	UNP Q16531
B	702	GLY	-	linker	UNP Q16531
B	703	ASN	-	linker	UNP Q16531
B	704	SER	-	linker	UNP Q16531
B	705	GLY	-	linker	UNP Q16531
E	700	GLY	-	linker	UNP Q16531
E	701	ASN	-	linker	UNP Q16531
E	702	GLY	-	linker	UNP Q16531
E	703	ASN	-	linker	UNP Q16531
E	704	SER	-	linker	UNP Q16531
E	705	GLY	-	linker	UNP Q16531

- Molecule 3 is a protein called Sal-like protein 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	53	Total	C	N	O	S	0	0	0
			395	248	76	67	4			
3	F	53	Total	C	N	O	S	0	0	0
			387	242	76	65	4			

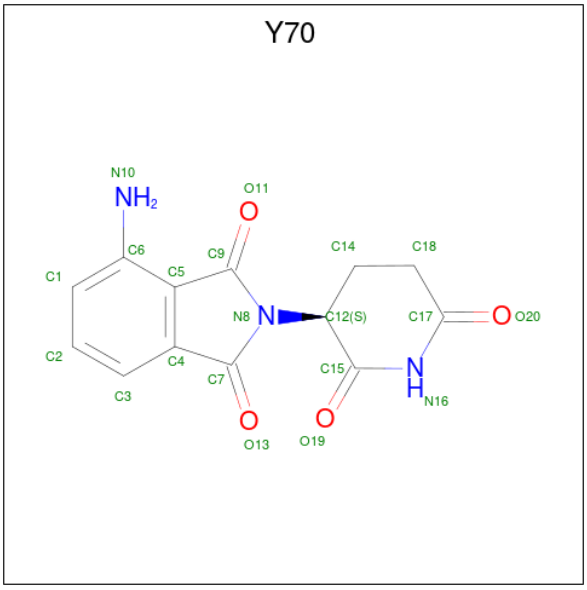
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	378	SER	-	expression tag	UNP Q9UJQ4
F	378	SER	-	expression tag	UNP Q9UJQ4

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

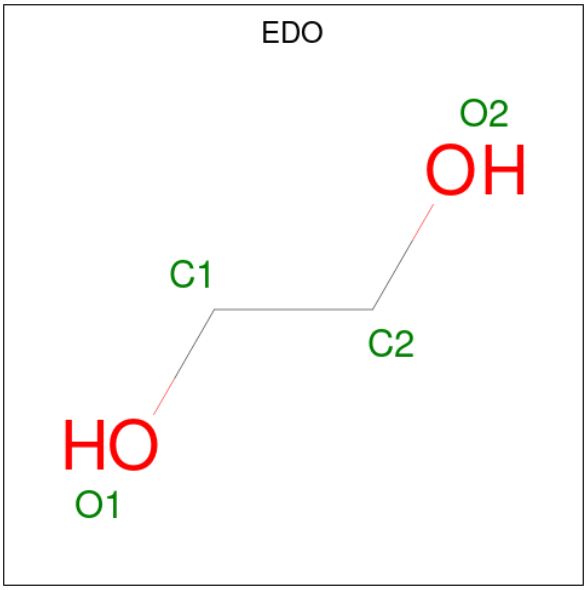
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Zn	0	0
			1	1		
4	C	2	Total	Zn	0	0
			2	2		
4	D	1	Total	Zn	0	0
			1	1		
4	F	2	Total	Zn	0	0
			2	2		

- Molecule 5 is S-Pomalidomide (three-letter code: Y70) (formula: $C_{13}H_{11}N_3O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O 20 13 3 4	0	0
5	D	1	Total C N O 20 13 3 4	0	0

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	E	1	Total C O 4 2 2	0	0

- Molecule 7 is water.

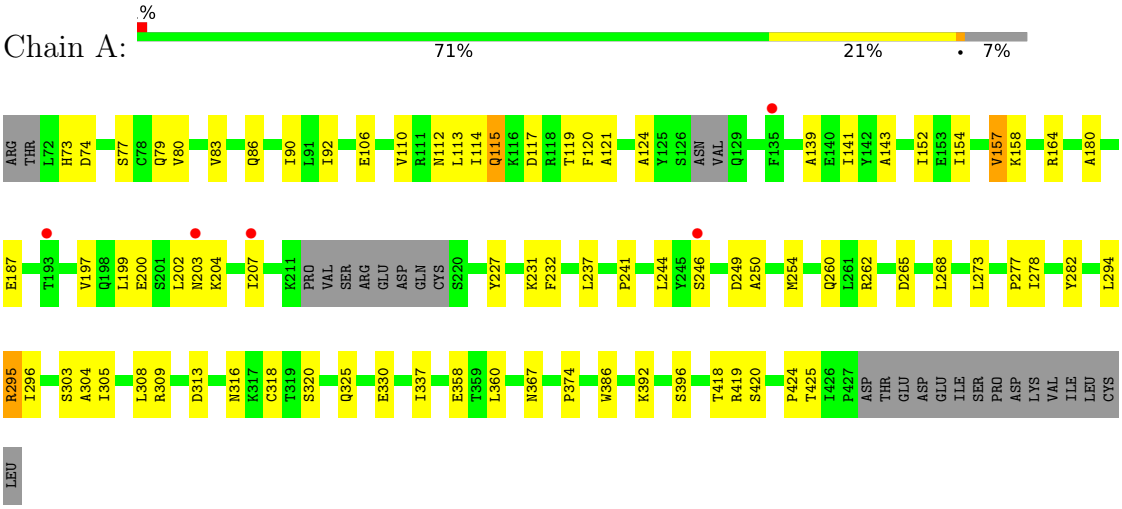
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	4	Total O 4 4	0	0
7	B	10	Total O 10 10	0	0
7	C	2	Total O 2 2	0	0
7	D	4	Total O 4 4	0	0
7	E	14	Total O 14 14	0	0
7	F	2	Total O 2 2	0	0

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.

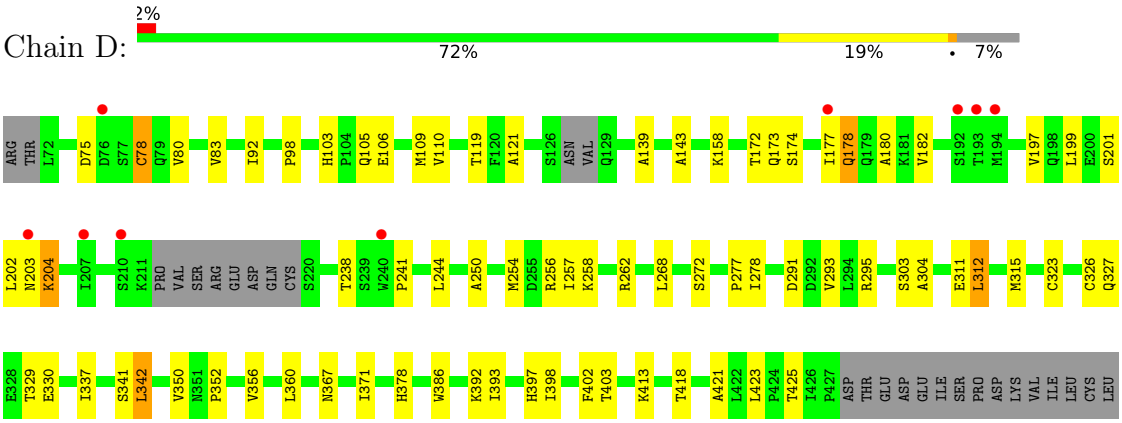
• Molecule 1: Protein cereblon

Chain A:



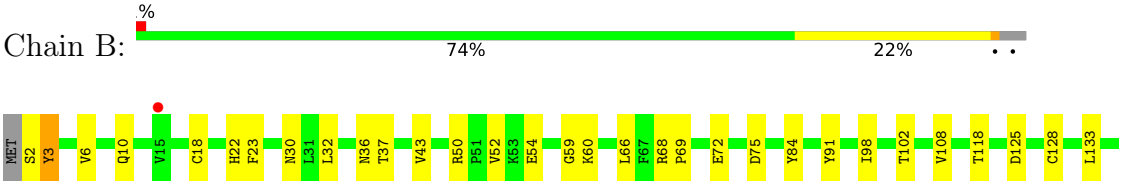
• Molecule 1: Protein cereblon

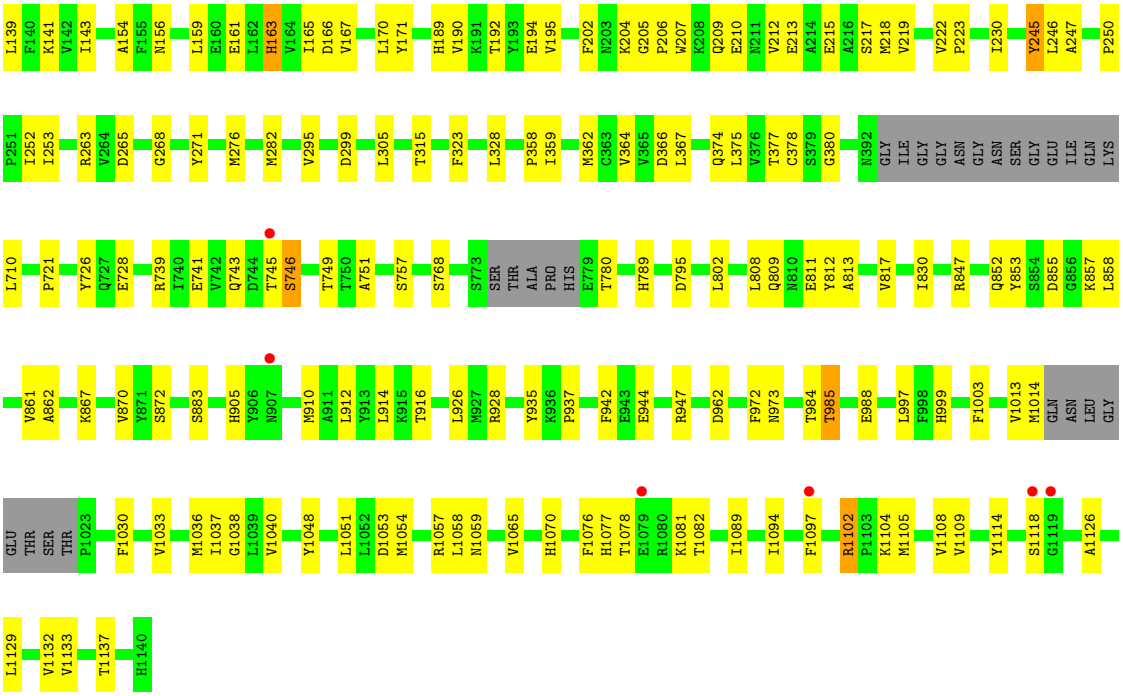
Chain D:



• Molecule 2: DNA damage-binding protein 1

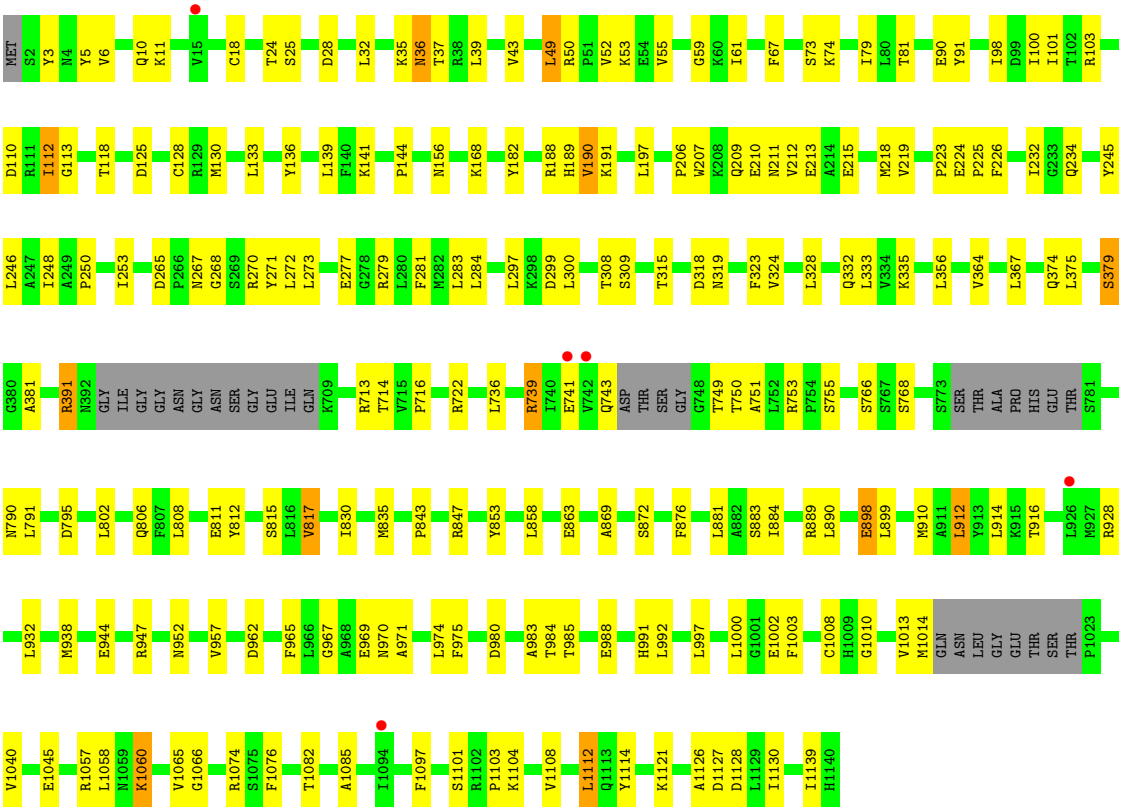
Chain B:





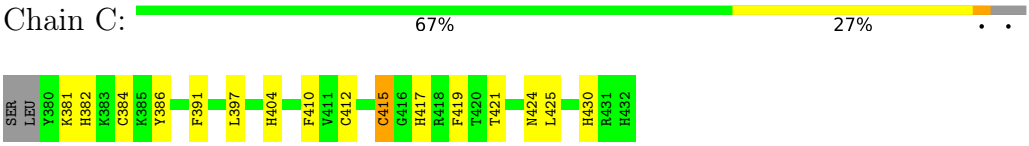
• Molecule 2: DNA damage-binding protein 1

Chain E:



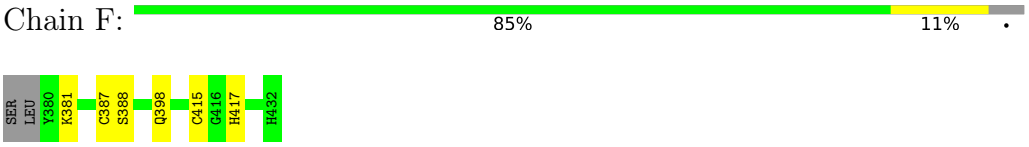
• Molecule 3: Sal-like protein 4

Chain C:



• Molecule 3: Sal-like protein 4

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	95.54Å 151.99Å 218.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.35 – 2.90 87.53 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.3 (49.35-2.90) 99.8 (87.53-2.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.92	Depositor
$< I/\sigma(I) >$ [1]	1.52 (at 2.91Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.219 , 0.273 0.227 , 0.281	Depositor DCC
R_{free} test set	3505 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å^2)	59.0	Xtriage
Anisotropy	0.291	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 43.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	18095	wwPDB-VP
Average B, all atoms (Å^2)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 53.52 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.1672e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: Y70, ZN, EDO

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	0.47	0/2664	0.67	1/3645 (0.0%)
1	D	0.47	0/2690	0.67	0/3671
2	B	0.49	2/6142 (0.0%)	0.70	1/8357 (0.0%)
2	E	0.49	1/6084 (0.0%)	0.70	3/8282 (0.0%)
3	C	0.45	1/407 (0.2%)	0.63	0/548
3	F	0.46	0/399	0.63	0/539
All	All	0.48	4/18386 (0.0%)	0.69	5/25042 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	E	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	898	GLU	CD-OE1	9.94	1.36	1.25
2	B	1102	ARG	CG-CD	7.04	1.69	1.51
2	B	1102	ARG	CB-CG	5.64	1.67	1.52
3	C	415	CYS	CB-SG	-5.08	1.73	1.81

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	294	LEU	CB-CG-CD2	7.70	124.09	111.00
2	E	898	GLU	CG-CD-OE2	-7.31	103.68	118.30
2	E	898	GLU	CB-CA-C	-6.45	97.51	110.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1102	ARG	N-CA-CB	6.01	121.43	110.60
2	E	898	GLU	CA-CB-CG	6.00	126.61	113.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	E	898	GLU	Sidechain

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	2600	0	2432	58	0
1	D	2627	0	2506	49	0
2	B	6027	0	5748	124	0
2	E	5973	0	5697	132	0
3	C	395	0	335	11	0
3	F	387	0	312	4	0
4	A	1	0	0	0	0
4	C	2	0	0	1	0
4	D	1	0	0	0	0
4	F	2	0	0	0	0
5	A	20	0	11	1	0
5	D	20	0	11	2	0
6	E	4	0	6	1	0
7	A	4	0	0	0	0
7	B	10	0	0	0	0
7	C	2	0	0	0	0
7	D	4	0	0	0	0
7	E	14	0	0	1	0
7	F	2	0	0	1	0
All	All	18095	0	17058	355	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 10.

All (355) 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)
2:B:1102:ARG:NH1	2:B:1126:ALA:HB3	1.77	0.97
3:C:415:CYS:HB2	3:C:417:HIS:H	1.35	0.89
1:D:278:ILE:HD13	1:D:304:ALA:HB2	1.58	0.83
2:E:10:GLN:NE2	2:E:11:LYS:O	2.12	0.83
2:B:6:VAL:HG22	2:B:1040:VAL:HG22	1.62	0.81
1:D:83:VAL:HG12	1:D:178:GLN:HB3	1.63	0.80
1:D:257:ILE:HG12	1:D:312:LEU:HG	1.63	0.79
2:E:985:THR:HG23	2:E:988:GLU:HG3	1.64	0.79
2:E:1058:LEU:HD11	2:E:1097:PHE:HB2	1.65	0.79
1:A:143:ALA:HB3	1:A:158:LYS:HB2	1.65	0.78
2:B:743:GLN:HA	2:B:749:THR:HG22	1.65	0.77
2:E:315:THR:HG22	2:E:323:PHE:HB3	1.66	0.75
2:E:952:ASN:ND2	2:E:969:GLU:OE1	2.20	0.73
1:D:398:ILE:HD13	1:D:421:ALA:HB1	1.69	0.73
3:C:421:THR:HG23	3:C:424:ASN:H	1.54	0.72
2:B:1102:ARG:HH11	2:B:1126:ALA:HB3	1.53	0.71
2:B:1051:LEU:HB2	2:B:1089:ILE:HD13	1.73	0.71
1:D:143:ALA:HB3	1:D:158:LYS:HB2	1.72	0.71
1:D:291:ASP:OD2	1:D:293:VAL:HG22	1.91	0.70
2:B:250:PRO:HG2	2:B:253:ILE:HG12	1.74	0.69
1:A:254:MET:CE	1:A:277:PRO:HA	2.23	0.69
2:B:768:SER:HB3	2:B:808:LEU:HD11	1.73	0.69
1:A:199:LEU:HD21	1:A:237:LEU:HD11	1.76	0.68
2:B:997:LEU:HD22	2:B:1076:PHE:CD1	2.28	0.68
1:A:254:MET:HE3	1:A:277:PRO:HA	1.76	0.68
2:B:739:ARG:HH11	2:B:757:SER:HB3	1.60	0.67
1:D:329:THR:HG21	1:D:393:ILE:HG13	1.77	0.67
2:E:190:VAL:HG13	2:E:209:GLN:HB3	1.75	0.67
2:E:248:ILE:HG13	2:E:250:PRO:HD3	1.76	0.67
2:E:741:GLU:HG2	2:E:750:THR:O	1.94	0.67
2:B:189:HIS:ND1	2:B:210:GLU:O	2.29	0.66
2:B:853:TYR:HB2	2:B:858:LEU:HD12	1.77	0.66
1:D:337:ILE:HD13	1:D:360:LEU:HD11	1.77	0.66
2:E:49:LEU:HD12	2:E:333:LEU:HD11	1.78	0.65
2:E:168:LYS:NZ	2:E:219:VAL:O	2.27	0.65
2:B:139:LEU:HD13	2:B:156:ASN:ND2	2.12	0.65
1:D:199:LEU:HB2	1:D:202:LEU:HD12	1.79	0.65
2:E:210:GLU:C	2:E:211:ASN:HD22	2.00	0.64
1:A:358:GLU:OE2	1:A:419:ARG:NH1	2.30	0.64
2:E:213:GLU:OE2	2:E:234:GLN:N	2.31	0.64
2:E:743:GLN:HA	2:E:749:THR:HG22	1.80	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:386:TRP:CG	5:D:502:Y70:H181	2.33	0.64
2:E:248:ILE:HD13	2:E:300:LEU:HB2	1.80	0.62
3:C:410:PHE:HB3	3:C:425:LEU:HD22	1.81	0.62
2:E:928:ARG:NH1	2:E:928:ARG:HG2	2.14	0.62
2:E:944:GLU:OE1	2:E:947:ARG:NH2	2.32	0.62
2:E:997:LEU:HD22	2:E:1076:PHE:CD2	2.35	0.62
2:B:133:LEU:HB2	2:B:141:LYS:HB3	1.81	0.62
2:E:188:ARG:NH1	2:E:215:GLU:HA	2.15	0.62
2:E:985:THR:CG2	2:E:988:GLU:HG3	2.30	0.62
1:D:250:ALA:O	1:D:254:MET:HG3	2.00	0.61
3:C:415:CYS:SG	4:C:502:ZN:ZN	1.88	0.61
1:D:83:VAL:HG23	1:D:121:ALA:O	2.01	0.61
2:B:1102:ARG:HA	2:B:1105:MET:HB3	1.82	0.61
2:E:277:GLU:OE1	2:E:279:ARG:NH2	2.33	0.61
2:E:1126:ALA:O	2:E:1130:ILE:HD12	2.02	0.60
2:B:1129:LEU:HA	2:B:1132:VAL:HG12	1.82	0.60
2:E:795:ASP:HB2	2:E:802:LEU:HD21	1.83	0.60
1:A:278:ILE:HD13	1:A:304:ALA:HB2	1.84	0.60
2:E:768:SER:OG	2:E:863:GLU:OE2	2.19	0.59
2:E:35:LYS:HE3	6:E:1201:EDO:H22	1.84	0.59
2:E:374:GLN:HG2	2:E:391:ARG:HE	1.67	0.59
2:E:928:ARG:HG2	2:E:928:ARG:HH11	1.65	0.59
1:D:106:GLU:O	1:D:110:VAL:HG13	2.02	0.59
2:B:43:VAL:HG21	2:B:50:ARG:CZ	2.33	0.59
2:B:362:MET:HE2	2:B:375:LEU:HG	1.84	0.58
2:B:1078:THR:OG1	2:B:1081:LYS:N	2.35	0.58
2:E:189:HIS:ND1	2:E:210:GLU:O	2.37	0.58
2:B:811:GLU:OE2	2:B:847:ARG:HD3	2.04	0.58
2:E:74:LYS:NZ	7:E:1302:HOH:O	2.36	0.57
2:E:881:LEU:HD13	2:E:890:LEU:HD13	1.86	0.57
1:A:207:ILE:HD13	2:B:163:HIS:HB3	1.85	0.57
2:B:245:TYR:HE1	2:B:247:ALA:HB2	1.70	0.57
2:B:213:GLU:HG2	2:B:215:GLU:H	1.68	0.57
2:E:974:LEU:HD11	2:E:1000:LEU:HD13	1.86	0.57
2:B:195:VAL:HG22	2:B:202:PHE:HE1	1.69	0.56
2:B:367:LEU:HB2	2:B:374:GLN:NE2	2.21	0.56
2:E:1057:ARG:NH1	2:E:1112:LEU:HB2	2.21	0.56
1:A:106:GLU:O	1:A:110:VAL:HG23	2.05	0.56
2:B:1053:ASP:O	2:B:1057:ARG:HG3	2.06	0.56
2:E:741:GLU:HG2	2:E:750:THR:C	2.26	0.55
2:B:22:HIS:HB2	2:B:75:ASP:OD2	2.07	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:119:THR:HA	1:D:139:ALA:O	2.06	0.55
1:D:398:ILE:O	1:D:418:THR:HG22	2.07	0.55
2:E:356:LEU:O	2:E:379:SER:HB3	2.07	0.55
1:A:250:ALA:HB2	1:A:305:ILE:HD11	1.88	0.55
3:C:421:THR:CG2	3:C:424:ASN:H	2.20	0.54
2:E:245:TYR:O	2:E:246:LEU:HD23	2.08	0.54
2:E:250:PRO:HG2	2:E:253:ILE:HG12	1.89	0.54
2:E:883:SER:OG	2:E:914:LEU:HD22	2.07	0.54
2:B:739:ARG:NH1	2:B:757:SER:HB3	2.21	0.54
1:D:371:ILE:HD13	3:F:417:HIS:NE2	2.22	0.54
1:A:237:LEU:HD21	2:B:328:LEU:HD22	1.90	0.53
1:A:141:ILE:HD12	1:A:157:VAL:HG21	1.89	0.53
2:E:139:LEU:HD13	2:E:156:ASN:ND2	2.24	0.53
2:B:69:PRO:HG2	2:B:72:GLU:HG3	1.89	0.53
2:B:139:LEU:HD13	2:B:156:ASN:HD22	1.73	0.53
2:E:843:PRO:HG2	2:E:869:ALA:HB2	1.90	0.53
2:E:853:TYR:HB2	2:E:858:LEU:HD13	1.90	0.53
2:E:928:ARG:HD2	2:E:969:GLU:OE1	2.09	0.53
2:B:359:ILE:HG23	2:B:377:THR:HB	1.90	0.52
2:E:225:PRO:HG2	2:E:267:ASN:HB2	1.91	0.52
2:E:741:GLU:CG	2:E:751:ALA:HA	2.40	0.52
2:B:23:PHE:N	2:B:30:ASN:OD1	2.42	0.52
2:E:1127:ASP:HA	2:E:1130:ILE:HD13	1.91	0.52
2:B:739:ARG:HH11	2:B:757:SER:CB	2.23	0.52
2:E:1074:ARG:O	2:E:1085:ALA:HB2	2.10	0.52
2:B:10:GLN:HB3	2:B:1037:ILE:HB	1.91	0.52
1:D:83:VAL:CG1	1:D:178:GLN:HB3	2.37	0.52
1:A:207:ILE:HD12	2:B:165:ILE:HD13	1.91	0.51
2:B:263:ARG:HG3	2:B:271:TYR:CE2	2.46	0.51
2:B:811:GLU:CD	2:B:847:ARG:HH11	2.13	0.51
2:B:1077:HIS:ND1	2:B:1082:THR:HG22	2.25	0.51
1:D:352:PRO:HG3	1:D:378:HIS:CG	2.45	0.51
1:A:119:THR:HA	1:A:139:ALA:O	2.10	0.51
2:E:90:GLU:OE1	2:E:101:ILE:HD11	2.10	0.51
2:E:223:PRO:HD2	2:E:268:GLY:HA3	1.93	0.51
1:D:241:PRO:HB3	2:E:812:TYR:CZ	2.45	0.51
2:B:246:LEU:HD22	2:B:299:ASP:HA	1.92	0.51
1:A:325:GLN:HG3	1:A:396:SER:OG	2.11	0.51
1:A:386:TRP:CG	5:A:502:Y70:H181	2.46	0.51
1:D:397:HIS:HD2	7:F:602:HOH:O	1.92	0.51
2:B:102:THR:OG1	2:B:1065:VAL:O	2.29	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:741:GLU:HG2	2:B:751:ALA:HA	1.93	0.51
2:B:1133:VAL:O	2:B:1137:THR:HG23	2.11	0.50
2:B:250:PRO:HB2	2:B:252:ILE:HG22	1.92	0.50
2:B:358:PRO:HD2	2:B:380:GLY:HA2	1.94	0.50
2:B:1104:LYS:O	2:B:1108:VAL:HG13	2.10	0.50
2:E:133:LEU:HB2	2:E:141:LYS:HB3	1.92	0.50
1:A:244:LEU:HD11	2:B:912:LEU:HD21	1.93	0.50
2:E:273:LEU:HB2	2:E:281:PHE:HB2	1.93	0.50
2:B:795:ASP:HB2	2:B:802:LEU:HD21	1.94	0.50
2:B:817:VAL:HG12	2:B:830:ILE:HB	1.93	0.50
2:B:60:LYS:HE2	2:B:972:PHE:CE2	2.47	0.50
2:E:817:VAL:HG12	2:E:830:ILE:HB	1.94	0.50
2:E:59:GLY:HA3	2:E:81:THR:HG21	1.92	0.50
2:E:110:ASP:HB2	2:E:136:TYR:CE2	2.46	0.50
1:A:241:PRO:HB3	2:B:812:TYR:OH	2.12	0.50
2:E:246:LEU:HD13	2:E:299:ASP:HA	1.92	0.50
1:D:173:GLN:CB	1:D:177:ILE:HD11	2.42	0.50
2:E:3:TYR:OH	2:E:1045:GLU:HG3	2.11	0.49
2:E:215:GLU:OE1	2:E:234:GLN:HG3	2.11	0.49
1:A:318:CYS:HB3	1:A:424:PRO:HB2	1.93	0.49
2:B:171:TYR:CD2	2:B:223:PRO:HA	2.46	0.49
2:B:855:ASP:C	2:B:857:LYS:H	2.16	0.49
1:A:241:PRO:HB3	2:B:812:TYR:CZ	2.47	0.49
2:B:84:TYR:HB3	2:B:108:VAL:HG23	1.94	0.49
1:D:350:VAL:HG22	1:D:356:VAL:HG22	1.95	0.49
1:A:141:ILE:HD12	1:A:157:VAL:CG2	2.43	0.49
2:B:3:TYR:HB3	2:B:1048:TYR:CD1	2.48	0.49
2:E:328:LEU:HD13	2:E:381:ALA:HB3	1.94	0.49
1:A:320:SER:OG	1:A:330:GLU:HG3	2.13	0.49
1:A:309:ARG:HH22	2:B:910:MET:HE3	1.76	0.49
1:D:423:LEU:O	1:D:425:THR:HG23	2.12	0.49
2:E:364:VAL:HG23	2:E:1008:CYS:SG	2.52	0.49
2:B:1102:ARG:HA	2:B:1105:MET:CB	2.42	0.49
2:E:24:THR:HA	2:E:91:TYR:CD1	2.48	0.49
2:E:808:LEU:O	2:E:811:GLU:HB2	2.12	0.49
2:B:944:GLU:CD	2:B:947:ARG:HH21	2.17	0.48
1:D:172:THR:HG23	1:D:178:GLN:HG2	1.94	0.48
1:A:337:ILE:HD13	1:A:360:LEU:HD11	1.95	0.48
2:E:112:ILE:HG12	2:E:113:GLY:N	2.27	0.48
2:E:768:SER:HB3	2:E:808:LEU:HD11	1.96	0.48
1:A:199:LEU:HD12	1:A:202:LEU:HD13	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:ARG:HG3	1:A:268:LEU:HD23	1.94	0.48
2:B:190:VAL:CG1	2:B:209:GLN:HB3	2.44	0.48
1:D:326:CYS:SG	1:D:329:THR:OG1	2.62	0.48
1:A:318:CYS:HA	1:A:425:THR:O	2.14	0.48
1:D:238:THR:O	2:E:722:ARG:NH2	2.39	0.47
2:E:3:TYR:CZ	2:E:1045:GLU:HG3	2.49	0.47
2:E:226:PHE:CE1	2:E:297:LEU:HD13	2.49	0.47
2:B:1030:PHE:CZ	2:B:1038:GLY:HA3	2.49	0.47
2:B:1102:ARG:HH12	2:B:1126:ALA:HB3	1.72	0.47
1:A:92:ILE:HD11	1:A:295:ARG:HG2	1.97	0.47
2:B:32:LEU:HD22	2:B:66:LEU:HD11	1.95	0.47
3:C:412:CYS:HA	3:C:425:LEU:HD11	1.95	0.47
2:E:884:ILE:HD13	2:E:889:ARG:NH1	2.30	0.47
1:A:367:ASN:HA	1:A:392:LYS:HD2	1.97	0.47
1:D:80:VAL:HA	1:D:180:ALA:O	2.15	0.47
2:E:367:LEU:HG	2:E:374:GLN:OE1	2.15	0.47
2:E:1104:LYS:O	2:E:1108:VAL:HG13	2.14	0.47
2:E:318:ASP:OD1	2:E:319:ASN:N	2.48	0.47
1:A:202:LEU:HD21	2:B:276:MET:SD	2.55	0.46
2:B:1036:MET:HG2	2:B:1037:ILE:N	2.29	0.46
2:E:811:GLU:HG3	2:E:835:MET:SD	2.55	0.46
2:E:899:LEU:HA	2:E:899:LEU:HD23	1.54	0.46
2:B:378:CYS:HB3	2:B:721:PRO:HB2	1.97	0.46
2:E:714:THR:HG22	2:E:716:PRO:HD3	1.96	0.46
1:A:268:LEU:HD11	1:A:273:LEU:HD21	1.98	0.46
1:D:201:SER:O	1:D:204:LYS:HD2	2.15	0.46
2:E:18:CYS:HA	2:E:32:LEU:O	2.16	0.46
2:E:206:PRO:HB2	2:E:207:TRP:CD1	2.49	0.46
1:A:152:ILE:O	1:A:154:ILE:HD12	2.15	0.46
2:E:952:ASN:OD1	2:E:970:ASN:HB3	2.15	0.46
2:E:218:MET:CE	2:E:232:ILE:HD12	2.46	0.46
1:D:311:GLU:O	1:D:315:MET:HG3	2.16	0.46
2:B:223:PRO:HD2	2:B:268:GLY:HA3	1.96	0.45
2:E:37:THR:HG22	2:E:59:GLY:O	2.16	0.45
2:E:364:VAL:HG22	2:E:375:LEU:HD13	1.98	0.45
2:B:163:HIS:ND1	2:B:163:HIS:N	2.64	0.45
2:E:39:LEU:HB3	2:E:55:VAL:HG22	1.99	0.45
3:F:387:CYS:O	3:F:388:SER:HB3	2.17	0.45
1:A:113:LEU:O	1:A:115:GLN:N	2.43	0.45
3:C:421:THR:HG22	3:C:424:ASN:CG	2.36	0.45
1:D:386:TRP:CD1	5:D:502:Y70:H181	2.50	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:308:THR:OG1	2:E:309:SER:N	2.49	0.45
2:E:766:SER:HB3	2:E:808:LEU:HD23	1.98	0.45
2:B:378:CYS:HB3	2:B:721:PRO:HG2	1.98	0.45
2:E:980:ASP:HB3	2:E:983:ALA:HB2	1.98	0.45
2:E:1065:VAL:HG12	2:E:1066:GLY:N	2.31	0.45
1:A:197:VAL:HG13	2:B:1003:PHE:CE2	2.51	0.45
1:A:203:ASN:HB3	2:B:118:THR:O	2.17	0.45
2:B:811:GLU:OE1	2:B:847:ARG:NH1	2.50	0.45
1:D:103:HIS:HB2	1:D:106:GLU:OE2	2.16	0.45
2:B:861:VAL:O	2:B:862:ALA:HB3	2.17	0.45
1:D:371:ILE:HD13	3:F:417:HIS:HE2	1.81	0.45
2:B:305:LEU:HD23	2:B:305:LEU:HA	1.74	0.45
1:A:73:HIS:ND1	1:A:79:GLN:HG3	2.32	0.45
2:E:271:TYR:HB2	2:E:283:LEU:HB3	1.99	0.45
2:B:159:LEU:HD23	2:B:159:LEU:HA	1.83	0.45
2:B:914:LEU:HD12	2:B:914:LEU:HA	1.73	0.45
1:D:256:ARG:HB2	1:D:312:LEU:HD11	1.97	0.45
2:E:967:GLY:HA3	2:E:975:PHE:CE1	2.52	0.45
3:C:391:PHE:CD1	3:C:397:LEU:HD12	2.52	0.45
2:E:790:ASN:OD1	2:E:806:GLN:HA	2.17	0.45
2:E:1101:SER:HB2	2:E:1103:PRO:HD2	1.99	0.45
1:A:187:GLU:OE1	1:A:278:ILE:HD12	2.17	0.44
1:D:203:ASN:HB3	2:E:118:THR:O	2.17	0.44
2:E:1101:SER:CB	2:E:1103:PRO:HD2	2.46	0.44
1:A:74:ASP:HB3	1:A:77:SER:HB3	1.98	0.44
1:A:83:VAL:HG22	1:A:121:ALA:HB3	2.00	0.44
2:B:125:ASP:OD2	2:B:128:CYS:N	2.50	0.44
2:B:212:VAL:HG22	2:B:213:GLU:H	1.82	0.44
2:B:222:VAL:HA	2:B:223:PRO:HD3	1.85	0.44
2:B:870:VAL:HA	2:B:883:SER:O	2.18	0.44
2:B:1051:LEU:CB	2:B:1089:ILE:HD13	2.45	0.44
1:D:244:LEU:HD11	2:E:912:LEU:HD11	2.00	0.44
1:A:164:ARG:NE	1:A:282:TYR:OH	2.49	0.44
2:E:5:TYR:HE1	2:E:1139:ILE:HD11	1.83	0.44
2:B:867:LYS:HE2	2:B:867:LYS:HB2	1.76	0.44
1:D:342:LEU:H	1:D:342:LEU:HG	1.32	0.44
2:E:144:PRO:HB3	2:E:197:LEU:HD21	1.98	0.44
2:E:218:MET:HE3	2:E:232:ILE:HD12	1.99	0.44
1:A:117:ASP:HB2	1:A:119:THR:HG22	2.00	0.44
2:B:141:LYS:HD2	2:B:154:ALA:HB3	1.99	0.44
2:E:43:VAL:HG22	2:E:50:ARG:CG	2.48	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:374:PRO:HA	1:A:386:TRP:O	2.18	0.44
2:B:192:THR:O	2:B:205:GLY:HA3	2.18	0.44
2:B:1051:LEU:HB2	2:B:1089:ILE:CD1	2.45	0.44
2:B:910:MET:HG2	2:B:912:LEU:CD1	2.48	0.44
2:E:1076:PHE:O	2:E:1082:THR:HA	2.18	0.44
2:B:905:HIS:HB2	2:B:942:PHE:CD2	2.53	0.44
2:E:43:VAL:HG22	2:E:50:ARG:HG2	2.00	0.44
2:E:970:ASN:HA	2:E:971:ALA:HA	1.84	0.44
2:B:91:TYR:OH	2:B:98:ILE:HD13	2.17	0.43
2:B:125:ASP:OD2	2:B:125:ASP:C	2.56	0.43
2:B:170:LEU:HD23	2:B:170:LEU:HA	1.84	0.43
3:C:386:TYR:HB2	3:C:404:HIS:CD2	2.53	0.43
2:E:182:TYR:CE2	2:E:189:HIS:HD2	2.36	0.43
2:E:932:LEU:HD22	2:E:965:PHE:CZ	2.53	0.43
2:B:985:THR:HG23	2:B:988:GLU:CB	2.48	0.43
1:A:120:PHE:HE1	1:A:141:ILE:HD11	1.83	0.43
2:B:1054:MET:SD	2:B:1129:LEU:HD22	2.58	0.43
2:B:1059:ASN:ND2	2:B:1070:HIS:HB3	2.34	0.43
2:E:67:PHE:HB2	2:E:128:CYS:SG	2.57	0.43
1:A:232:PHE:HZ	1:A:249:ASP:HB2	1.83	0.43
2:B:367:LEU:HB2	2:B:374:GLN:HE22	1.84	0.43
2:B:789:HIS:CD2	2:B:813:ALA:H	2.36	0.43
2:B:1057:ARG:HD3	2:B:1108:VAL:O	2.18	0.43
2:E:43:VAL:HG13	2:E:52:VAL:HG21	2.00	0.43
2:E:910:MET:HG2	2:E:912:LEU:HD13	2.00	0.43
1:A:207:ILE:CD1	2:B:163:HIS:HB3	2.49	0.43
1:A:237:LEU:HD22	2:B:358:PRO:HG3	2.00	0.43
2:B:143:ILE:HG12	2:B:154:ALA:HB2	2.00	0.43
2:B:852:GLN:O	2:B:853:TYR:HB3	2.19	0.43
1:D:371:ILE:HG21	3:F:417:HIS:CE1	2.53	0.43
2:E:356:LEU:O	2:E:379:SER:CB	2.65	0.43
1:D:262:ARG:HG2	1:D:268:LEU:CD2	2.49	0.43
2:E:270:ARG:HG2	2:E:284:LEU:HD23	2.00	0.43
1:A:260:GLN:HE22	1:A:316:ASN:HD21	1.65	0.43
2:B:358:PRO:HA	2:B:1033:VAL:O	2.19	0.43
1:D:323:CYS:O	1:D:327:GLN:HA	2.19	0.43
1:D:254:MET:CE	1:D:277:PRO:HA	2.49	0.43
1:A:112:ASN:HD22	1:A:112:ASN:HA	1.53	0.42
1:A:200:GLU:HA	1:A:203:ASN:ND2	2.33	0.42
2:B:364:VAL:HG22	2:B:375:LEU:HD13	2.01	0.42
2:E:182:TYR:HE1	2:E:191:LYS:HB2	1.84	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:308:THR:OG1	2:E:324:VAL:HG11	2.19	0.42
2:E:315:THR:CG2	2:E:323:PHE:HB3	2.44	0.42
2:E:811:GLU:OE2	2:E:847:ARG:NH1	2.52	0.42
1:A:80:VAL:HA	1:A:180:ALA:O	2.20	0.42
2:B:195:VAL:HG22	2:B:202:PHE:CE1	2.52	0.42
1:A:90:ILE:HD13	1:A:296:ILE:HG13	2.02	0.42
2:E:6:VAL:HB	2:E:1040:VAL:HG22	2.02	0.42
2:E:364:VAL:HG21	2:E:1010:GLY:HA3	2.01	0.42
2:E:876:PHE:HD1	2:E:916:THR:HG21	1.84	0.42
2:B:18:CYS:HA	2:B:32:LEU:O	2.18	0.42
1:A:237:LEU:HD21	2:B:328:LEU:CD2	2.50	0.42
2:E:1060:LYS:HD2	2:E:1060:LYS:HA	1.79	0.42
2:B:1058:LEU:HD11	2:B:1097:PHE:HB2	2.02	0.42
1:D:197:VAL:HG13	2:E:1003:PHE:CE2	2.54	0.42
2:E:308:THR:HG23	2:E:309:SER:O	2.20	0.42
2:E:1013:VAL:HG23	2:E:1014:MET:N	2.33	0.42
2:B:37:THR:HG22	2:B:59:GLY:O	2.20	0.42
1:D:204:LYS:HE2	2:E:218:MET:SD	2.60	0.42
2:E:741:GLU:HG3	2:E:751:ALA:HA	2.01	0.42
1:A:86:GLN:OE1	1:A:86:GLN:HA	2.20	0.42
1:A:90:ILE:HG12	1:A:124:ALA:HB1	2.01	0.42
1:A:250:ALA:O	1:A:254:MET:HG3	2.19	0.42
2:B:1094:ILE:HD13	2:B:1094:ILE:HA	1.86	0.42
3:C:419:PHE:CD2	3:C:425:LEU:HD13	2.55	0.42
2:E:53:LYS:HD3	2:E:98:ILE:HG22	2.02	0.42
1:D:257:ILE:CG1	1:D:312:LEU:HG	2.42	0.41
2:E:139:LEU:HD13	2:E:156:ASN:HD22	1.85	0.41
2:B:935:TYR:O	2:B:937:PRO:HD3	2.20	0.41
2:B:43:VAL:HG13	2:B:52:VAL:HG21	2.03	0.41
3:C:421:THR:HG22	3:C:424:ASN:ND2	2.36	0.41
2:E:61:ILE:HG23	2:E:79:ILE:HG23	2.02	0.41
2:B:853:TYR:HA	2:B:857:LYS:O	2.21	0.41
2:B:1105:MET:O	2:B:1109:VAL:HG13	2.20	0.41
1:D:105:GLN:O	1:D:109:MET:HB2	2.20	0.41
2:E:43:VAL:HG13	2:E:52:VAL:CG2	2.50	0.41
2:E:991:HIS:HD2	2:E:992:LEU:N	2.18	0.41
1:D:204:LYS:H	1:D:204:LYS:HG3	1.65	0.41
2:E:90:GLU:OE1	2:E:103:ARG:HD3	2.21	0.41
2:E:36:ASN:ND2	2:E:1002:GLU:OE2	2.53	0.41
2:B:166:ASP:OD1	2:B:167:VAL:N	2.53	0.41
2:B:166:ASP:HB3	2:B:219:VAL:HG23	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:367:LEU:HD12	2:B:374:GLN:NE2	2.35	0.41
2:E:736:LEU:HD23	2:E:791:LEU:HD13	2.03	0.41
2:E:100:ILE:HD12	2:E:100:ILE:N	2.36	0.41
1:D:78:CYS:HA	1:D:182:VAL:O	2.21	0.41
1:D:386:TRP:HB3	1:D:402:PHE:CE2	2.56	0.41
2:E:49:LEU:HD11	2:E:333:LEU:HD21	2.02	0.41
1:A:204:LYS:HE3	2:B:218:MET:SD	2.61	0.40
2:B:315:THR:HG23	2:B:323:PHE:HB3	2.02	0.40
2:B:926:LEU:HD12	2:B:926:LEU:HA	1.93	0.40
2:B:1013:VAL:HG23	2:B:1014:MET:N	2.36	0.40
2:E:1130:ILE:HD12	2:E:1130:ILE:H	1.86	0.40
1:A:141:ILE:HG23	1:A:157:VAL:HG23	2.02	0.40
2:B:194:GLU:HG3	2:B:204:LYS:O	2.21	0.40
2:B:206:PRO:HB2	2:B:207:TRP:CD1	2.56	0.40
2:B:973:ASN:OD1	2:B:999:HIS:CD2	2.75	0.40
2:B:1097:PHE:CE1	2:B:1105:MET:HG3	2.56	0.40
1:A:227:TYR:CZ	1:A:231:LYS:HD3	2.56	0.40
2:B:133:LEU:HD23	2:B:133:LEU:HA	1.83	0.40
1:D:367:ASN:HA	1:D:392:LYS:HD2	2.03	0.40
2:E:25:SER:OG	2:E:28:ASP:OD2	2.15	0.40
2:B:726:TYR:CZ	2:B:728:GLU:HA	2.57	0.40
1:D:92:ILE:HD11	1:D:295:ARG:HG3	2.04	0.40
2:E:53:LYS:HD3	2:E:98:ILE:CG2	2.51	0.40
2:E:391:ARG:HE	2:E:391:ARG:HB2	1.61	0.40
2:E:739:ARG:HH12	2:E:790:ASN:HD21	1.68	0.40
1:A:265:ASP:HB3	1:A:268:LEU:HB2	2.04	0.40
2:E:272:LEU:O	2:E:273:LEU:HD23	2.22	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	340/373 (91%)	324 (95%)	14 (4%)	2 (1%)	25 58
1	D	340/373 (91%)	324 (95%)	15 (4%)	1 (0%)	41 71
2	B	802/836 (96%)	752 (94%)	47 (6%)	3 (0%)	34 66
2	E	794/836 (95%)	748 (94%)	44 (6%)	2 (0%)	41 71
3	C	51/55 (93%)	47 (92%)	3 (6%)	1 (2%)	7 27
3	F	51/55 (93%)	46 (90%)	4 (8%)	1 (2%)	7 27
All	All	2378/2528 (94%)	2241 (94%)	127 (5%)	10 (0%)	34 66

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	174	SER
1	A	114	ILE
2	B	36	ASN
2	E	36	ASN
1	A	115	GLN
2	B	780	THR
3	F	381	LYS
2	B	746	SER
2	E	1121	LYS
3	C	381	LYS

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	258/340 (76%)	250 (97%)	8 (3%)	40 74
1	D	265/340 (78%)	251 (95%)	14 (5%)	22 54
2	B	615/727 (85%)	590 (96%)	25 (4%)	30 64
2	E	607/727 (84%)	578 (95%)	29 (5%)	25 58
3	C	38/51 (74%)	35 (92%)	3 (8%)	12 34
3	F	34/51 (67%)	32 (94%)	2 (6%)	19 49

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1817/2236 (81%)	1736 (96%)	81 (4%)	27 61

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	157	VAL
1	A	246	SER
1	A	295	ARG
1	A	303	SER
1	A	308	LEU
1	A	313	ASP
1	A	418	THR
1	A	420	SER
2	B	2	SER
2	B	3	TYR
2	B	54	GLU
2	B	68	ARG
2	B	161	GLU
2	B	163	HIS
2	B	217	SER
2	B	230	ILE
2	B	245	TYR
2	B	265	ASP
2	B	282	MET
2	B	295	VAL
2	B	366	ASP
2	B	710	LEU
2	B	745	THR
2	B	746	SER
2	B	809	GLN
2	B	872	SER
2	B	916	THR
2	B	928	ARG
2	B	962	ASP
2	B	984	THR
2	B	985	THR
2	B	1114	TYR
2	B	1118	SER
3	C	382	HIS
3	C	384	CYS
3	C	430	HIS
1	D	75	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	78	CYS
1	D	98	PRO
1	D	178	GLN
1	D	204	LYS
1	D	258	LYS
1	D	272	SER
1	D	303	SER
1	D	312	LEU
1	D	330	GLU
1	D	341	SER
1	D	342	LEU
1	D	403	THR
1	D	413	LYS
2	E	49	LEU
2	E	73	SER
2	E	112	ILE
2	E	125	ASP
2	E	130	MET
2	E	190	VAL
2	E	212	VAL
2	E	224	GLU
2	E	265	ASP
2	E	332	GLN
2	E	335	LYS
2	E	379	SER
2	E	391	ARG
2	E	713	ARG
2	E	739	ARG
2	E	753	ARG
2	E	755	SER
2	E	815	SER
2	E	817	VAL
2	E	872	SER
2	E	912	LEU
2	E	938	MET
2	E	957	VAL
2	E	962	ASP
2	E	984	THR
2	E	1060	LYS
2	E	1112	LEU
2	E	1114	TYR
2	E	1128	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	F	398	GLN
3	F	415	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	112	ASN
1	A	316	ASN
1	A	367	ASN
2	B	999	HIS
1	D	397	HIS
2	E	211	ASN
2	E	759	GLN
2	E	991	HIS

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 9 ligands modelled in this entry, 6 are monoatomic - leaving 3 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	$\#\|Z\|>2$
6	EDO	E	1201	-	3,3,3	0.51	0	2,2,2	0.16	0
5	Y70	A	502	-	22,22,22	0.78	0	31,33,33	1.46	8 (25%)
5	Y70	D	502	-	22,22,22	0.98	1 (4%)	31,33,33	1.40	5 (16%)

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
6	EDO	E	1201	-	-	0/1/1/1	-
5	Y70	A	502	-	-	1/4/33/33	0/3/3/3
5	Y70	D	502	-	-	0/4/33/33	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	502	Y70	C5-C6	-2.64	1.38	1.42

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	502	Y70	C18-C14-C12	3.66	116.66	109.77
5	A	502	Y70	C18-C14-C12	2.99	115.39	109.77
5	D	502	Y70	C2-C3-C4	-2.71	114.69	119.81
5	A	502	Y70	C5-C6-N10	2.64	125.24	121.66
5	A	502	Y70	C1-C6-C5	-2.58	114.80	118.29
5	D	502	Y70	C1-C6-C5	-2.57	114.82	118.29
5	A	502	Y70	C14-C12-C15	2.40	115.73	111.61
5	A	502	Y70	C12-C15-N16	2.38	119.45	116.25
5	D	502	Y70	C12-C15-N16	2.33	119.38	116.25
5	D	502	Y70	C14-C12-C15	2.24	115.47	111.61
5	A	502	Y70	C15-C12-N8	2.23	111.11	109.08
5	A	502	Y70	C2-C1-C6	2.13	124.01	121.04
5	A	502	Y70	C2-C3-C4	-2.06	115.91	119.81

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	502	Y70	C14-C12-N8-C9

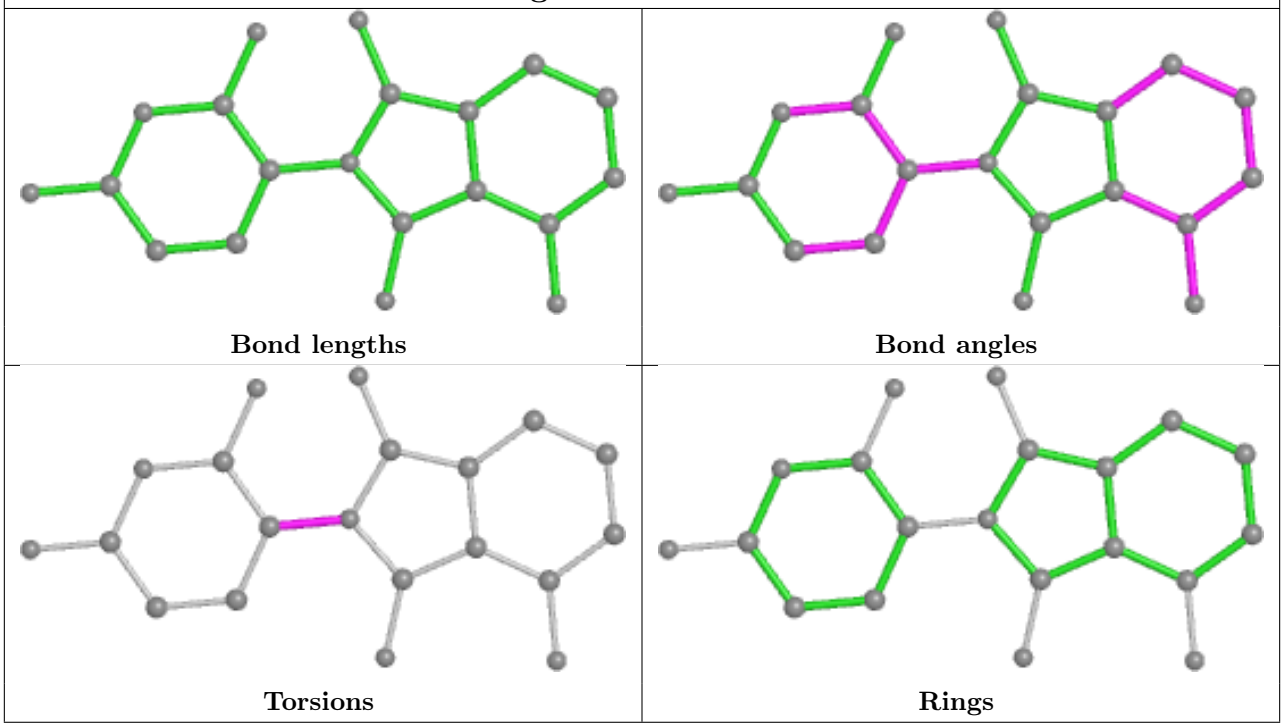
There are no ring outliers.

3 monomers are involved in 4 short contacts:

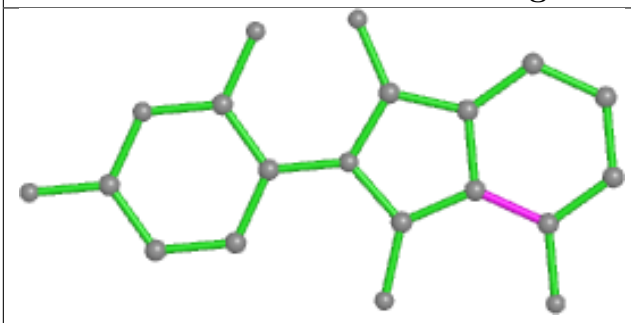
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	E	1201	EDO	1	0
5	A	502	Y70	1	0
5	D	502	Y70	2	0

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.

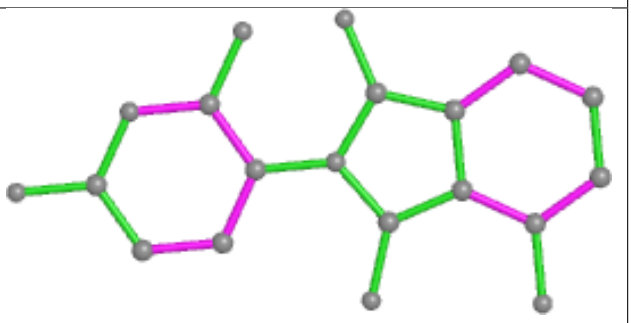
Ligand Y70 A 502



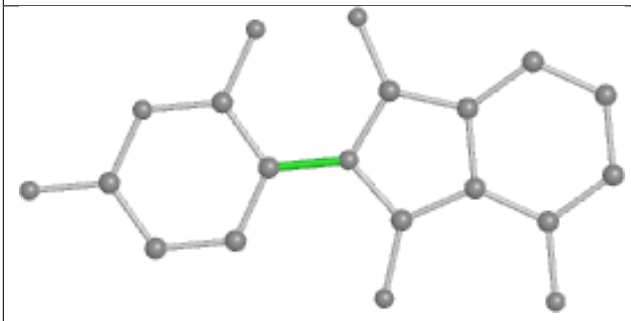
Ligand Y70 D 502



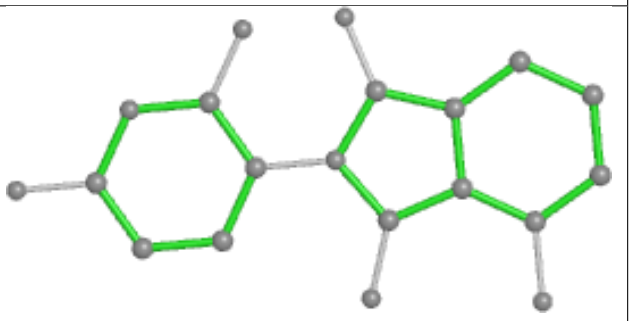
Bond lengths



Bond angles



Torsions



Rings

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, 95^{th} 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	346/373 (92%)	0.08	5 (1%) 75 75	43, 72, 119, 162	0
1	D	346/373 (92%)	0.02	9 (2%) 56 52	44, 64, 116, 152	0
2	B	809/836 (96%)	-0.00	7 (0%) 84 84	40, 64, 107, 147	0
2	E	804/836 (96%)	0.01	5 (0%) 89 89	43, 69, 115, 146	0
3	C	53/55 (96%)	-0.27	0 100 100	63, 85, 111, 116	0
3	F	53/55 (96%)	-0.44	0 100 100	54, 80, 113, 121	0
All	All	2411/2528 (95%)	0.00	26 (1%) 80 80	40, 68, 114, 162	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	203	ASN	3.0
1	A	207	ILE	3.0
2	B	15	VAL	3.0
2	B	1119	GLY	2.8
1	D	194	MET	2.6
1	D	210	SER	2.6
1	D	193	THR	2.6
1	A	246	SER	2.6
2	B	1079	GLU	2.5
1	D	192	SER	2.4
1	D	76	ASP	2.4
2	B	745	THR	2.3
2	E	742	VAL	2.3
2	B	1118	SER	2.3
2	E	15	VAL	2.3
1	D	203	ASN	2.2
2	E	926	LEU	2.2
1	A	135	PHE	2.1
1	D	240	TRP	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	193	THR	2.0
1	D	207	ILE	2.0
2	B	1097	PHE	2.0
2	E	1094	ILE	2.0
2	E	741	GLU	2.0
1	D	177	ILE	2.0
2	B	907	ASN	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

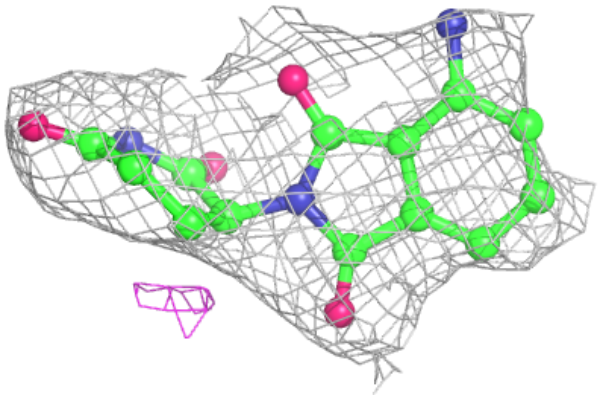
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

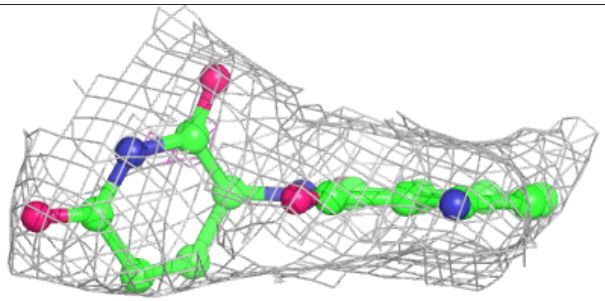
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	EDO	E	1201	4/4	0.91	0.35	62,64,64,64	0
5	Y70	A	502	20/20	0.95	0.24	60,69,73,76	0
5	Y70	D	502	20/20	0.96	0.21	47,54,56,62	0
4	ZN	C	501	1/1	0.97	0.14	86,86,86,86	0
4	ZN	A	501	1/1	0.98	0.15	69,69,69,69	0
4	ZN	C	502	1/1	0.99	0.17	86,86,86,86	0
4	ZN	F	501	1/1	0.99	0.14	79,79,79,79	0
4	ZN	F	502	1/1	0.99	0.15	56,56,56,56	0
4	ZN	D	501	1/1	1.00	0.14	57,57,57,57	0

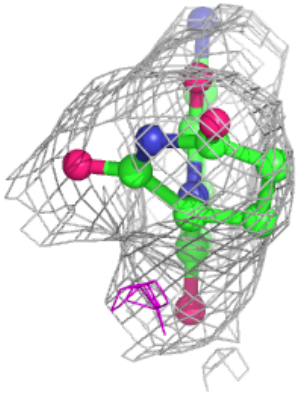
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around Y70 A 502:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

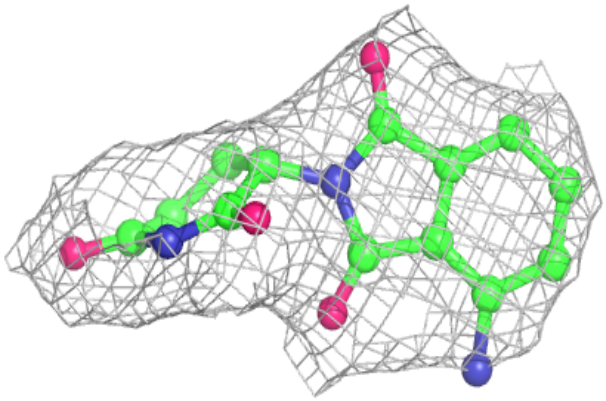


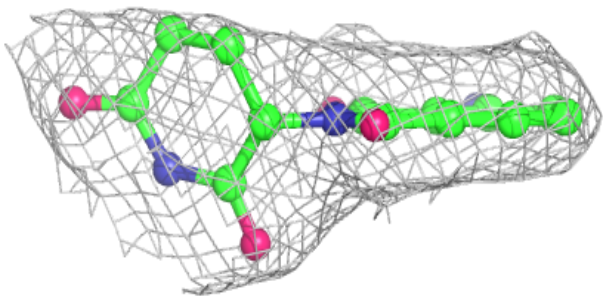


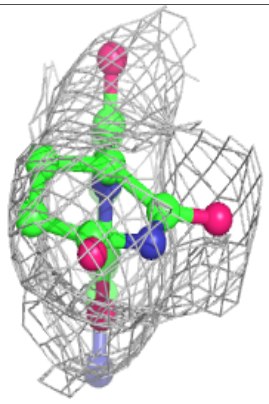


Electron density around Y70 D 502:

$2mF_o$-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.