Full wwPDB X-ray Structure Validation Report (i)

Jun 30, 2022 – 01:39 am BST

PDB ID	:	7ZAZ
Title	:	macrocyclase OphP with ZPP
Authors	:	Song, H.; Naismith, J.H.
Deposited on	:	2022-03-23
Resolution	:	2.00 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:

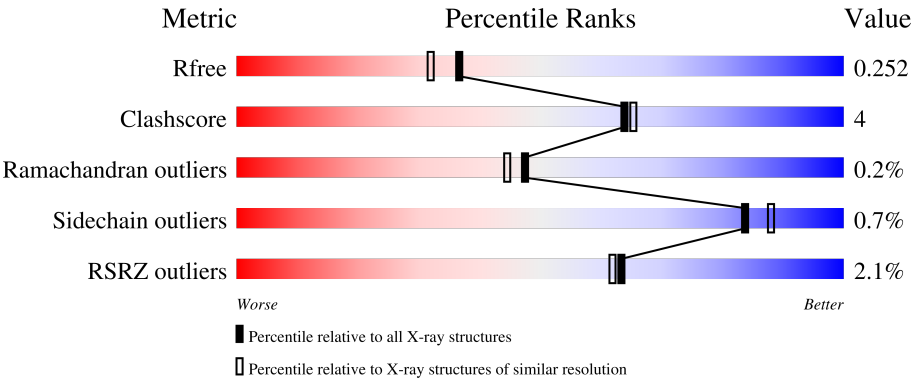
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.29
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

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 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	AAA	745	2% 89% 8%
1	BBB	745	3% 85% 10% 5%
1	CCC	745	2% 83% 9% 7%
1	DDD	745	% 87% 9%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ZPR	CCC	806	-	-	-	X
3	DMS	BBB	802	-	-	X	-

2 Entry composition

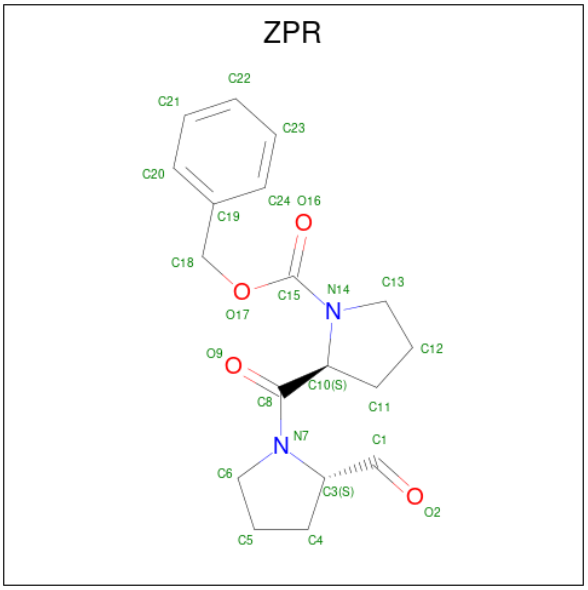
There are 9 unique types of molecules in this entry. The entry contains 24384 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Prolyl endopeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	727	Total	C	N	O	S	0	2	0
			5834	3722	982	1104	26			
1	BBB	706	Total	C	N	O	S	0	1	0
			5663	3617	946	1073	27			
1	CCC	690	Total	C	N	O	S	0	0	0
			5549	3556	926	1041	26			
1	DDD	716	Total	C	N	O	S	0	2	0
			5753	3672	970	1085	26			

- Molecule 2 is N-BENZYLOXYCARBONYL-L-PROLYL-L-PROLINAL (three-letter code: ZPR) (formula: $C_{18}H_{22}N_2O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	AAA	1	Total	C	N	O	0	0
			24	18	2	4		
2	BBB	1	Total	C	N	O	0	0
			24	18	2	4		

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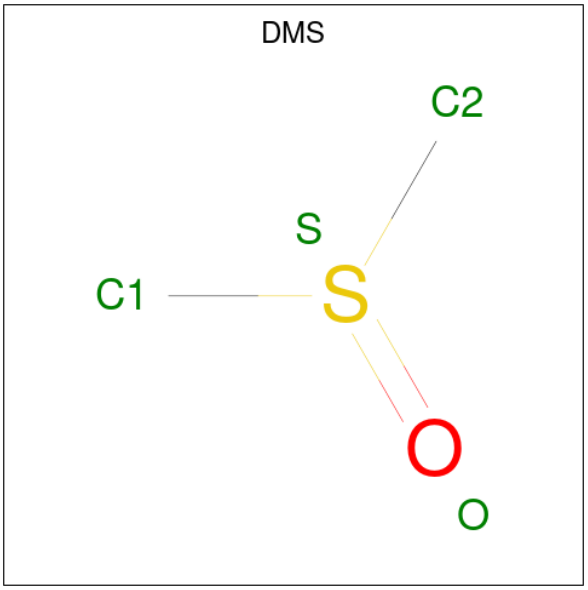
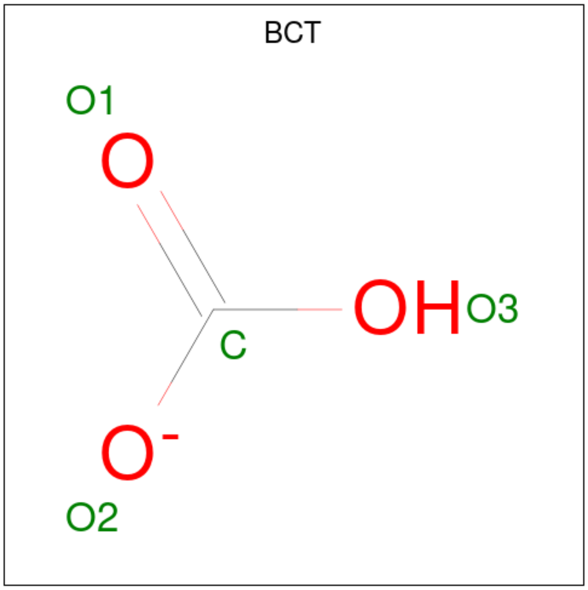
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	CCC	1	Total	C	N	O	0	0
			24	18	2	4		
2	DDD	1	Total	C	N	O	0	0
			24	18	2	4		

- Molecule 3 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	AAA	1	Total	C	O	S	0	0
			4	2	1	1		
3	AAA	1	Total	C	O	S	0	0
			4	2	1	1		
3	BBB	1	Total	C	O	S	0	0
			4	2	1	1		
3	DDD	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 4 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	AAA	1	Total C O 4 1 3	0	0
4	AAA	1	Total C O 4 1 3	0	0
4	AAA	1	Total C O 4 1 3	0	0
4	AAA	1	Total C O 4 1 3	0	0
4	AAA	1	Total C O 4 1 3	0	0
4	AAA	1	Total C O 4 1 3	0	0
4	AAA	1	Total C O 4 1 3	0	0
4	BBB	1	Total C O 4 1 3	0	0
4	BBB	1	Total C O 4 1 3	0	0
4	BBB	1	Total C O 4 1 3	0	0
4	BBB	1	Total C O 4 1 3	0	0
4	BBB	1	Total C O 4 1 3	0	0
4	BBB	1	Total C O 4 1 3	0	0
4	BBB	1	Total C O 4 1 3	0	0

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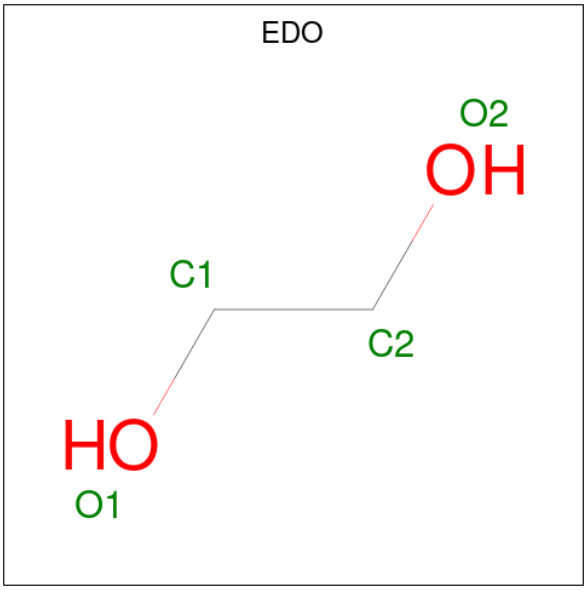
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	CCC	1	Total C O 4 1 3	0	0
4	CCC	1	Total C O 4 1 3	0	0
4	CCC	1	Total C O 4 1 3	0	0
4	CCC	1	Total C O 4 1 3	0	0
4	CCC	1	Total C O 4 1 3	0	0
4	DDD	1	Total C O 4 1 3	0	0
4	DDD	1	Total C O 4 1 3	0	0
4	DDD	1	Total C O 4 1 3	0	0
4	DDD	1	Total C O 4 1 3	0	0
4	DDD	1	Total C O 4 1 3	0	0

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	AAA	1	Total C O 4 2 2	0	0

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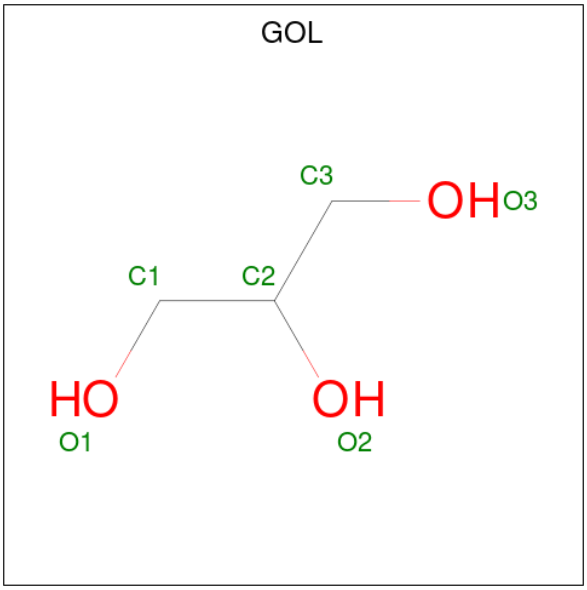
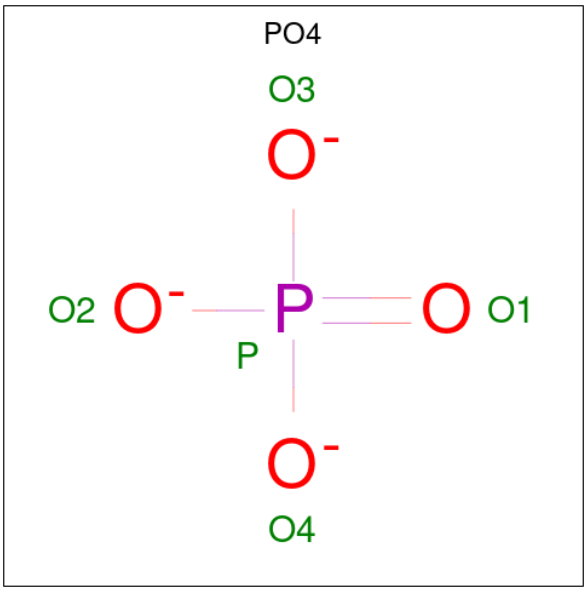
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	AAA	1	Total	C	O	0	0
			4	2	2		
5	AAA	1	Total	C	O	0	0
			4	2	2		
5	BBB	1	Total	C	O	0	0
			4	2	2		
5	CCC	1	Total	C	O	0	0
			4	2	2		
5	CCC	1	Total	C	O	0	0
			4	2	2		
5	DDD	1	Total	C	O	0	0
			4	2	2		
5	DDD	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	CCC	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	DDD	1	Total O P 5 4 1	0	0
7	DDD	1	Total O P 5 4 1	0	0

- Molecule 8 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	DDD	1	Total Na 1 1	0	0

- Molecule 9 is water.

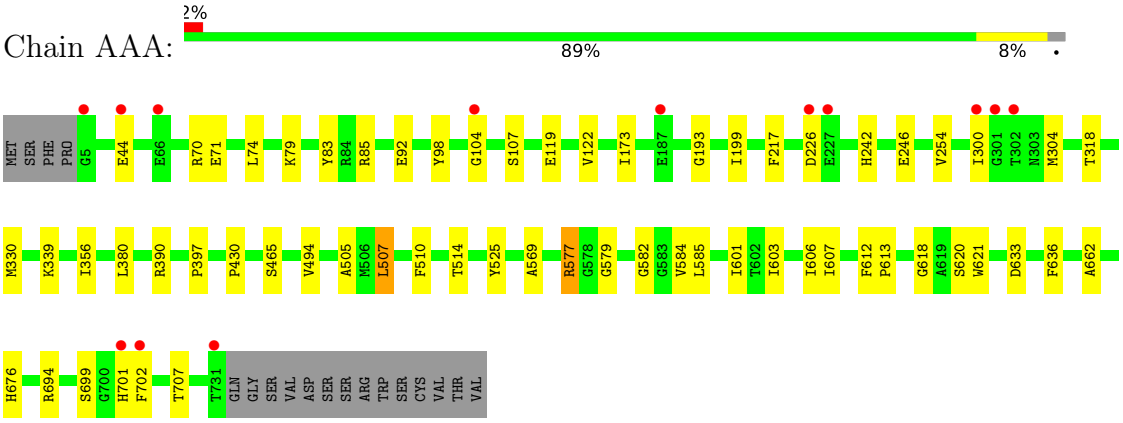
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	AAA	339	Total O 339 339	0	0
9	BBB	288	Total O 288 288	0	0
9	CCC	306	Total O 306 306	0	0
9	DDD	395	Total O 395 395	0	0

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.

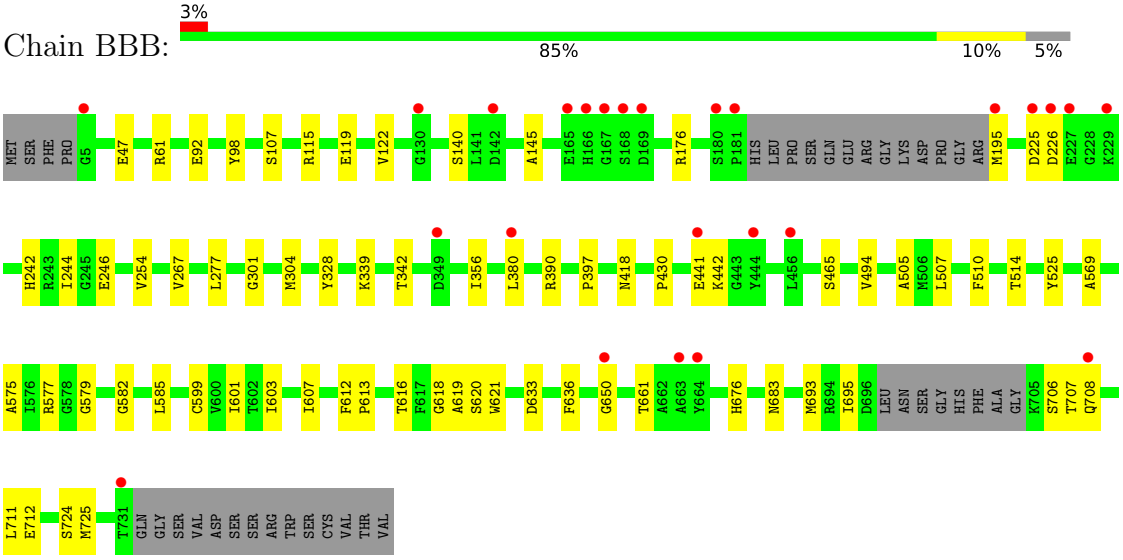
• Molecule 1: Prolyl endopeptidase

Chain AAA:



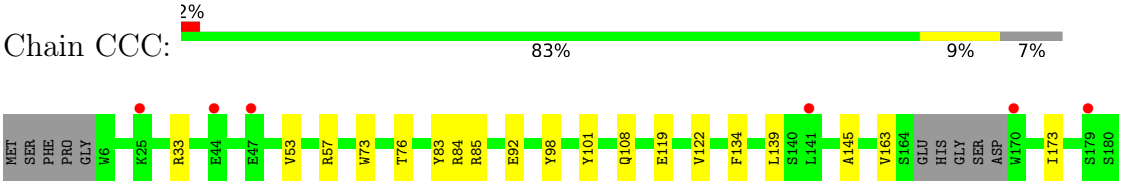
• Molecule 1: Prolyl endopeptidase

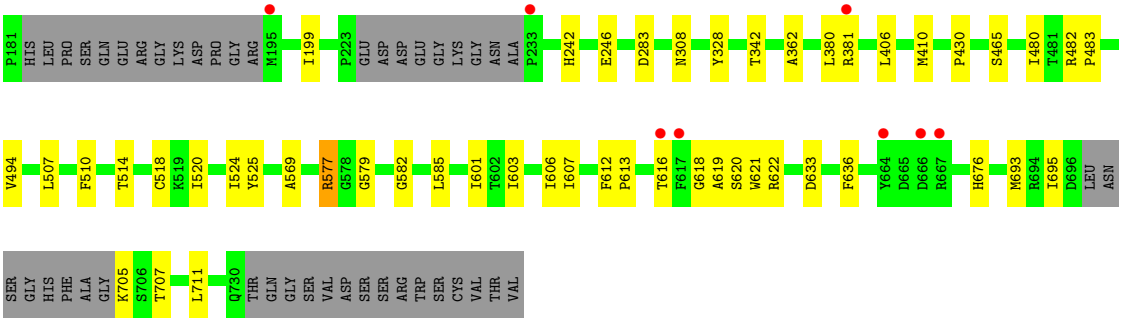
Chain BBB:



• Molecule 1: Prolyl endopeptidase

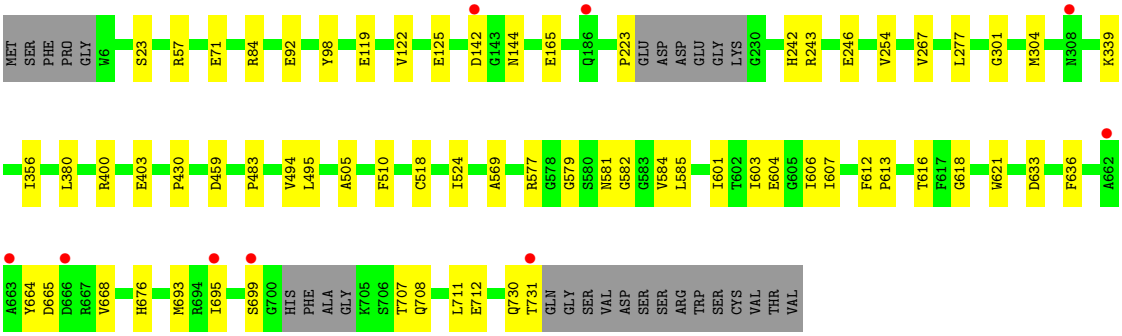
Chain CCC:





• Molecule 1: Prolyl endopeptidase

Chain DDD:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	69.68Å 102.65Å 110.27Å 116.23° 101.09° 92.18°	Depositor
Resolution (Å)	67.80 – 2.00 67.71 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.5 (67.80-2.00) 97.6 (67.71-2.00)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.49 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.209 , 0.245 0.218 , 0.252	Depositor DCC
R_{free} test set	8559 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å^2)	26.0	Xtriage
Anisotropy	0.381	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.000 for -h,k,-k-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	24384	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.53% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, EDO, PO4, ZPR, GOL, DMS, BCT

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	AAA	0.65	0/6004	0.75	0/8145
1	BBB	0.64	0/5826	0.74	0/7903
1	CCC	0.65	0/5709	0.75	0/7741
1	DDD	0.65	0/5919	0.75	0/8029
All	All	0.65	0/23458	0.75	0/31818

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
1	CCC	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	CCC	163	VAL	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AAA	5834	0	5566	47	0
1	BBB	5663	0	5393	50	0
1	CCC	5549	0	5314	46	0
1	DDD	5753	0	5493	45	0
2	AAA	24	0	21	0	0
2	BBB	24	0	21	1	0
2	CCC	24	0	21	4	0
2	DDD	24	0	21	0	0
3	AAA	8	0	12	2	0
3	BBB	4	0	6	4	0
3	DDD	4	0	6	0	0
4	AAA	28	0	0	0	0
4	BBB	28	0	0	0	0
4	CCC	20	0	0	0	0
4	DDD	20	0	0	0	0
5	AAA	12	0	18	0	0
5	BBB	4	0	6	0	0
5	CCC	8	0	12	0	0
5	DDD	8	0	12	0	0
6	CCC	6	0	8	1	0
7	DDD	10	0	0	0	0
8	DDD	1	0	0	0	0
9	AAA	339	0	0	3	0
9	BBB	288	0	0	2	0
9	CCC	306	0	0	0	0
9	DDD	395	0	0	1	0
All	All	24384	0	21930	187	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 4.

All (187) 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:AAA:584:VAL:CG2	1:AAA:606:ILE:HG23	1.99	0.93
1:DDD:693:MET:HE2	1:DDD:695:ILE:HD11	1.57	0.83
1:DDD:581:ASN:O	1:DDD:584:VAL:HG12	1.79	0.83
1:BBB:599[B]:CYS:SG	1:BBB:724:SER:HB2	2.21	0.81
1:AAA:107:SER:HA	1:AAA:707:THR:HG23	1.65	0.79
1:DDD:664:TYR:O	1:DDD:699:SER:HA	1.84	0.78
1:CCC:693:MET:HE2	1:CCC:695:ILE:HD11	1.67	0.75
1:DDD:494:VAL:HG22	1:DDD:524:ILE:HG12	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:584:VAL:HG22	1:AAA:606:ILE:HG23	1.69	0.72
1:DDD:494:VAL:HG22	1:DDD:524:ILE:CG1	2.21	0.71
1:AAA:70:ARG:NH1	1:AAA:74[B]:LEU:HD11	2.06	0.71
1:CCC:606:ILE:HD11	2:CCC:806:ZPR:H41	1.71	0.70
1:AAA:584:VAL:HG23	1:AAA:606:ILE:HG23	1.72	0.70
1:CCC:514:THR:HG21	1:CCC:525:TYR:CD2	2.28	0.69
1:BBB:254:VAL:HG13	1:BBB:304:MET:HE2	1.76	0.67
1:AAA:494:VAL:CG2	1:AAA:569:ALA:HB2	2.23	0.67
1:BBB:514:THR:HG21	1:BBB:525:TYR:CD2	2.30	0.67
1:CCC:693:MET:CE	1:CCC:695:ILE:HD11	2.24	0.67
1:CCC:57:ARG:HB2	1:CCC:695:ILE:HD12	1.74	0.67
1:BBB:494:VAL:CG2	1:BBB:569:ALA:HB2	2.26	0.66
1:DDD:693:MET:CE	1:DDD:695:ILE:HD11	2.26	0.66
1:AAA:494:VAL:HG23	1:AAA:569:ALA:HB2	1.79	0.64
1:DDD:604:GLU:HG3	1:DDD:668:VAL:HB	1.78	0.64
1:DDD:494:VAL:CG2	1:DDD:569:ALA:HB2	2.28	0.64
1:AAA:662:ALA:HB1	1:AAA:699:SER:O	1.98	0.63
1:DDD:84[B]:ARG:NH2	1:DDD:125:GLU:OE1	2.30	0.63
1:CCC:283:ASP:HA	1:CCC:620:SER:HB2	1.81	0.62
1:BBB:254:VAL:HG13	1:BBB:304:MET:CE	2.28	0.62
1:CCC:494:VAL:CG2	1:CCC:569:ALA:HB2	2.28	0.62
1:BBB:693:MET:CE	1:BBB:695:ILE:HD11	2.30	0.61
1:BBB:494:VAL:HG23	1:BBB:569:ALA:HB2	1.84	0.60
1:DDD:254:VAL:HG13	1:DDD:304:MET:HE2	1.83	0.59
1:CCC:119:GLU:O	1:CCC:122:VAL:HG22	2.02	0.59
1:AAA:119:GLU:O	1:AAA:122:VAL:HG22	2.03	0.59
1:AAA:514:THR:HG21	1:AAA:525:TYR:CD2	2.37	0.59
1:BBB:575:ALA:HB2	1:BBB:725:MET:CE	2.33	0.58
1:BBB:620:SER:N	3:BBB:802:DMS:H13	2.18	0.58
1:BBB:119:GLU:O	1:BBB:122:VAL:HG22	2.03	0.58
1:DDD:119:GLU:O	1:DDD:122:VAL:HG22	2.04	0.58
1:BBB:599[B]:CYS:SG	1:BBB:724:SER:CB	2.93	0.57
1:CCC:619:ALA:HB1	1:CCC:622:ARG:NH2	2.19	0.56
3:BBB:802:DMS:C1	9:BBB:1077:HOH:O	2.54	0.55
1:CCC:53:VAL:HG13	1:CCC:695:ILE:HD13	1.89	0.54
1:DDD:604:GLU:HG2	1:DDD:665:ASP:OD2	2.07	0.54
1:AAA:71:GLU:HA	1:AAA:74[B]:LEU:HD12	1.90	0.53
1:CCC:621:TRP:CZ2	2:CCC:806:ZPR:H42	2.43	0.53
1:AAA:70:ARG:HH11	1:AAA:74[B]:LEU:HD11	1.70	0.53
1:AAA:584:VAL:HG23	1:AAA:606:ILE:CG2	2.40	0.52
1:CCC:494:VAL:HG23	1:CCC:569:ALA:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DDD:254:VAL:HG13	1:DDD:304:MET:CE	2.39	0.51
1:AAA:607:ILE:HG21	1:AAA:676:HIS:CG	2.46	0.51
1:CCC:108:GLN:HG3	1:CCC:145:ALA:O	2.10	0.51
1:BBB:607:ILE:HG21	1:BBB:676:HIS:CG	2.45	0.51
1:AAA:514:THR:HG21	1:AAA:525:TYR:CG	2.46	0.51
9:AAA:902:HOH:O	1:DDD:71:GLU:HG3	2.11	0.51
1:CCC:607:ILE:HG21	1:CCC:676:HIS:CG	2.47	0.50
1:DDD:607:ILE:HG21	1:DDD:676:HIS:CG	2.46	0.50
1:BBB:621:TRP:CZ2	2:BBB:807:ZPR:H42	2.45	0.50
1:CCC:134:PHE:HZ	1:CCC:139:LEU:HD11	1.77	0.50
1:CCC:606:ILE:HD11	2:CCC:806:ZPR:C4	2.40	0.49
1:BBB:575:ALA:HB2	1:BBB:725:MET:HE3	1.93	0.49
1:AAA:494:VAL:HG21	1:AAA:569:ALA:HB2	1.94	0.49
1:CCC:84:ARG:NH1	1:CCC:101:TYR:OH	2.35	0.49
1:CCC:494:VAL:HG21	1:CCC:569:ALA:HB2	1.93	0.49
1:CCC:482:ARG:HB3	1:CCC:524:ILE:HG13	1.95	0.49
1:BBB:494:VAL:HG21	1:BBB:569:ALA:HB2	1.95	0.48
1:BBB:693:MET:HE3	1:BBB:695:ILE:HD11	1.94	0.48
1:BBB:107:SER:HB3	1:BBB:706:SER:HB2	1.96	0.48
1:BBB:514:THR:HG21	1:BBB:525:TYR:CE2	2.48	0.48
1:CCC:514:THR:HG21	1:CCC:525:TYR:CE2	2.49	0.48
1:DDD:494:VAL:HG22	1:DDD:524:ILE:CD1	2.44	0.48
1:CCC:406:LEU:HD23	1:CCC:406:LEU:C	2.34	0.47
1:AAA:44:GLU:OE2	1:AAA:226:ASP:HB3	2.14	0.47
1:BBB:441:GLU:HA	1:BBB:441:GLU:OE2	2.14	0.47
1:AAA:380:LEU:HD21	1:AAA:505:ALA:HB2	1.95	0.47
1:AAA:507:LEU:H	1:AAA:507:LEU:CD2	2.28	0.47
1:BBB:575:ALA:HB2	1:BBB:725:MET:HE1	1.96	0.47
1:BBB:579:GLY:HA2	1:BBB:603:ILE:O	2.15	0.47
1:AAA:584:VAL:CG2	1:AAA:606:ILE:CG2	2.85	0.47
1:BBB:430:PRO:HA	1:BBB:510:PHE:CG	2.50	0.47
1:AAA:254:VAL:HG13	1:AAA:304:MET:HE2	1.97	0.47
1:BBB:619:ALA:HB3	3:BBB:802:DMS:C1	2.45	0.46
1:AAA:579:GLY:HA2	1:AAA:603:ILE:O	2.15	0.46
1:DDD:494:VAL:HG23	1:DDD:569:ALA:HB2	1.95	0.46
1:CCC:579:GLY:HA2	1:CCC:603:ILE:O	2.15	0.46
1:AAA:606:ILE:HD12	1:AAA:621:TRP:CZ3	2.51	0.46
1:DDD:242:HIS:HE1	1:DDD:246:GLU:O	1.98	0.46
1:AAA:254:VAL:HG13	1:AAA:304:MET:CE	2.45	0.46
1:BBB:47:GLU:CD	1:DDD:223:PRO:CB	2.84	0.46
1:AAA:79:LYS:HG3	9:AAA:909:HOH:O	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:193:GLY:N	9:AAA:902:HOH:O	2.37	0.45
1:AAA:514:THR:HG21	1:AAA:525:TYR:CE2	2.51	0.45
1:BBB:380:LEU:HD21	1:BBB:505:ALA:HB2	1.97	0.45
1:CCC:73:TRP:CH2	1:CCC:520:ILE:HD12	2.51	0.45
1:CCC:618:GLY:HA2	1:CCC:621:TRP:CE3	2.52	0.45
1:CCC:707:THR:O	1:CCC:711:LEU:HG	2.16	0.45
1:BBB:577:ARG:HA	1:BBB:601:ILE:O	2.17	0.45
1:CCC:242:HIS:HE1	1:CCC:246:GLU:O	2.00	0.45
1:BBB:418:ASN:HB3	9:BBB:904:HOH:O	2.16	0.45
1:DDD:57:ARG:HB2	1:DDD:695:ILE:HD13	1.98	0.45
1:DDD:579:GLY:HA2	1:DDD:603:ILE:O	2.16	0.45
1:DDD:577:ARG:HA	1:DDD:601:ILE:O	2.17	0.45
1:BBB:619:ALA:HB3	3:BBB:802:DMS:H13	1.99	0.45
1:DDD:707:THR:O	1:DDD:711:LEU:HG	2.17	0.45
1:AAA:620:SER:H	3:AAA:803:DMS:H22	1.82	0.44
1:DDD:400:ARG:HB3	1:DDD:403:GLU:HG3	1.98	0.44
1:BBB:242:HIS:HE1	1:BBB:246:GLU:O	1.99	0.44
1:CCC:577:ARG:HA	1:CCC:601:ILE:O	2.18	0.44
1:DDD:633:ASP:HA	1:DDD:636:PHE:CE2	2.53	0.44
1:AAA:633:ASP:HA	1:AAA:636:PHE:CE2	2.53	0.44
1:DDD:142:ASP:OD2	1:DDD:144:ASN:HB3	2.17	0.44
1:AAA:242:HIS:HE1	1:AAA:246:GLU:O	1.99	0.44
1:AAA:620:SER:H	3:AAA:803:DMS:C2	2.30	0.44
1:CCC:362:ALA:HB2	1:CCC:381:ARG:CD	2.47	0.44
1:DDD:92:GLU:HG3	1:DDD:98:TYR:CD1	2.53	0.44
1:AAA:92:GLU:HG3	1:AAA:98:TYR:CD1	2.53	0.44
1:AAA:430:PRO:HA	1:AAA:510:PHE:CG	2.53	0.44
1:AAA:577:ARG:HA	1:AAA:601:ILE:O	2.16	0.44
1:BBB:612:PHE:CG	1:BBB:613:PRO:HD3	2.53	0.44
1:DDD:430:PRO:HA	1:DDD:510:PHE:CG	2.52	0.44
1:AAA:701:HIS:CG	1:AAA:702:PHE:H	2.36	0.44
1:DDD:494:VAL:HG23	1:DDD:569:ALA:CB	2.48	0.44
1:BBB:633:ASP:HA	1:BBB:636:PHE:CE2	2.53	0.43
1:CCC:92:GLU:HG3	1:CCC:98:TYR:CD1	2.53	0.43
1:DDD:612:PHE:CG	1:DDD:613:PRO:HD3	2.53	0.43
1:CCC:33:ARG:CZ	1:CCC:33:ARG:HB3	2.49	0.43
1:CCC:480:ILE:HG23	1:CCC:524:ILE:HG23	1.99	0.43
1:CCC:173:ILE:HB	1:CCC:199:ILE:HB	1.99	0.43
1:CCC:612:PHE:N	1:CCC:613:PRO:CD	2.81	0.43
1:DDD:243:ARG:NH2	9:DDD:902:HOH:O	2.38	0.43
1:DDD:708:GLN:O	1:DDD:712:GLU:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:612:PHE:CG	1:AAA:613:PRO:HD3	2.53	0.43
1:BBB:195:MET:CE	1:BBB:244:ILE:CG2	2.97	0.43
1:BBB:582:GLY:O	1:BBB:585:LEU:HB3	2.19	0.43
1:CCC:633:ASP:HA	1:CCC:636:PHE:CE2	2.53	0.43
1:DDD:618:GLY:HA2	1:DDD:621:TRP:CE3	2.53	0.43
1:BBB:612:PHE:N	1:BBB:613:PRO:CD	2.82	0.43
1:CCC:308:ASN:OD1	1:DDD:23:SER:HB2	2.19	0.43
1:BBB:707:THR:O	1:BBB:711:LEU:HG	2.18	0.43
1:AAA:612:PHE:N	1:AAA:613:PRO:CD	2.82	0.43
1:BBB:140:SER:OG	1:BBB:145:ALA:HB2	2.19	0.43
1:CCC:134:PHE:CZ	1:CCC:139:LEU:HD11	2.53	0.43
1:CCC:380:LEU:CD1	1:CCC:507:LEU:HD21	2.48	0.43
1:CCC:483:PRO:HD3	1:CCC:518:CYS:HB3	1.99	0.43
1:BBB:328:TYR:CD1	1:BBB:342:THR:HG22	2.54	0.43
1:DDD:494:VAL:HG22	1:DDD:524:ILE:HD11	2.00	0.42
1:BBB:92:GLU:HG3	1:BBB:98:TYR:CD1	2.54	0.42
1:DDD:582:GLY:O	1:DDD:585:LEU:HB3	2.19	0.42
1:AAA:582:GLY:O	1:AAA:585:LEU:HB3	2.19	0.42
1:BBB:380:LEU:CD1	1:BBB:507:LEU:HD21	2.50	0.42
1:BBB:514:THR:CG2	1:BBB:525:TYR:CG	3.03	0.42
1:DDD:606:ILE:HD12	1:DDD:621:TRP:CZ3	2.55	0.42
1:BBB:514:THR:HG21	1:BBB:525:TYR:CG	2.54	0.42
1:DDD:612:PHE:N	1:DDD:613:PRO:CD	2.83	0.42
1:BBB:693:MET:SD	1:BBB:695:ILE:HD11	2.60	0.42
1:AAA:339:LYS:HB2	1:AAA:356:ILE:O	2.20	0.42
1:CCC:612:PHE:CG	1:CCC:613:PRO:HD3	2.54	0.42
1:DDD:730:GLN:O	1:DDD:731:THR:C	2.58	0.42
1:CCC:582:GLY:O	1:CCC:585:LEU:HB3	2.19	0.42
1:DDD:339:LYS:HB2	1:DDD:356:ILE:O	2.20	0.42
1:DDD:495:LEU:HD11	1:DDD:577:ARG:HD2	2.02	0.41
1:AAA:173:ILE:HB	1:AAA:199:ILE:HB	2.02	0.41
1:AAA:217:PHE:HZ	1:AAA:300:ILE:HD12	1.85	0.41
1:DDD:301:GLY:O	1:DDD:304:MET:HE2	2.20	0.41
1:AAA:83:TYR:CE2	1:AAA:85:ARG:HG2	2.56	0.41
1:CCC:430:PRO:HA	1:CCC:510:PHE:CG	2.55	0.41
1:BBB:708:GLN:O	1:BBB:712:GLU:HG3	2.21	0.41
1:AAA:494:VAL:HG23	1:AAA:569:ALA:CB	2.49	0.41
1:CCC:83:TYR:CE2	1:CCC:85:ARG:HG2	2.55	0.41
1:AAA:318:THR:OG1	1:AAA:330:MET:HB3	2.21	0.41
1:CCC:76:THR:HG21	1:CCC:520:ILE:HD11	2.03	0.41
1:BBB:301:GLY:O	1:BBB:304:MET:HE2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DDD:267:VAL:HA	1:DDD:277:LEU:O	2.21	0.41
1:AAA:577:ARG:HB2	1:AAA:601:ILE:HB	2.03	0.41
1:CCC:410:MET:HA	6:CCC:807:GOL:H2	2.02	0.41
1:CCC:621:TRP:CE2	2:CCC:806:ZPR:H42	2.56	0.41
1:AAA:390:ARG:HD3	1:AAA:397:PRO:HA	2.03	0.40
1:AAA:618:GLY:HA2	1:AAA:621:TRP:CE3	2.56	0.40
1:BBB:494:VAL:HG23	1:BBB:569:ALA:CB	2.49	0.40
1:BBB:339:LYS:HB2	1:BBB:356:ILE:O	2.21	0.40
1:BBB:390:ARG:HD3	1:BBB:397:PRO:HA	2.04	0.40
1:BBB:618:GLY:HA2	1:BBB:621:TRP:CE3	2.56	0.40
1:CCC:328:TYR:CD1	1:CCC:342:THR:HG22	2.56	0.40
1:DDD:380:LEU:HD11	1:DDD:505:ALA:CB	2.50	0.40
1:BBB:267:VAL:HA	1:BBB:277:LEU:O	2.22	0.40
1:BBB:661:THR:HG23	1:BBB:695:ILE:HD13	2.03	0.40
1:DDD:483:PRO:HD3	1:DDD:518:CYS:HB3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AAA	727/745 (98%)	704 (97%)	22 (3%)	1 (0%)	51	49
1	BBB	701/745 (94%)	678 (97%)	20 (3%)	3 (0%)	34	30
1	CCC	680/745 (91%)	661 (97%)	18 (3%)	1 (0%)	51	49
1	DDD	712/745 (96%)	688 (97%)	23 (3%)	1 (0%)	51	49
All	All	2820/2980 (95%)	2731 (97%)	83 (3%)	6 (0%)	47	44

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	BBB	226	ASP
1	BBB	650	GLY
1	BBB	616	THR
1	CCC	616	THR
1	DDD	616	THR
1	AAA	104	GLY

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	AAA	630/645 (98%)	626 (99%)	4 (1%)	86 90
1	BBB	612/645 (95%)	605 (99%)	7 (1%)	73 78
1	CCC	601/645 (93%)	598 (100%)	3 (0%)	88 92
1	DDD	622/645 (96%)	620 (100%)	2 (0%)	92 95
All	All	2465/2580 (96%)	2449 (99%)	16 (1%)	84 90

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	465	SER
1	AAA	507	LEU
1	AAA	577	ARG
1	AAA	694	ARG
1	BBB	61	ARG
1	BBB	115	ARG
1	BBB	176	ARG
1	BBB	225	ASP
1	BBB	442	LYS
1	BBB	465	SER
1	BBB	683	ASN
1	CCC	465	SER
1	CCC	577	ARG
1	CCC	705	LYS
1	DDD	165	GLU
1	DDD	459	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 44 ligands modelled in this entry, 1 is monoatomic - leaving 43 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	$\#\|Z\| > 2$
4	BCT	AAA	807	-	2,3,3	0.98	0	2,3,3	1.65	1 (50%)
2	ZPR	DDD	801	1	25,26,26	1.46	2 (8%)	31,35,35	1.99	4 (12%)
6	GOL	CCC	807	-	5,5,5	0.09	0	5,5,5	0.31	0
4	BCT	AAA	809	-	2,3,3	1.37	0	2,3,3	0.81	0
4	BCT	DDD	804	-	2,3,3	0.99	0	2,3,3	1.59	1 (50%)
5	EDO	AAA	811	-	3,3,3	0.09	0	2,2,2	0.11	0
2	ZPR	CCC	806	1	25,26,26	1.37	1 (4%)	31,35,35	1.94	4 (12%)
4	BCT	DDD	811	-	2,3,3	0.96	0	2,3,3	1.67	1 (50%)
4	BCT	BBB	804	-	2,3,3	0.97	0	2,3,3	1.68	1 (50%)
2	ZPR	AAA	801	1	25,26,26	1.32	1 (4%)	31,35,35	1.75	3 (9%)
4	BCT	CCC	804	-	2,3,3	0.97	0	2,3,3	1.58	1 (50%)
4	BCT	AAA	804	-	2,3,3	0.95	0	2,3,3	1.69	1 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	BCT	BBB	803	-	2,3,3	1.34	0	2,3,3	0.88	0
4	BCT	CCC	801	-	2,3,3	0.99	0	2,3,3	1.67	1 (50%)
4	BCT	CCC	805	-	2,3,3	1.35	0	2,3,3	0.85	0
3	DMS	AAA	803	-	3,3,3	0.21	0	3,3,3	0.16	0
5	EDO	CCC	809	-	3,3,3	0.03	0	2,2,2	0.17	0
4	BCT	CCC	803	-	2,3,3	1.29	0	2,3,3	0.91	0
4	BCT	DDD	802	-	2,3,3	0.96	0	2,3,3	1.67	1 (50%)
4	BCT	CCC	802	-	2,3,3	0.99	0	2,3,3	1.71	1 (50%)
5	EDO	BBB	809	-	3,3,3	0.04	0	2,2,2	0.35	0
2	ZPR	BBB	807	1	25,26,26	1.31	1 (4%)	31,35,35	1.98	4 (12%)
4	BCT	AAA	805	-	2,3,3	1.00	0	2,3,3	1.59	1 (50%)
5	EDO	AAA	813	-	3,3,3	0.04	0	2,2,2	0.12	0
4	BCT	BBB	808	-	2,3,3	1.36	0	2,3,3	0.79	0
5	EDO	CCC	808	-	3,3,3	0.09	0	2,2,2	0.12	0
3	DMS	DDD	803	-	3,3,3	0.25	0	3,3,3	0.07	0
4	BCT	AAA	806	-	2,3,3	0.98	0	2,3,3	1.60	1 (50%)
5	EDO	DDD	810	-	3,3,3	0.10	0	2,2,2	0.09	0
3	DMS	AAA	802	-	3,3,3	0.22	0	3,3,3	0.08	0
4	BCT	DDD	806	-	2,3,3	1.33	0	2,3,3	0.76	0
7	PO4	DDD	805	-	4,4,4	0.60	0	6,6,6	0.46	0
4	BCT	BBB	810	-	2,3,3	1.34	0	2,3,3	0.84	0
4	BCT	DDD	807	-	2,3,3	1.00	0	2,3,3	1.72	1 (50%)
4	BCT	BBB	806	-	2,3,3	0.99	0	2,3,3	1.52	1 (50%)
5	EDO	AAA	812	-	3,3,3	0.11	0	2,2,2	0.19	0
7	PO4	DDD	808	-	4,4,4	0.71	0	6,6,6	0.45	0
4	BCT	BBB	805	-	2,3,3	0.99	0	2,3,3	1.65	1 (50%)
4	BCT	BBB	801	-	2,3,3	1.33	0	2,3,3	0.80	0
4	BCT	AAA	810	-	2,3,3	0.98	0	2,3,3	1.65	1 (50%)
5	EDO	DDD	809	-	3,3,3	0.09	0	2,2,2	0.07	0
4	BCT	AAA	808	-	2,3,3	0.93	0	2,3,3	1.63	1 (50%)
3	DMS	BBB	802	-	3,3,3	0.22	0	3,3,3	0.32	0

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
2	ZPR	AAA	801	1	-	3/17/39/39	0/3/3/3
2	ZPR	DDD	801	1	-	5/17/39/39	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	CCC	807	-	-	1/4/4/4	-
5	EDO	AAA	812	-	-	0/1/1/1	-
5	EDO	AAA	813	-	-	1/1/1/1	-
5	EDO	CCC	808	-	-	1/1/1/1	-
5	EDO	AAA	811	-	-	1/1/1/1	-
5	EDO	BBB	809	-	-	1/1/1/1	-
5	EDO	DDD	809	-	-	0/1/1/1	-
2	ZPR	CCC	806	1	-	6/17/39/39	0/3/3/3
5	EDO	DDD	810	-	-	1/1/1/1	-
5	EDO	CCC	809	-	-	0/1/1/1	-
2	ZPR	BBB	807	1	-	7/17/39/39	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	CCC	806	ZPR	O17-C15	6.20	1.46	1.34
2	DDD	801	ZPR	O17-C15	6.17	1.46	1.34
2	BBB	807	ZPR	O17-C15	5.82	1.45	1.34
2	AAA	801	ZPR	O17-C15	5.72	1.45	1.34
2	DDD	801	ZPR	C3-N7	-2.95	1.45	1.48

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	DDD	801	ZPR	O17-C15-N14	8.70	120.61	111.05
2	BBB	807	ZPR	O17-C15-N14	8.21	120.06	111.05
2	CCC	806	ZPR	O17-C15-N14	7.56	119.35	111.05
2	AAA	801	ZPR	O17-C15-N14	7.11	118.86	111.05
2	BBB	807	ZPR	O17-C15-O16	-4.78	116.64	124.78
2	CCC	806	ZPR	C4-C3-C1	-4.67	106.27	112.70
2	DDD	801	ZPR	O17-C15-O16	-4.41	117.27	124.78
2	CCC	806	ZPR	O17-C15-O16	-3.93	118.08	124.78
2	AAA	801	ZPR	O17-C15-O16	-3.89	118.16	124.78
2	BBB	807	ZPR	C4-C3-C1	-2.85	108.78	112.70
2	AAA	801	ZPR	C18-O17-C15	2.35	121.77	115.53
4	DDD	807	BCT	O2-C-O1	2.30	125.50	119.55
4	CCC	802	BCT	O2-C-O1	2.26	125.40	119.55
2	BBB	807	ZPR	C18-O17-C15	2.24	121.46	115.53
4	CCC	801	BCT	O2-C-O1	2.24	125.34	119.55
4	BBB	804	BCT	O2-C-O1	2.23	125.33	119.55
4	DDD	802	BCT	O2-C-O1	2.23	125.33	119.55
4	AAA	804	BCT	O2-C-O1	2.22	125.30	119.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	DDD	811	BCT	O2-C-O1	2.20	125.27	119.55
4	BBB	805	BCT	O2-C-O1	2.20	125.25	119.55
4	AAA	810	BCT	O2-C-O1	2.19	125.21	119.55
4	AAA	807	BCT	O2-C-O1	2.18	125.20	119.55
2	DDD	801	ZPR	C18-O17-C15	2.14	121.22	115.53
4	AAA	805	BCT	O2-C-O1	2.14	125.09	119.55
4	AAA	808	BCT	O2-C-O1	2.13	125.06	119.55
4	AAA	806	BCT	O2-C-O1	2.12	125.06	119.55
2	DDD	801	ZPR	C13-N14-C15	2.11	128.17	122.95
4	DDD	804	BCT	O2-C-O1	2.11	125.03	119.55
4	CCC	804	BCT	O2-C-O1	2.09	124.97	119.55
2	CCC	806	ZPR	C18-O17-C15	2.06	121.01	115.53
4	BBB	806	BCT	O2-C-O1	2.02	124.77	119.55

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	BBB	807	ZPR	O16-C15-O17-C18
2	BBB	807	ZPR	N14-C15-O17-C18
2	BBB	807	ZPR	C10-C8-N7-C6
2	BBB	807	ZPR	C10-C8-N7-C3
2	BBB	807	ZPR	O9-C8-N7-C6
2	BBB	807	ZPR	O9-C8-N7-C3
2	CCC	806	ZPR	O16-C15-O17-C18
2	CCC	806	ZPR	N14-C15-O17-C18
2	CCC	806	ZPR	C10-C8-N7-C6
2	CCC	806	ZPR	C10-C8-N7-C3
2	CCC	806	ZPR	O9-C8-N7-C6
2	CCC	806	ZPR	O9-C8-N7-C3
2	DDD	801	ZPR	O16-C15-O17-C18
2	DDD	801	ZPR	N14-C15-O17-C18
6	CCC	807	GOL	C1-C2-C3-O3
5	AAA	811	EDO	O1-C1-C2-O2
5	BBB	809	EDO	O1-C1-C2-O2
2	AAA	801	ZPR	N14-C15-O17-C18
5	DDD	810	EDO	O1-C1-C2-O2
2	AAA	801	ZPR	O16-C15-O17-C18
5	AAA	813	EDO	O1-C1-C2-O2
2	DDD	801	ZPR	O17-C15-N14-C10
2	DDD	801	ZPR	C19-C18-O17-C15
2	DDD	801	ZPR	O16-C15-N14-C10

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Mol	Chain	Res	Type	Atoms
2	BBB	807	ZPR	N14-C10-C8-N7
5	CCC	808	EDO	O1-C1-C2-O2
2	AAA	801	ZPR	C19-C18-O17-C15

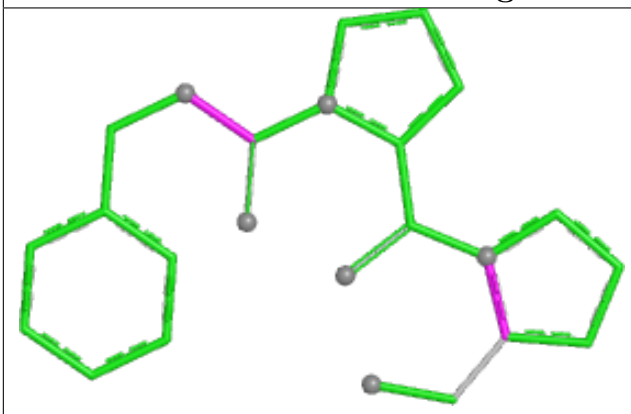
There are no ring outliers.

5 monomers are involved in 12 short contacts:

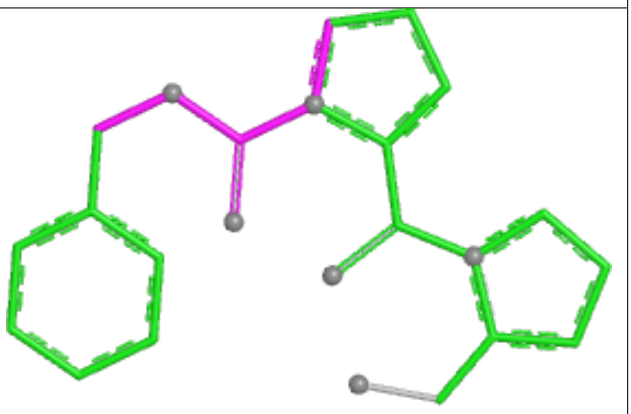
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	CCC	807	GOL	1	0
2	CCC	806	ZPR	4	0
3	AAA	803	DMS	2	0
2	BBB	807	ZPR	1	0
3	BBB	802	DMS	4	0

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.

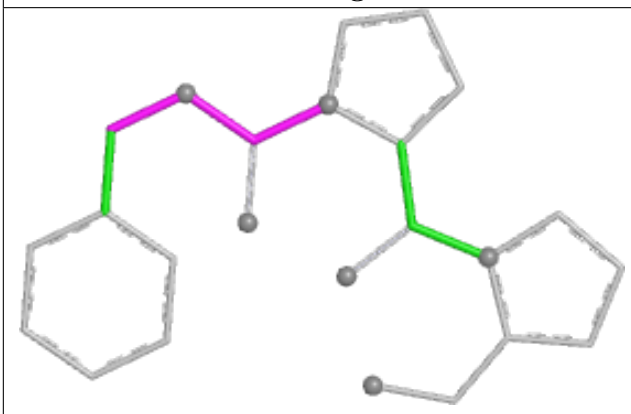
Ligand ZPR DDD 801



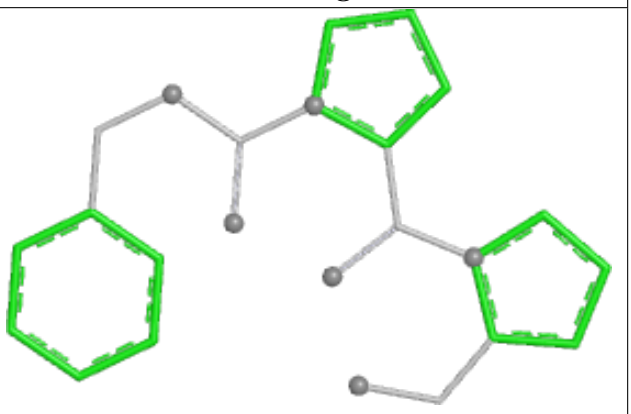
Bond lengths



Bond angles

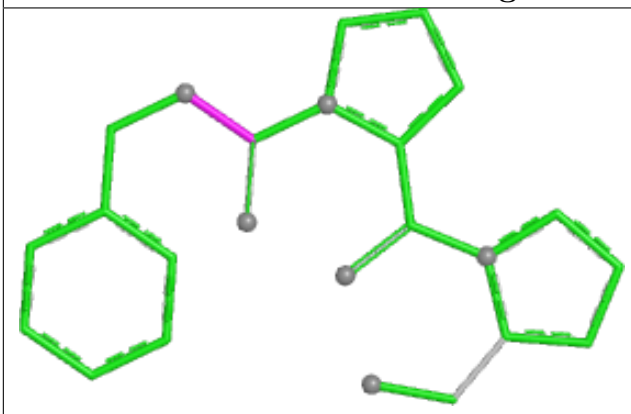


Torsions

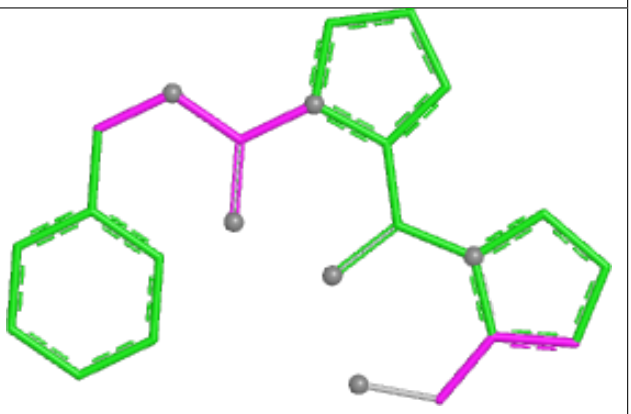


Rings

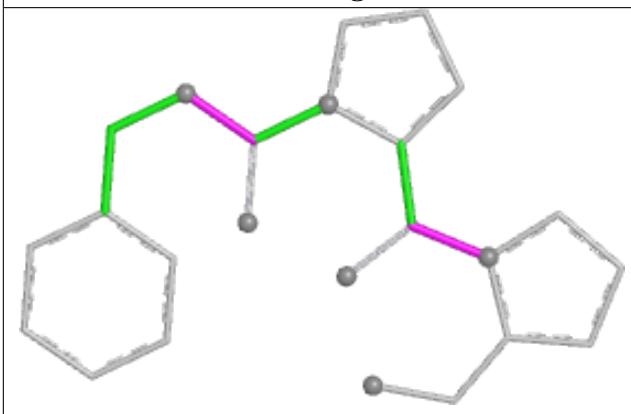
Ligand ZPR CCC 806



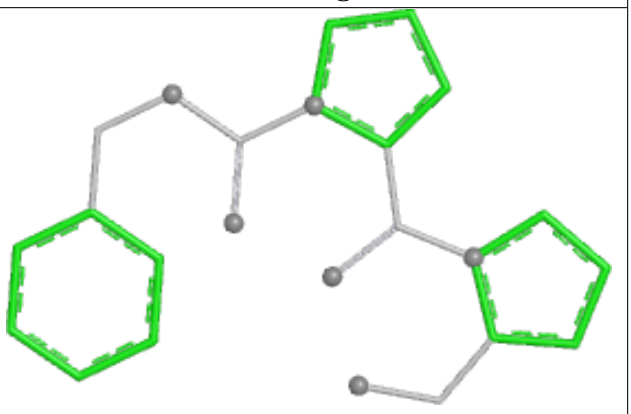
Bond lengths



Bond angles

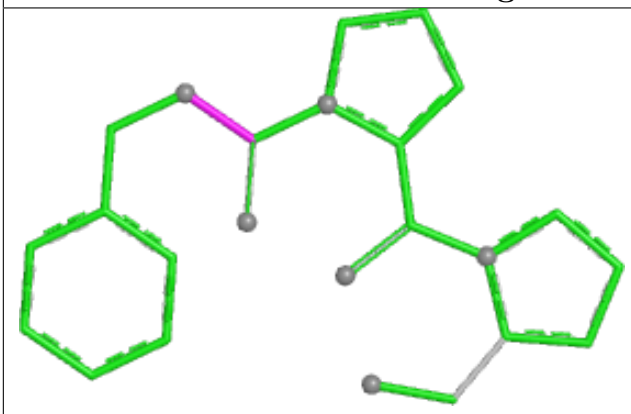


Torsions

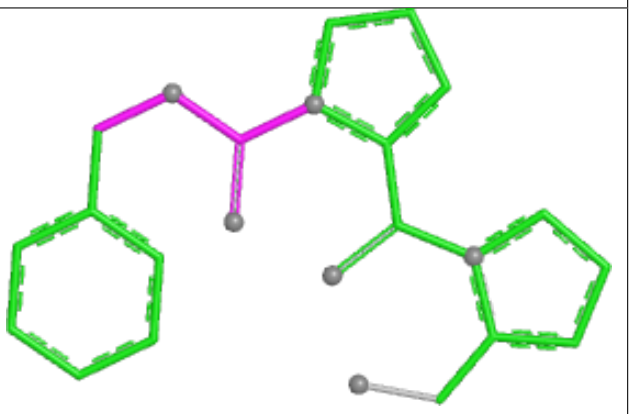


Rings

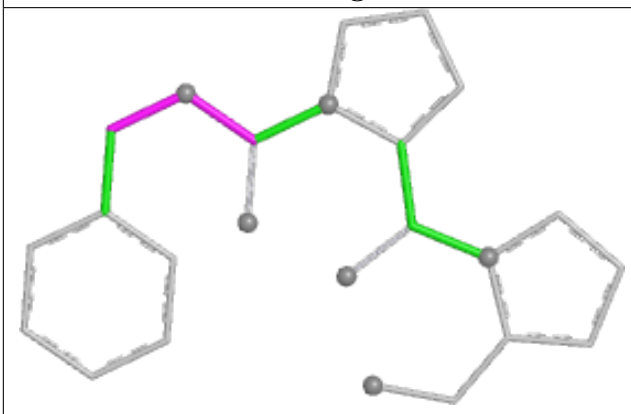
Ligand ZPR AAA 801



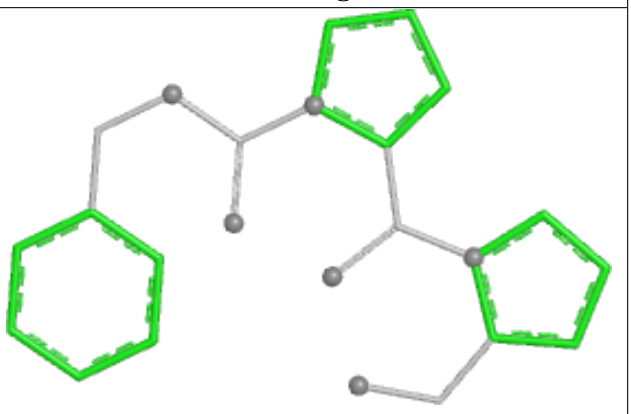
Bond lengths



Bond angles

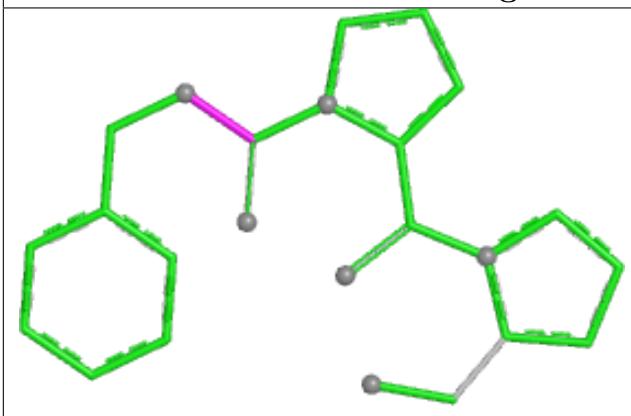


Torsions

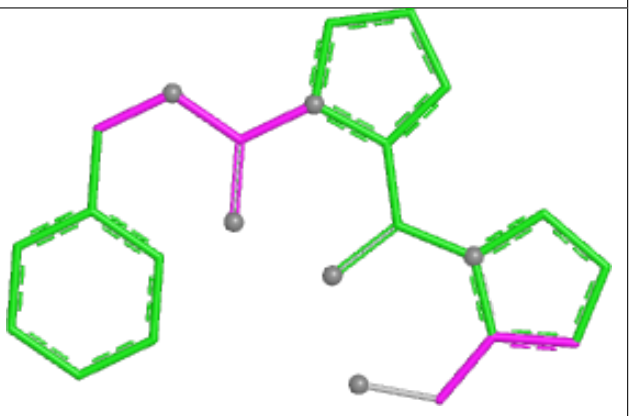


Rings

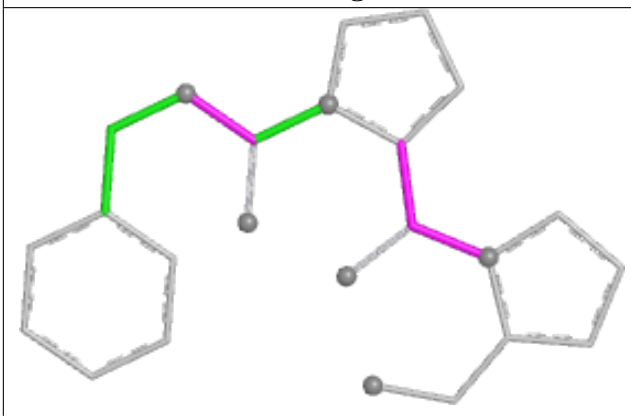
Ligand ZPR BBB 807



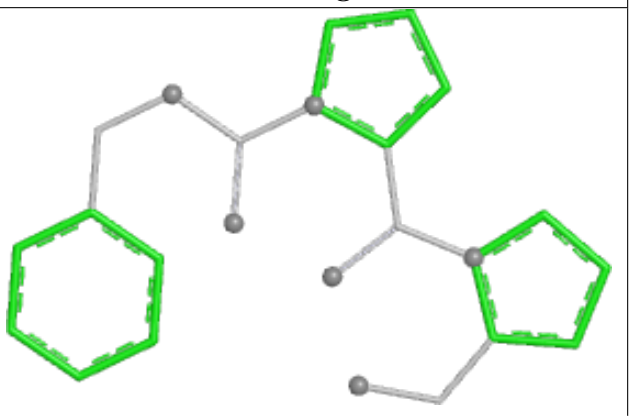
Bond lengths



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	AAA	727/745 (97%)	-0.04	13 (1%)	68	66	22, 33, 55, 91	0
1	BBB	706/745 (94%)	0.06	25 (3%)	44	43	22, 36, 64, 111	0
1	CCC	690/745 (92%)	0.02	14 (2%)	65	63	24, 35, 61, 94	0
1	DDD	716/745 (96%)	-0.16	9 (1%)	77	76	19, 30, 49, 80	0
All	All	2839/2980 (95%)	-0.03	61 (2%)	63	62	19, 33, 58, 111	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	166	HIS	7.3
1	AAA	731	THR	6.4
1	BBB	664	TYR	5.9
1	CCC	617	PHE	5.0
1	BBB	226	ASP	4.9
1	BBB	444	TYR	4.8
1	CCC	233	PRO	4.5
1	BBB	142	ASP	4.5
1	AAA	226	ASP	4.5
1	AAA	302	THR	4.4
1	CCC	666	ASP	4.3
1	BBB	5	GLY	4.0
1	CCC	141	LEU	4.0
1	DDD	731	THR	4.0
1	BBB	167	GLY	3.9
1	BBB	225	ASP	3.8
1	DDD	699	SER	3.7
1	CCC	667	ARG	3.7
1	AAA	227	GLU	3.6
1	AAA	301	GLY	3.6
1	BBB	227	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
1	CCC	179	SER	3.5
1	AAA	702	PHE	3.4
1	BBB	180	SER	3.4
1	CCC	44	GLU	3.3
1	BBB	229	LYS	3.1
1	BBB	708	GLN	3.1
1	BBB	650	GLY	3.1
1	CCC	616	THR	3.1
1	DDD	662	ALA	2.9
1	DDD	186	GLN	2.9
1	BBB	168	SER	2.9
1	AAA	187	GLU	2.9
1	BBB	169	ASP	2.8
1	BBB	731	THR	2.7
1	CCC	47	GLU	2.7
1	AAA	44	GLU	2.6
1	BBB	349	ASP	2.6
1	CCC	170	TRP	2.6
1	BBB	663	ALA	2.6
1	CCC	664	TYR	2.5
1	DDD	695	ILE	2.5
1	AAA	701	HIS	2.5
1	DDD	663	ALA	2.5
1	BBB	181	PRO	2.5
1	AAA	300	ILE	2.5
1	AAA	104	GLY	2.3
1	DDD	308	ASN	2.3
1	AAA	66	GLU	2.3
1	DDD	142	ASP	2.3
1	AAA	5	GLY	2.3
1	BBB	165	GLU	2.3
1	BBB	130	GLY	2.3
1	CCC	381	ARG	2.3
1	CCC	25	LYS	2.2
1	DDD	666	ASP	2.1
1	BBB	195	MET	2.1
1	BBB	380	LEU	2.1
1	CCC	195	MET	2.0
1	BBB	456	LEU	2.0
1	BBB	441	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, 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
4	BCT	AAA	810	4/4	0.56	0.24	54,56,61,63	0
2	ZPR	CCC	806	24/24	0.73	0.46	59,95,109,116	0
4	BCT	BBB	806	4/4	0.73	0.26	49,54,55,56	0
5	EDO	DDD	809	4/4	0.74	0.17	47,48,49,52	0
4	BCT	AAA	806	4/4	0.75	0.21	52,53,55,60	0
4	BCT	BBB	804	4/4	0.75	0.17	51,54,60,62	0
2	ZPR	BBB	807	24/24	0.76	0.28	47,92,100,102	0
4	BCT	CCC	803	4/4	0.80	0.17	55,56,59,60	0
4	BCT	AAA	804	4/4	0.82	0.14	53,54,58,59	0
5	EDO	AAA	812	4/4	0.84	0.18	32,32,36,38	0
4	BCT	CCC	805	4/4	0.84	0.13	50,55,55,62	0
5	EDO	DDD	810	4/4	0.85	0.15	47,49,52,53	0
4	BCT	CCC	801	4/4	0.86	0.14	42,50,53,56	0
4	BCT	AAA	809	4/4	0.86	0.17	44,49,50,55	0
6	GOL	CCC	807	6/6	0.86	0.26	40,43,46,52	0
5	EDO	BBB	809	4/4	0.87	0.14	36,42,43,44	0
4	BCT	DDD	811	4/4	0.87	0.22	57,58,60,61	0
7	PO4	DDD	808	5/5	0.87	0.15	47,53,55,56	0
2	ZPR	AAA	801	24/24	0.88	0.17	35,48,59,62	0
5	EDO	CCC	808	4/4	0.88	0.14	40,42,44,46	0
4	BCT	BBB	808	4/4	0.89	0.10	41,43,44,46	0
4	BCT	DDD	804	4/4	0.89	0.11	45,49,50,51	0
5	EDO	AAA	813	4/4	0.89	0.12	46,47,47,49	0
2	ZPR	DDD	801	24/24	0.90	0.16	31,45,78,84	0
4	BCT	BBB	805	4/4	0.90	0.15	51,51,51,54	0
4	BCT	BBB	803	4/4	0.90	0.10	43,44,45,48	0
7	PO4	DDD	805	5/5	0.90	0.14	58,60,64,75	0

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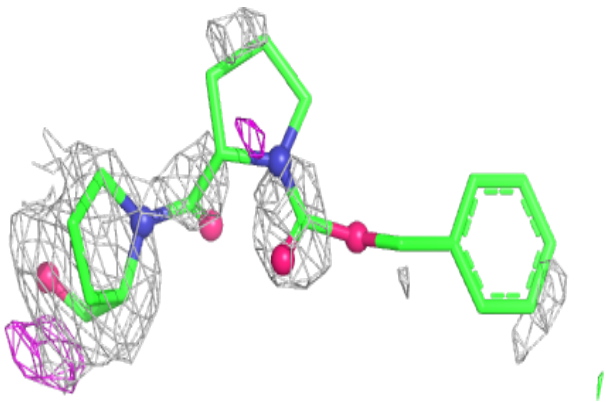
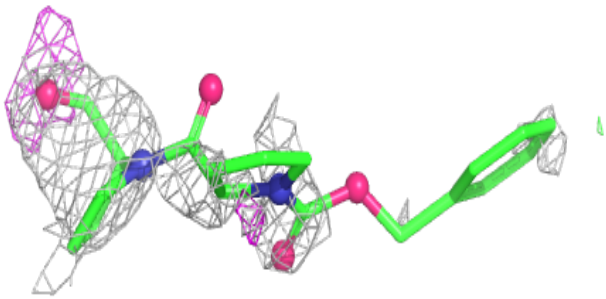
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	EDO	AAA	811	4/4	0.90	0.12	43,44,45,47	0
8	NA	DDD	812	1/1	0.90	0.26	44,44,44,44	0
4	BCT	AAA	805	4/4	0.91	0.11	44,49,49,50	0
4	BCT	BBB	810	4/4	0.91	0.10	41,42,42,45	0
4	BCT	AAA	807	4/4	0.91	0.08	42,45,51,57	0
4	BCT	BBB	801	4/4	0.93	0.13	41,45,45,48	0
4	BCT	DDD	802	4/4	0.93	0.08	38,39,39,47	0
3	DMS	BBB	802	4/4	0.93	0.17	28,30,31,38	0
4	BCT	DDD	806	4/4	0.93	0.14	42,45,45,46	0
4	BCT	AAA	808	4/4	0.93	0.13	43,47,50,51	0
5	EDO	CCC	809	4/4	0.93	0.13	40,44,47,48	0
4	BCT	CCC	804	4/4	0.94	0.11	39,40,45,45	0
4	BCT	CCC	802	4/4	0.94	0.10	43,46,47,52	0
4	BCT	DDD	807	4/4	0.94	0.08	37,42,45,48	0
3	DMS	AAA	803	4/4	0.94	0.14	24,30,30,31	0
3	DMS	AAA	802	4/4	0.95	0.09	48,50,55,57	0
3	DMS	DDD	803	4/4	0.98	0.09	36,39,40,40	0

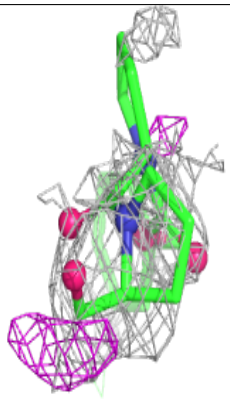
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ZPR CCC 806:

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

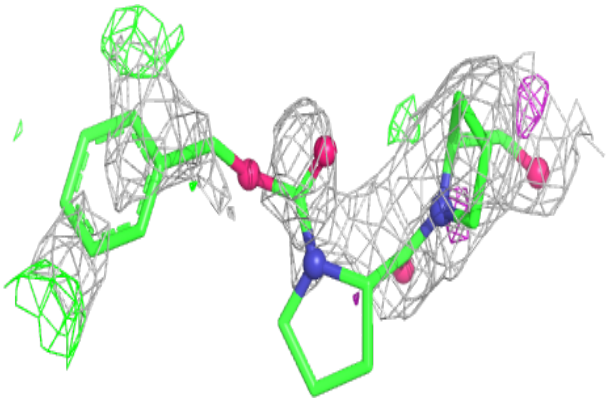


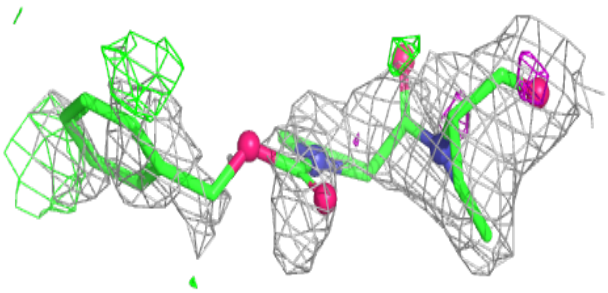


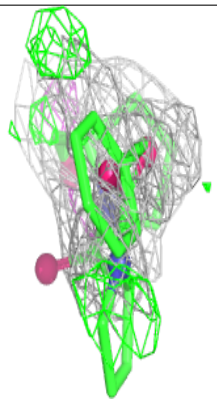


Electron density around ZPR BBB 807:

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

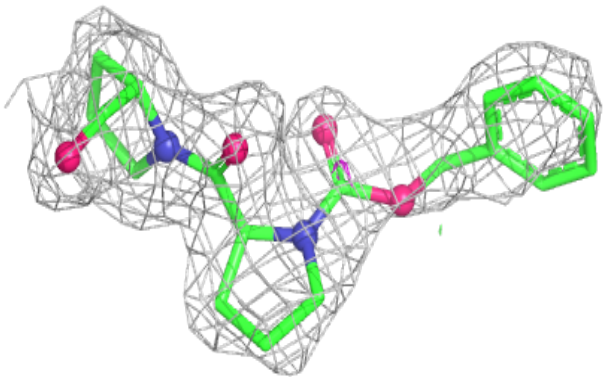


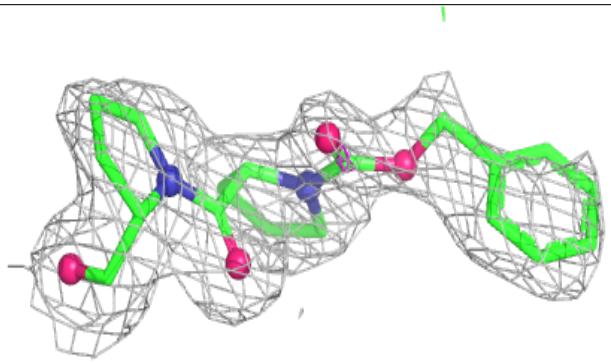


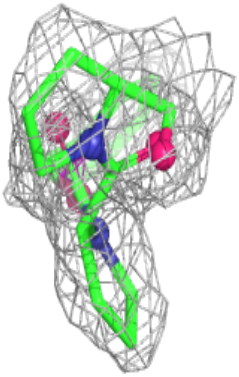


Electron density around ZPR AAA 801:

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

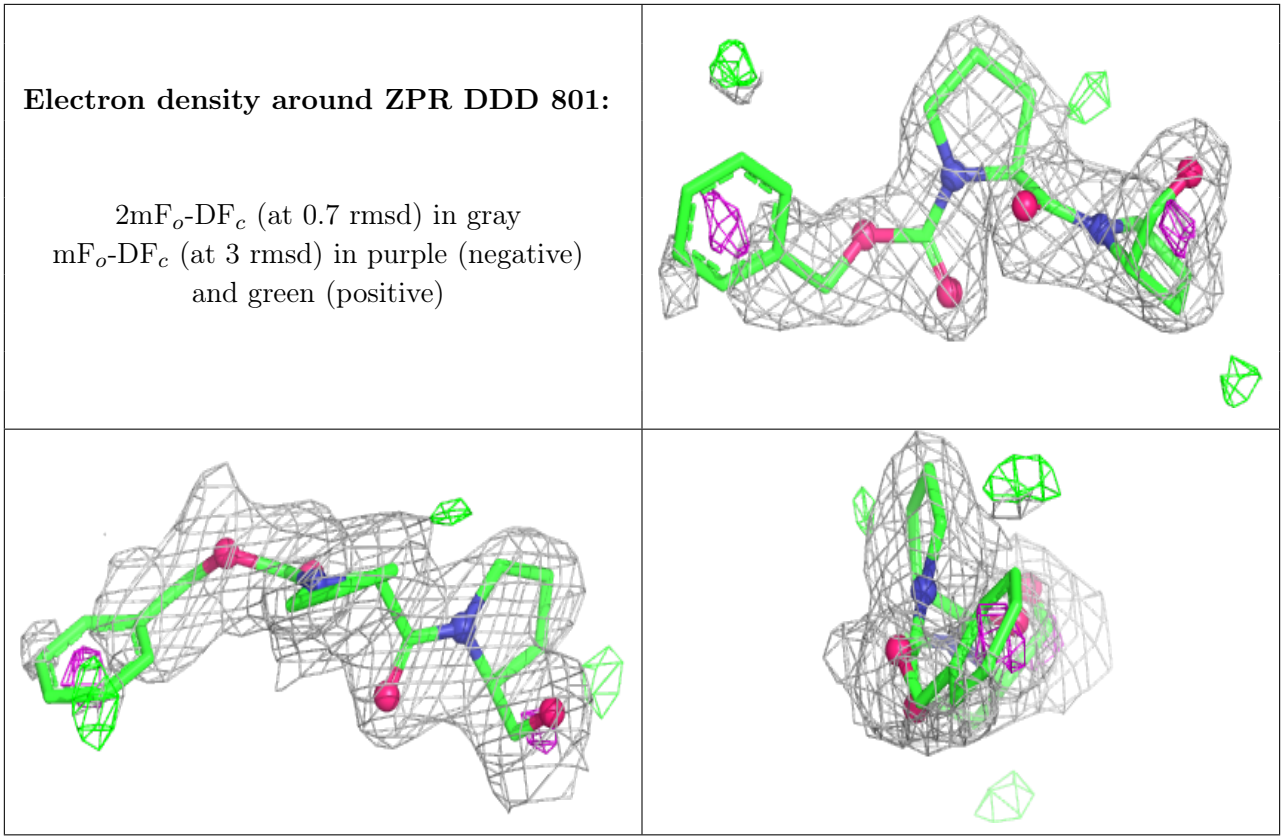






Electron density around ZPR DDD 801:

$2mF_o$-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.