Full wwPDB X-ray Structure Validation Report (i)

Sep 22, 2022 – 05:14 pm BST

PDB ID	:	7OR4
Title	:	Crystal structure of DPP8 in complex with a 4-oxo-b-lactam based inhibitor, B142
Authors	:	Ross, B.; Huber, R.
Deposited on	:	2021-06-04
Resolution	:	2.44 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:

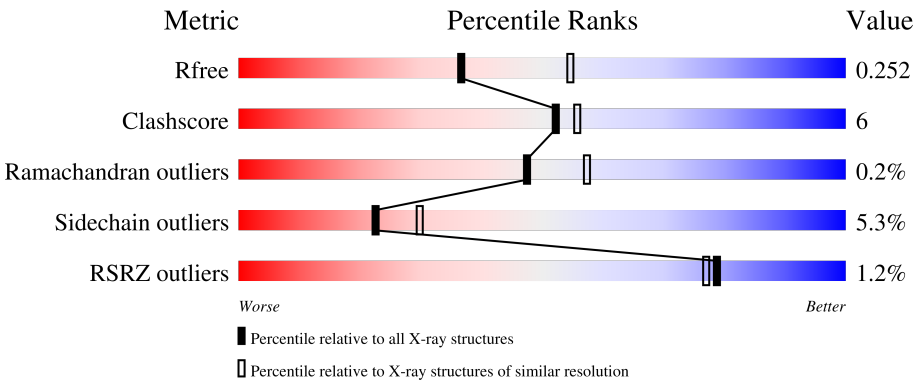
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.30
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.30

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 2.44 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	1564 (2.46-2.42)
Clashscore	141614	1631 (2.46-2.42)
Ramachandran outliers	138981	1617 (2.46-2.42)
Sidechain outliers	138945	1617 (2.46-2.42)
RSRZ outliers	127900	1547 (2.46-2.42)

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	898	% 76% 13% 10%
1	B	898	% 75% 15% • 9%

2 Entry composition (i)

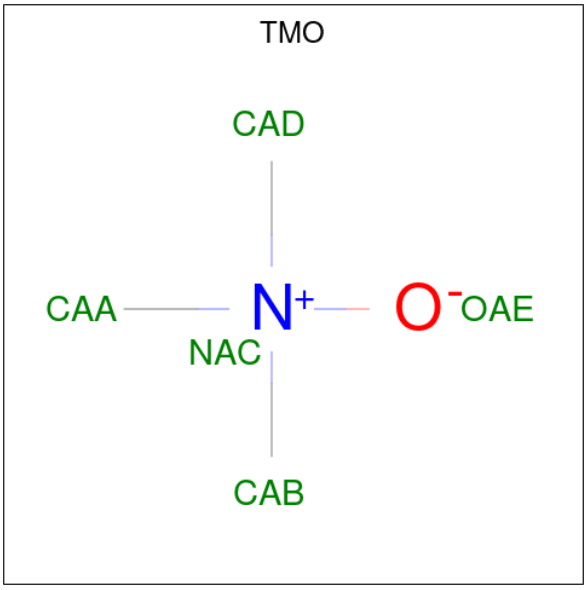
There are 4 unique types of molecules in this entry. The entry contains 13408 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Dipeptidyl peptidase 8.

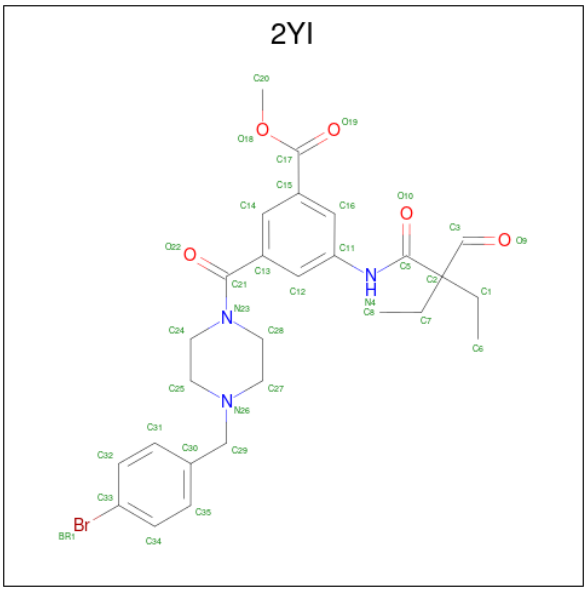
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	B	815	6622	4262	1105	1228	27	0	0	0
1	A	805	6536	4209	1087	1213	27	0	1	0

- Molecule 2 is trimethylamine oxide (three-letter code: TMO) (formula: C_3H_9NO).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	B	1	5	3	1	1	0	0
2	A	1	5	3	1	1	0	0

- Molecule 3 is methyl 3-[4-[(4-bromophenyl)methyl]piperazin-1-yl]carbonyl-5-[(2-ethyl-2-methanoyl-butanoyl)amino]benzoate (three-letter code: 2YI) (formula: $C_{27}H_{32}BrN_3O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	Br	C	N	O		
3	B	1	36	1	27	3	5	0	0
			Total	Br	C	N	O		
3	A	1	36	1	27	3	5	0	0

- Molecule 4 is water.

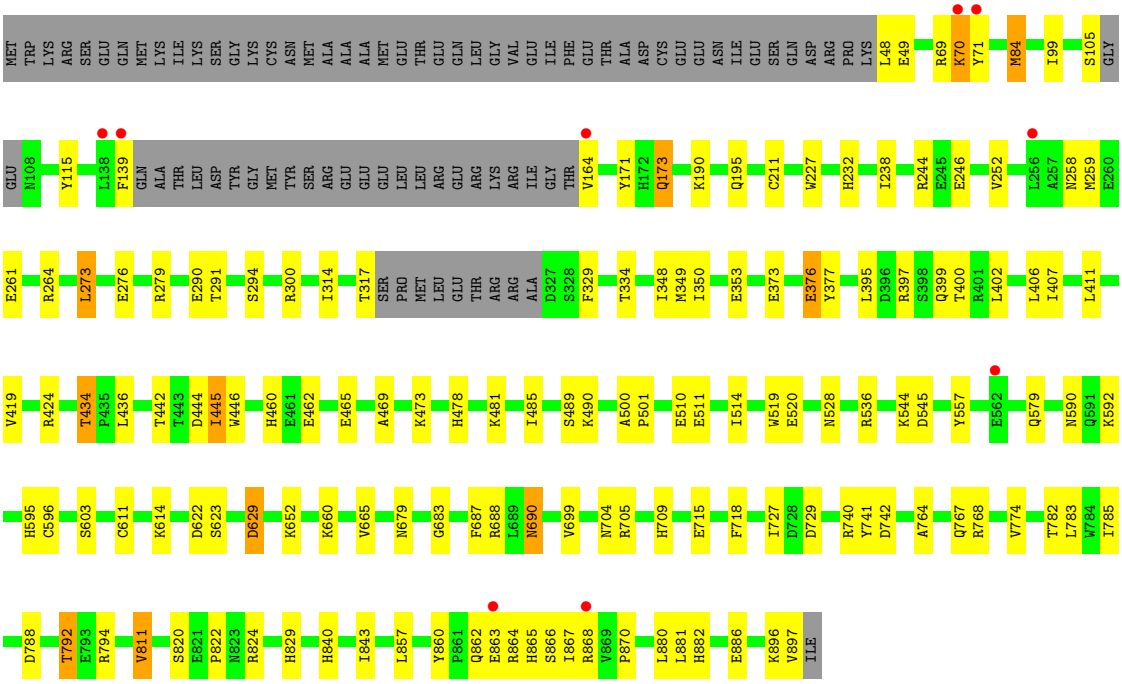
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	B	96	96	96	0	0
			Total	O		
4	A	72	72	72	0	0

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.

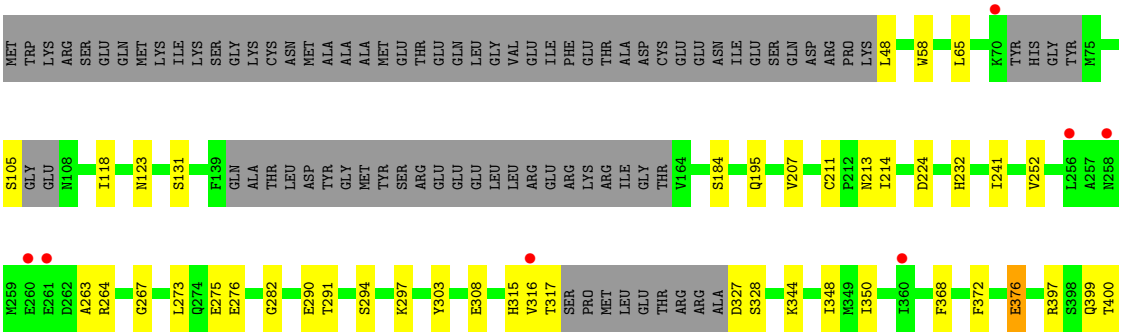
• Molecule 1: Dipeptidyl peptidase 8

Chain B:



• Molecule 1: Dipeptidyl peptidase 8

Chain A:



V405
D417
Q423
T442
I445
E462
E465
K473
Y480
K481
I485
L486
K487
E488
S489
K490
Y491
A500
P501
S502
D503
W519
E520
K544
D545
R569
S574
N590
K601
D608
P609
T610
C611
K614
E639
S640
F644
Y651
D655
L666
V677
N678
N679
V699
V700
D703
N704
R705
G706
H709
K713
F718
K719
Y720
I725
D729
I776
A779
L783
F786
Y787
D788
T792
E793
R794
Q804
P822
H829
G830
F831
L832
D833
E834
N835
V836
H837
H840
I843
R850
I859
Q862
GLU
ARG
HIS
SER
ILE
ARG
V869
G873
Y876
E877
L880
L881
H882
E886
R891
V897
ILE

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α, β, γ	149.44Å 149.44Å 269.39Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.74 – 2.44 49.74 – 2.44	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.74-2.44) 100.0 (49.74-2.44)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.98 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.215 , 0.253 0.218 , 0.252	Depositor DCC
R_{free} test set	6301 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	62.3	Xtriage
Anisotropy	0.286	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	0.228 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	13408	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 2.10% 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: TMO, 2YI

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	0.70	0/6720	0.86	0/9116
1	B	0.70	0/6808	0.87	0/9237
All	All	0.70	0/13528	0.86	0/18353

There are no bond length outliers.

There are no bond angle outliers.

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	6536	0	6356	67	0
1	B	6622	0	6434	82	0
2	A	5	0	9	0	0
2	B	5	0	9	0	0
3	A	36	0	0	2	0
3	B	36	0	0	1	0
4	A	72	0	0	10	0
4	B	96	0	0	7	0
All	All	13408	0	12808	144	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 6.

All (144) 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)
1:B:611:CYS:HB2	4:B:1051:HOH:O	1.27	1.34
1:A:611:CYS:HB2	4:A:1067:HOH:O	1.54	1.07
1:B:788:ASP:O	1:B:792:THR:HG23	1.78	0.83
1:A:705:ARG:HD3	1:A:729:ASP:OD2	1.78	0.81
1:B:244:ARG:HD3	4:B:1017:HOH:O	1.83	0.78
1:B:334:THR:CG2	1:B:785:ILE:HA	2.14	0.77
1:B:705:ARG:HD3	1:B:729:ASP:OD2	1.84	0.77
1:B:173:GLN:HE22	1:B:579:GLN:HE22	1.34	0.76
1:B:465:GLU:OE1	1:B:481:LYS:NZ	2.22	0.73
1:B:290:GLU:OE2	1:B:300:ARG:NH2	2.22	0.72
1:B:334:THR:HG22	1:B:785:ILE:HA	1.71	0.70
1:A:399:GLN:OE1	1:A:794:ARG:HD3	1.91	0.70
1:A:788:ASP:O	1:A:792:THR:CG2	2.41	0.69
1:B:84:MET:SD	1:B:171:TYR:CD2	2.86	0.69
1:B:822:PRO:HG3	1:A:882:HIS:CE1	2.28	0.68
1:B:596:CYS:SG	1:B:623:SER:N	2.66	0.68
1:A:611:CYS:CB	4:A:1067:HOH:O	2.27	0.67
1:B:611:CYS:CB	4:B:1051:HOH:O	2.05	0.67
1:A:788:ASP:O	1:A:792:THR:HG23	1.95	0.67
1:B:596:CYS:SG	1:B:623:SER:HB2	2.35	0.66
1:B:882:HIS:CE1	1:A:822:PRO:HG3	2.31	0.65
1:B:258:ASN:HB2	4:B:1087:HOH:O	1.95	0.65
1:A:224:ASP:OD2	1:A:297:LYS:NZ	2.21	0.65
1:A:195:GLN:HB2	4:A:1068:HOH:O	1.96	0.65
1:B:48:LEU:HD11	1:B:742:ASP:HB2	1.79	0.64
1:B:446:TRP:HZ2	1:B:715:GLU:HG2	1.61	0.64
1:B:595:HIS:HB3	4:B:1092:HOH:O	1.96	0.64
1:B:376:GLU:HG2	1:B:397:ARG:HB2	1.82	0.62
1:A:840:HIS:HE1	4:A:1017:HOH:O	1.81	0.62
1:A:184:SER:HA	1:A:214:ILE:CD1	2.29	0.61
1:A:400:THR:O	1:A:442:THR:HA	2.00	0.61
1:A:376:GLU:HG2	1:A:397:ARG:HB2	1.83	0.61
1:B:882:HIS:CE1	1:B:886:GLU:HG3	2.36	0.61
1:B:865:HIS:HB3	1:B:868:ARG:HB3	1.84	0.60
1:B:481:LYS:HB2	1:B:514:ILE:HD11	1.84	0.60
1:B:407:ILE:HG23	1:B:411:LEU:HD12	1.84	0.60
1:A:48:LEU:HD23	4:A:1026:HOH:O	2.02	0.59
1:A:639:GLU:CD	4:A:1005:HOH:O	2.39	0.59
1:A:713:LYS:HE2	4:A:1030:HOH:O	2.02	0.59
1:B:880:LEU:HD23	3:B:902:2YI:BR1	2.59	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:348:ILE:HG22	1:B:350:ILE:CD1	2.34	0.57
1:B:434:THR:HG21	1:B:489:SER:HB2	1.87	0.57
1:B:896:LYS:O	1:B:897:VAL:C	2.44	0.56
1:A:252:VAL:HG13	1:A:264:ARG:HB3	1.87	0.56
1:B:402:LEU:C	1:B:402:LEU:HD23	2.26	0.56
1:A:779:ALA:O	1:A:836:VAL:HG11	2.05	0.56
1:A:880:LEU:HD23	3:A:902:2YI:BR1	2.61	0.56
1:B:376:GLU:CG	1:B:397:ARG:HB2	2.37	0.55
1:A:608:ASP:OD1	1:A:610:THR:HB	2.07	0.55
1:B:683:GLY:O	1:B:687:PHE:HB2	2.07	0.55
1:B:211:CYS:HB3	1:B:232:HIS:CD2	2.42	0.54
1:A:882:HIS:CE1	1:A:886:GLU:HG3	2.42	0.54
1:B:767:GLN:O	1:B:768:ARG:HD2	2.08	0.54
1:A:491:TYR:HB2	1:A:503:ASP:OD2	2.08	0.53
1:B:473:LYS:HE3	1:B:511:GLU:OE2	2.08	0.53
1:B:820:SER:O	1:A:58:TRP:HB3	2.09	0.53
1:B:406:LEU:HB2	1:B:436:LEU:HB2	1.90	0.52
1:B:473:LYS:CE	1:B:511:GLU:OE2	2.57	0.52
1:B:400:THR:O	1:B:442:THR:HA	2.10	0.52
1:B:446:TRP:CZ2	1:B:715:GLU:HG2	2.43	0.52
1:B:252:VAL:CG1	1:B:264:ARG:HB3	2.40	0.52
1:A:677:VAL:HB	1:A:703:ASP:OD2	2.10	0.51
1:B:519:TRP:CZ2	1:B:544:LYS:HD2	2.45	0.51
1:B:99:ILE:O	1:B:115:TYR:HA	2.09	0.51
1:B:882:HIS:CE1	1:A:822:PRO:CG	2.93	0.51
1:A:118:ILE:N	1:A:118:ILE:HD13	2.25	0.50
1:B:349:MET:SD	1:B:349:MET:N	2.84	0.50
1:A:520:GLU:OE2	1:A:709:HIS:HA	2.11	0.50
1:A:519:TRP:CG	1:A:544:LYS:HA	2.47	0.49
1:A:804:GLN:NE2	1:A:804:GLN:HA	2.27	0.49
1:B:276:GLU:OE1	1:B:276:GLU:HA	2.13	0.48
1:B:783:LEU:HD22	1:B:843:ILE:HD13	1.95	0.48
1:B:782:THR:HA	1:B:811:VAL:HG13	1.94	0.48
1:A:267:GLY:HA2	1:A:282:GLY:O	2.13	0.48
1:A:500:ALA:HB1	1:A:501:PRO:HD2	1.96	0.48
1:A:473:LYS:HD3	1:A:480:TYR:CZ	2.49	0.48
1:A:706:GLY:HA3	1:A:718:PHE:CE2	2.49	0.47
1:B:740:ARG:HD3	1:B:741:TYR:CE2	2.48	0.47
1:A:368:PHE:O	1:A:372:PHE:N	2.43	0.47
1:A:788:ASP:O	1:A:792:THR:HG22	2.14	0.47
3:A:902:2YI:O10	3:A:902:2YI:C16	2.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:SER:HA	1:A:214:ILE:HD12	1.95	0.47
1:B:227:TRP:CZ3	1:B:238:ILE:HD12	2.50	0.47
1:A:211:CYS:HB3	1:A:232:HIS:CD2	2.50	0.47
1:B:173:GLN:HE22	1:B:579:GLN:NE2	2.09	0.46
1:A:473:LYS:CD	1:A:480:TYR:CZ	2.99	0.46
1:A:804:GLN:HA	1:A:804:GLN:HE21	1.80	0.46
1:B:862:GLN:O	1:B:863:GLU:HB2	2.15	0.46
1:B:788:ASP:O	1:B:792:THR:CG2	2.57	0.46
1:B:460:HIS:CE1	1:B:462:GLU:HB2	2.51	0.46
1:A:873:GLY:O	1:A:877:GLU:HG3	2.14	0.46
1:B:399:GLN:OE1	1:B:794:ARG:HD3	2.16	0.46
1:B:870:PRO:HG2	4:B:1090:HOH:O	2.15	0.45
1:A:776:ILE:HG21	1:A:880:LEU:CD1	2.46	0.45
1:A:207:VAL:HG22	1:A:241:ILE:HG22	1.98	0.45
1:B:259:MET:HE1	1:B:329:PHE:HA	1.99	0.45
1:A:276:GLU:OE2	1:A:788:ASP:OD2	2.34	0.45
1:B:687:PHE:O	1:B:690:ASN:HB3	2.16	0.45
1:B:782:THR:H	1:B:840:HIS:CD2	2.34	0.44
1:B:70:LYS:HD3	1:B:70:LYS:HA	1.76	0.44
1:B:273:LEU:HD22	1:B:279:ARG:NH1	2.32	0.44
1:B:782:THR:H	1:B:840:HIS:HD2	1.65	0.44
1:A:48:LEU:CA	4:A:1026:HOH:O	2.65	0.44
1:B:705:ARG:NH1	1:B:729:ASP:OD1	2.51	0.44
1:A:48:LEU:CD2	4:A:1026:HOH:O	2.63	0.44
1:B:629:ASP:OD1	1:B:629:ASP:N	2.50	0.44
1:B:860:TYR:CE2	1:B:867:ILE:HD11	2.53	0.44
1:A:651:TYR:HB2	1:A:699:VAL:HB	1.99	0.43
1:B:520:GLU:OE2	1:B:709:HIS:HA	2.17	0.43
1:B:69:ARG:HB2	1:B:688:ARG:NH2	2.33	0.43
1:B:444:ASP:HB2	4:B:1096:HOH:O	2.18	0.43
1:A:213:ASN:HB2	1:A:232:HIS:NE2	2.33	0.43
1:A:372:PHE:HE1	1:A:405:VAL:HG11	1.81	0.43
1:B:500:ALA:HB1	1:B:501:PRO:HD2	1.99	0.43
1:B:49:GLU:O	1:B:660:LYS:HA	2.19	0.43
1:A:465:GLU:OE1	1:A:481:LYS:NZ	2.46	0.43
1:B:590:ASN:HB2	1:B:679:ASN:OD1	2.19	0.43
1:B:469:ALA:HA	1:B:478:HIS:O	2.19	0.42
1:A:719:LYS:HG2	1:A:720:TYR:CD2	2.54	0.42
1:B:857:LEU:HD21	1:A:859:ILE:HD12	2.00	0.42
1:B:349:MET:C	1:B:350:ILE:HD12	2.40	0.42
1:A:834:GLU:O	1:A:837[B]:HIS:CE1	2.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:519:TRP:CG	1:B:544:LYS:HA	2.54	0.42
1:B:536:ARG:HA	1:B:557:TYR:CE2	2.55	0.42
1:A:666:LEU:HD12	1:A:700:VAL:O	2.19	0.42
1:A:263:ALA:HB1	1:A:308:GLU:HB2	2.02	0.42
1:A:897:VAL:HG23	1:A:897:VAL:O	2.20	0.41
1:A:303:TYR:CZ	1:A:344:LYS:HB2	2.54	0.41
1:A:601:LYS:O	1:A:614:LYS:HA	2.20	0.41
1:A:640:SER:HB3	1:A:644:PHE:O	2.20	0.41
1:A:500:ALA:O	1:A:503:ASP:HB2	2.21	0.41
1:A:590:ASN:HB2	1:A:679:ASN:OD1	2.20	0.41
1:B:377:TYR:HB2	1:B:395:LEU:HB2	2.01	0.41
1:A:489:SER:OG	1:A:503:ASP:O	2.35	0.41
1:B:314:ILE:HD11	1:B:329:PHE:CZ	2.56	0.41
1:A:783:LEU:O	1:A:786:PHE:HB2	2.20	0.41
1:B:727:ILE:HD12	1:B:764:ALA:HB2	2.02	0.41
1:A:348:ILE:HG22	1:A:350:ILE:CD1	2.50	0.41
1:B:822:PRO:CG	1:A:882:HIS:CE1	3.00	0.41
1:B:348:ILE:HG22	1:B:350:ILE:HD11	2.02	0.41
1:B:774:VAL:HA	1:B:824:ARG:O	2.21	0.41
1:A:713:LYS:CE	4:A:1030:HOH:O	2.63	0.41
1:B:665:VAL:O	1:B:699:VAL:HA	2.21	0.40
1:A:65:LEU:HD11	1:A:881:LEU:HD22	2.01	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	794/898 (88%)	758 (96%)	35 (4%)	1 (0%)	51	64
1	B	807/898 (90%)	772 (96%)	33 (4%)	2 (0%)	47	57
All	All	1601/1796 (89%)	1530 (96%)	68 (4%)	3 (0%)	47	57

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	866	SER
1	B	445	ILE
1	A	445	ILE

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	715/795 (90%)	680 (95%)	35 (5%)	25	33
1	B	723/795 (91%)	682 (94%)	41 (6%)	20	26
All	All	1438/1590 (90%)	1362 (95%)	76 (5%)	22	30

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	70	LYS
1	B	71	TYR
1	B	84	MET
1	B	105	SER
1	B	139	PHE
1	B	164	VAL
1	B	173	GLN
1	B	190	LYS
1	B	195	GLN
1	B	246	GLU
1	B	261	GLU
1	B	273	LEU
1	B	291	THR
1	B	294	SER
1	B	317	THR
1	B	353	GLU
1	B	373	GLU
1	B	376	GLU
1	B	419	VAL
1	B	424	ARG

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Mol	Chain	Res	Type
1	B	434	THR
1	B	445	ILE
1	B	485	ILE
1	B	490	LYS
1	B	510	GLU
1	B	528	ASN
1	B	545	ASP
1	B	592	LYS
1	B	603	SER
1	B	614	LYS
1	B	622	ASP
1	B	629	ASP
1	B	652	LYS
1	B	690	ASN
1	B	704	ASN
1	B	718	PHE
1	B	792	THR
1	B	811	VAL
1	B	829	HIS
1	B	864	ARG
1	B	881	LEU
1	A	105	SER
1	A	123	ASN
1	A	131	SER
1	A	273	LEU
1	A	275	GLU
1	A	290	GLU
1	A	291	THR
1	A	294	SER
1	A	315	HIS
1	A	316	VAL
1	A	317	THR
1	A	327	ASP
1	A	328	SER
1	A	376	GLU
1	A	417	ASP
1	A	423	GLN
1	A	462	GLU
1	A	485	ILE
1	A	487	LYS
1	A	545	ASP
1	A	569	ARG

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Mol	Chain	Res	Type
1	A	574	SER
1	A	614	LYS
1	A	655	ASP
1	A	704	ASN
1	A	718	PHE
1	A	725	ILE
1	A	792	THR
1	A	829	HIS
1	A	831	PHE
1	A	833	ASP
1	A	843	ILE
1	A	850	ARG
1	A	876	TYR
1	A	891	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	111	ASN
1	B	123	ASN
1	B	173	GLN
1	B	199	GLN
1	B	258	ASN
1	B	306	ASN
1	B	423	GLN
1	B	460	HIS
1	B	840	HIS
1	B	882	HIS
1	A	111	ASN
1	A	123	ASN
1	A	200	GLN
1	A	550	HIS
1	A	804	GLN
1	A	840	HIS
1	A	862	GLN
1	A	879	HIS
1	A	882	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)

4 ligands are modelled in this entry.

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	$\#\|Z\| > 2$
3	2YI	A	902	1	36,38,38	1.40	2 (5%)	49,53,53	1.92	11 (22%)
2	TMO	A	901	-	4,4,4	0.72	0	6,6,6	0.30	0
2	TMO	B	901	-	4,4,4	1.06	0	6,6,6	0.43	0
3	2YI	B	902	1	36,38,38	1.34	1 (2%)	49,53,53	2.07	13 (26%)

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
3	2YI	B	902	1	-	18/34/47/47	0/3/3/3
3	2YI	A	902	1	-	16/34/47/47	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	902	2YI	O18-C17	7.26	1.49	1.33
3	B	902	2YI	O18-C17	6.62	1.48	1.33
3	A	902	2YI	C11-N4	-2.05	1.37	1.41

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	902	2YI	O18-C17-C15	7.39	123.55	112.34
3	A	902	2YI	C20-O18-C17	5.37	126.18	115.83
3	A	902	2YI	O18-C17-C15	5.32	120.41	112.34
3	B	902	2YI	C7-C2-C1	-5.19	101.51	110.61
3	A	902	2YI	C13-C21-N23	4.52	124.45	118.72
3	B	902	2YI	C25-C24-N23	-4.32	101.18	110.44
3	A	902	2YI	C30-C29-N26	3.70	120.31	113.12
3	B	902	2YI	C20-O18-C17	3.66	122.90	115.83
3	A	902	2YI	C11-N4-C5	-3.38	120.64	126.78
3	A	902	2YI	O10-C5-C2	-3.26	115.96	121.21
3	B	902	2YI	O18-C17-O19	-3.18	117.23	123.45
3	B	902	2YI	BR1-C33-C34	2.89	123.50	119.30
3	A	902	2YI	C2-C5-N4	2.80	119.58	115.43
3	B	902	2YI	O10-C5-C2	-2.74	116.80	121.21
3	B	902	2YI	C11-N4-C5	-2.72	121.85	126.78
3	B	902	2YI	C6-C1-C2	2.71	117.55	114.38
3	A	902	2YI	C29-N26-C25	2.65	116.97	111.06
3	A	902	2YI	C24-C25-N26	-2.50	105.52	110.64
3	A	902	2YI	C28-N23-C24	2.47	117.37	112.62
3	B	902	2YI	C2-C5-N4	2.41	119.01	115.43
3	A	902	2YI	O22-C21-C13	-2.24	115.87	120.23
3	B	902	2YI	C29-N26-C25	-2.16	106.26	111.06
3	B	902	2YI	C28-C27-N26	2.14	115.03	110.64
3	B	902	2YI	C30-C29-N26	2.08	117.17	113.12

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	902	2YI	C6-C1-C2-C3
3	B	902	2YI	C6-C1-C2-C5
3	B	902	2YI	C1-C2-C3-O9
3	B	902	2YI	C13-C21-N23-C24
3	B	902	2YI	C13-C21-N23-C28
3	B	902	2YI	O22-C21-N23-C24
3	B	902	2YI	O22-C21-N23-C28
3	A	902	2YI	C7-C2-C3-O9
3	A	902	2YI	C13-C21-N23-C24
3	A	902	2YI	C13-C21-N23-C28
3	A	902	2YI	O22-C21-N23-C24
3	A	902	2YI	O22-C21-N23-C28

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Mol	Chain	Res	Type	Atoms
3	A	902	2YI	C14-C15-C17-O19
3	A	902	2YI	C16-C15-C17-O18
3	A	902	2YI	C14-C15-C17-O18
3	A	902	2YI	C16-C15-C17-O19
3	A	902	2YI	C30-C29-N26-C27
3	A	902	2YI	C15-C17-O18-C20
3	A	902	2YI	C30-C29-N26-C25
3	B	902	2YI	C14-C15-C17-O18
3	A	902	2YI	O19-C17-O18-C20
3	B	902	2YI	C16-C15-C17-O18
3	B	902	2YI	C14-C15-C17-O19
3	B	902	2YI	C12-C13-C21-O22
3	B	902	2YI	C16-C15-C17-O19
3	B	902	2YI	C30-C29-N26-C27
3	B	902	2YI	C12-C13-C21-N23
3	B	902	2YI	C6-C1-C2-C7
3	B	902	2YI	C14-C13-C21-O22
3	B	902	2YI	C7-C2-C3-O9
3	A	902	2YI	C1-C2-C3-O9
3	A	902	2YI	C2-C5-N4-C11
3	B	902	2YI	C14-C13-C21-N23
3	A	902	2YI	C7-C2-C5-N4

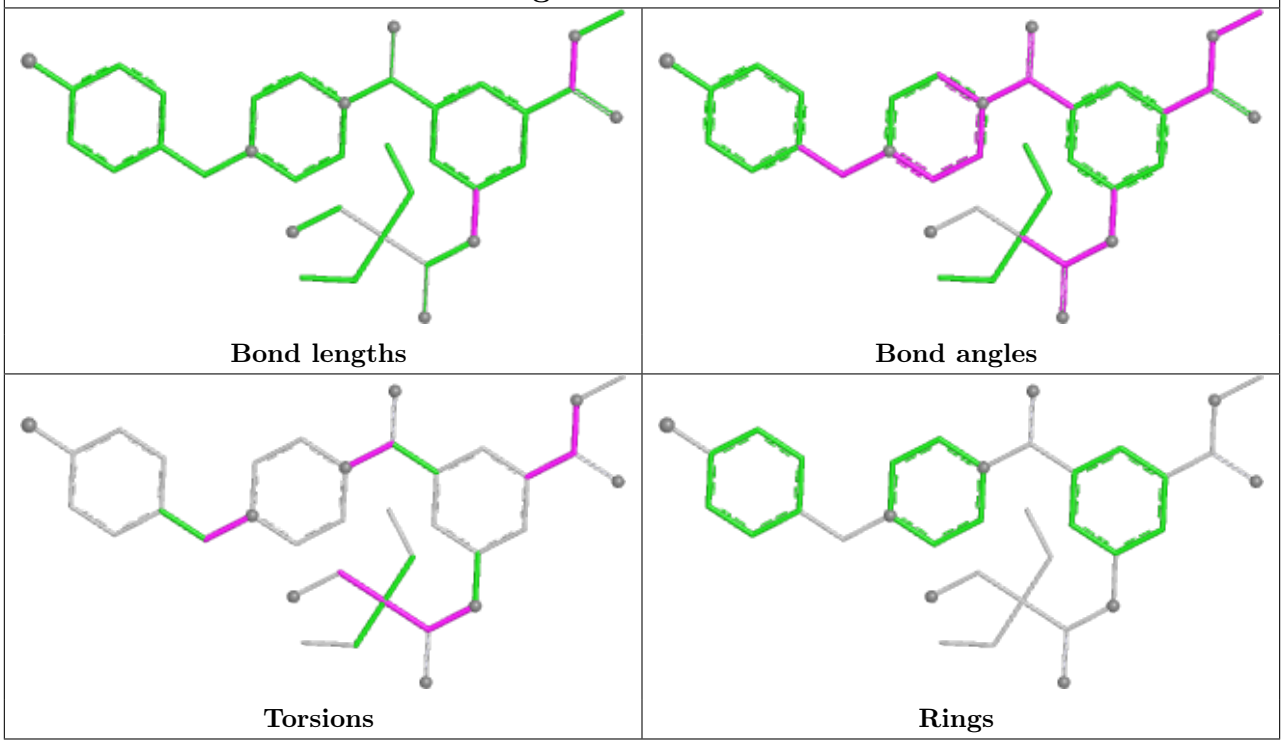
There are no ring outliers.

2 monomers are involved in 3 short contacts:

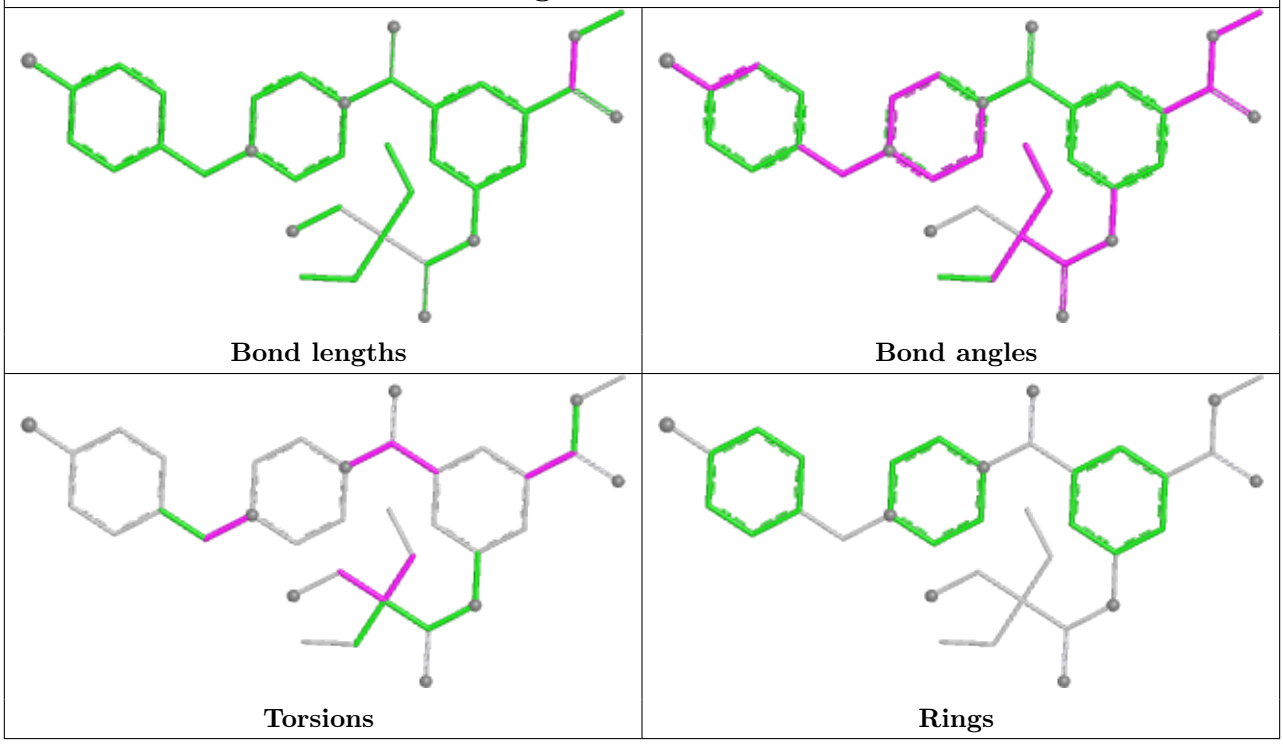
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	902	2YI	2	0
3	B	902	2YI	1	0

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 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 2YI A 902



Ligand 2YI B 902



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	805/898 (89%)	-0.05	10 (1%)	79	77	44, 66, 108, 164	0
1	B	815/898 (90%)	-0.06	9 (1%)	80	79	40, 61, 106, 159	0
All	All	1620/1796 (90%)	-0.05	19 (1%)	79	77	40, 63, 108, 164	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	139	PHE	10.8
1	B	164	VAL	6.6
1	A	256	LEU	5.9
1	B	71	TYR	4.1
1	A	831	PHE	3.8
1	A	832	LEU	3.6
1	B	256	LEU	3.4
1	B	70	LYS	3.3
1	B	868	ARG	3.2
1	A	835	ASN	3.0
1	A	70	LYS	2.9
1	A	316	VAL	2.9
1	B	138	LEU	2.8
1	A	258	ASN	2.8
1	A	260	GLU	2.4
1	A	261	GLU	2.3
1	A	360	ILE	2.1
1	B	562	GLU	2.0
1	B	863	GLU	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

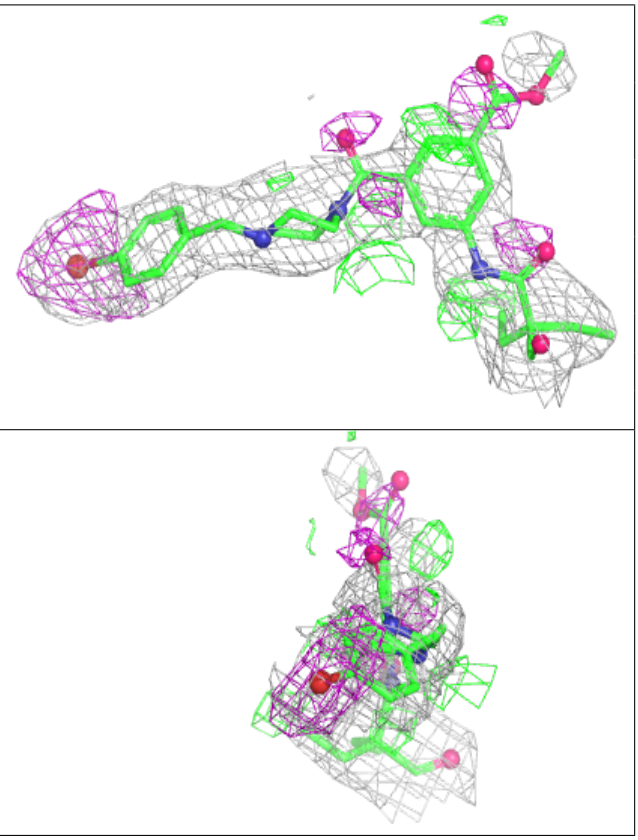
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

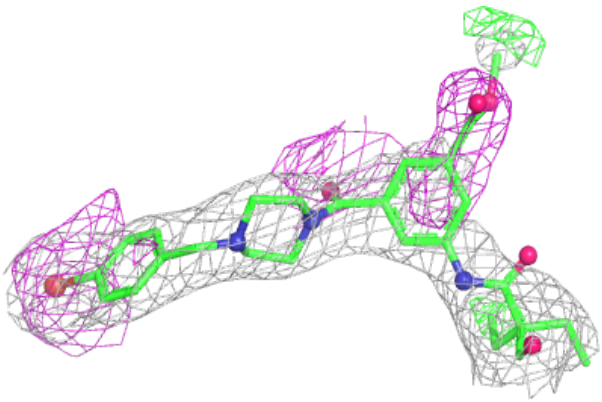
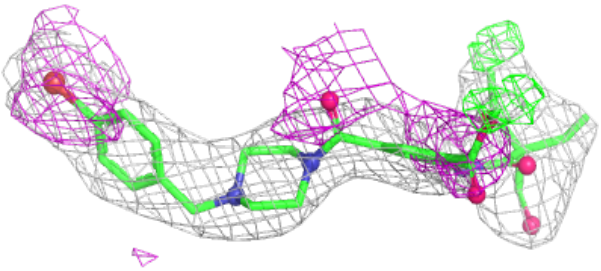
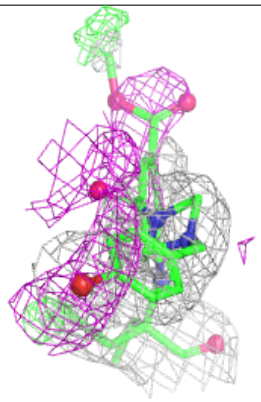
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	2YI	B	902	36/36	0.89	0.24	57,93,139,163	0
3	2YI	A	902	36/36	0.89	0.27	64,89,124,136	0
2	TMO	B	901	5/5	0.93	0.23	72,72,84,88	0
2	TMO	A	901	5/5	0.99	0.20	66,74,80,82	0

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 2YI B 902:

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 2YI A 902: 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.