Full wwPDB X-ray Structure Validation Report (i)

Sep 25, 2023 – 05:36 AM EDT

PDB ID	:	5WDK
Title	:	A processive dipeptidyl aminopeptidase secreted from an established commensal bacterium P. distasonis
Authors	:	Wolan, D.W.; Xu, J.H.; Solania, A.; Chatterjee, S.; Jiang, Z.; ODonoghue, A.J.
Deposited on	:	2017-07-05
Resolution	:	2.36 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

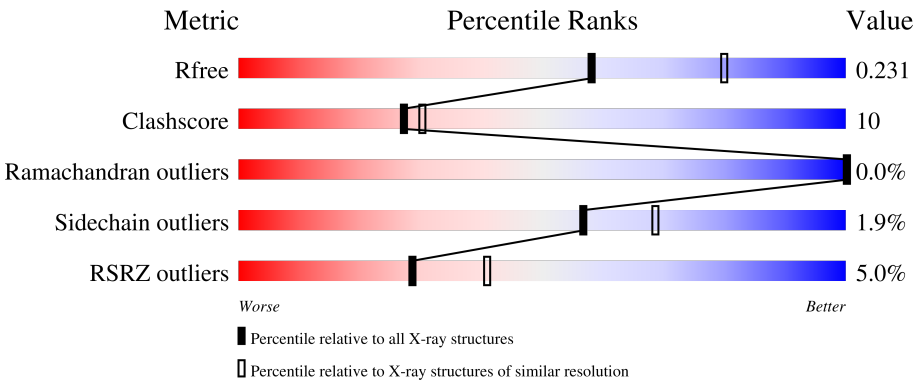
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh &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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.36 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	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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	401	5%, 78%, 12%, 9%
1	B	401	%, 72%, 14%, 14%
1	C	401	6%, 65%, 21%, •, 12%
1	D	401	9%, 67%, 22%, •, 9%

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Mol	Chain	Length	Quality of chain
1	E	401	%, 78%, 9%, 13%
1	F	401	3%, 84%, 9%, 7%

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
3	T1O	B	502	-	X	-	-
3	T1O	E	503	-	X	-	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 17403 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 Aminopeptidase C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	363	2821	1794	460	550	17	0	1	0
1	B	345	2721	1733	442	529	17	0	0	0
1	C	352	2715	1726	443	529	17	0	0	0
1	D	363	2775	1764	449	545	17	0	0	0
1	E	349	2739	1747	444	531	17	0	0	0
1	F	374	2943	1873	481	572	17	0	1	0

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	5	MET	-	expression tag	UNP A6LE66
A	6	GLY	-	expression tag	UNP A6LE66
A	7	SER	-	expression tag	UNP A6LE66
A	8	ASP	-	expression tag	UNP A6LE66
A	9	LYS	-	expression tag	UNP A6LE66
A	10	ILE	-	expression tag	UNP A6LE66
A	11	HIS	-	expression tag	UNP A6LE66
A	12	HIS	-	expression tag	UNP A6LE66
A	13	HIS	-	expression tag	UNP A6LE66
A	14	HIS	-	expression tag	UNP A6LE66
A	15	HIS	-	expression tag	UNP A6LE66
A	16	HIS	-	expression tag	UNP A6LE66
A	17	GLU	-	expression tag	UNP A6LE66
A	18	ASN	-	expression tag	UNP A6LE66
A	19	LEU	-	expression tag	UNP A6LE66
A	20	TYR	-	expression tag	UNP A6LE66
A	21	PHE	-	expression tag	UNP A6LE66

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Chain	Residue	Modelled	Actual	Comment	Reference
A	22	GLN	-	expression tag	UNP A6LE66
B	5	MET	-	expression tag	UNP A6LE66
B	6	GLY	-	expression tag	UNP A6LE66
B	7	SER	-	expression tag	UNP A6LE66
B	8	ASP	-	expression tag	UNP A6LE66
B	9	LYS	-	expression tag	UNP A6LE66
B	10	ILE	-	expression tag	UNP A6LE66
B	11	HIS	-	expression tag	UNP A6LE66
B	12	HIS	-	expression tag	UNP A6LE66
B	13	HIS	-	expression tag	UNP A6LE66
B	14	HIS	-	expression tag	UNP A6LE66
B	15	HIS	-	expression tag	UNP A6LE66
B	16	HIS	-	expression tag	UNP A6LE66
B	17	GLU	-	expression tag	UNP A6LE66
B	18	ASN	-	expression tag	UNP A6LE66
B	19	LEU	-	expression tag	UNP A6LE66
B	20	TYR	-	expression tag	UNP A6LE66
B	21	PHE	-	expression tag	UNP A6LE66
B	22	GLN	-	expression tag	UNP A6LE66
C	5	MET	-	expression tag	UNP A6LE66
C	6	GLY	-	expression tag	UNP A6LE66
C	7	SER	-	expression tag	UNP A6LE66
C	8	ASP	-	expression tag	UNP A6LE66
C	9	LYS	-	expression tag	UNP A6LE66
C	10	ILE	-	expression tag	UNP A6LE66
C	11	HIS	-	expression tag	UNP A6LE66
C	12	HIS	-	expression tag	UNP A6LE66
C	13	HIS	-	expression tag	UNP A6LE66
C	14	HIS	-	expression tag	UNP A6LE66
C	15	HIS	-	expression tag	UNP A6LE66
C	16	HIS	-	expression tag	UNP A6LE66
C	17	GLU	-	expression tag	UNP A6LE66
C	18	ASN	-	expression tag	UNP A6LE66
C	19	LEU	-	expression tag	UNP A6LE66
C	20	TYR	-	expression tag	UNP A6LE66
C	21	PHE	-	expression tag	UNP A6LE66
C	22	GLN	-	expression tag	UNP A6LE66
D	5	MET	-	expression tag	UNP A6LE66
D	6	GLY	-	expression tag	UNP A6LE66
D	7	SER	-	expression tag	UNP A6LE66
D	8	ASP	-	expression tag	UNP A6LE66
D	9	LYS	-	expression tag	UNP A6LE66

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Chain	Residue	Modelled	Actual	Comment	Reference
D	10	ILE	-	expression tag	UNP A6LE66
D	11	HIS	-	expression tag	UNP A6LE66
D	12	HIS	-	expression tag	UNP A6LE66
D	13	HIS	-	expression tag	UNP A6LE66
D	14	HIS	-	expression tag	UNP A6LE66
D	15	HIS	-	expression tag	UNP A6LE66
D	16	HIS	-	expression tag	UNP A6LE66
D	17	GLU	-	expression tag	UNP A6LE66
D	18	ASN	-	expression tag	UNP A6LE66
D	19	LEU	-	expression tag	UNP A6LE66
D	20	TYR	-	expression tag	UNP A6LE66
D	21	PHE	-	expression tag	UNP A6LE66
D	22	GLN	-	expression tag	UNP A6LE66
E	5	MET	-	expression tag	UNP A6LE66
E	6	GLY	-	expression tag	UNP A6LE66
E	7	SER	-	expression tag	UNP A6LE66
E	8	ASP	-	expression tag	UNP A6LE66
E	9	LYS	-	expression tag	UNP A6LE66
E	10	ILE	-	expression tag	UNP A6LE66
E	11	HIS	-	expression tag	UNP A6LE66
E	12	HIS	-	expression tag	UNP A6LE66
E	13	HIS	-	expression tag	UNP A6LE66
E	14	HIS	-	expression tag	UNP A6LE66
E	15	HIS	-	expression tag	UNP A6LE66
E	16	HIS	-	expression tag	UNP A6LE66
E	17	GLU	-	expression tag	UNP A6LE66
E	18	ASN	-	expression tag	UNP A6LE66
E	19	LEU	-	expression tag	UNP A6LE66
E	20	TYR	-	expression tag	UNP A6LE66
E	21	PHE	-	expression tag	UNP A6LE66
E	22	GLN	-	expression tag	UNP A6LE66
F	5	MET	-	expression tag	UNP A6LE66
F	6	GLY	-	expression tag	UNP A6LE66
F	7	SER	-	expression tag	UNP A6LE66
F	8	ASP	-	expression tag	UNP A6LE66
F	9	LYS	-	expression tag	UNP A6LE66
F	10	ILE	-	expression tag	UNP A6LE66
F	11	HIS	-	expression tag	UNP A6LE66
F	12	HIS	-	expression tag	UNP A6LE66
F	13	HIS	-	expression tag	UNP A6LE66
F	14	HIS	-	expression tag	UNP A6LE66
F	15	HIS	-	expression tag	UNP A6LE66

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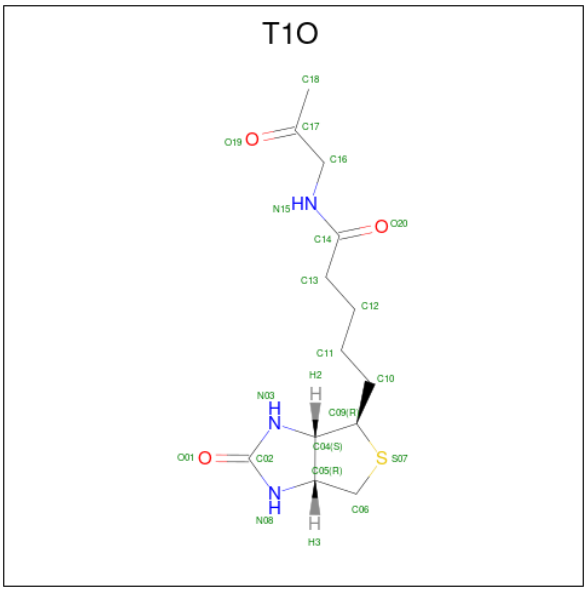
Chain	Residue	Modelled	Actual	Comment	Reference
F	16	HIS	-	expression tag	UNP A6LE66
F	17	GLU	-	expression tag	UNP A6LE66
F	18	ASN	-	expression tag	UNP A6LE66
F	19	LEU	-	expression tag	UNP A6LE66
F	20	TYR	-	expression tag	UNP A6LE66
F	21	PHE	-	expression tag	UNP A6LE66
F	22	GLN	-	expression tag	UNP A6LE66

- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total K 2 2	0	0
2	B	1	Total K 1 1	0	0
2	C	2	Total K 2 2	0	0
2	D	2	Total K 2 2	0	0
2	E	2	Total K 2 2	0	0
2	F	2	Total K 2 2	0	0

- Molecule 3 is 5-[(3aS,4R,6aR)-2-oxohexahydro-1H-thieno[3,4-d]imidazol-4-yl]-N-(2-oxopropyl)pentanamide (three-letter code: T1O) (formula: $C_{13}H_{21}N_3O_3S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
3	A	1	20	13	3	3	1	0	0
3	B	1	20	13	3	3	1	0	0
3	C	1	20	13	3	3	1	0	0
3	D	1	20	13	3	3	1	0	0
3	E	1	20	13	3	3	1	0	0
3	F	1	20	13	3	3	1	0	0

- Molecule 4 is water.

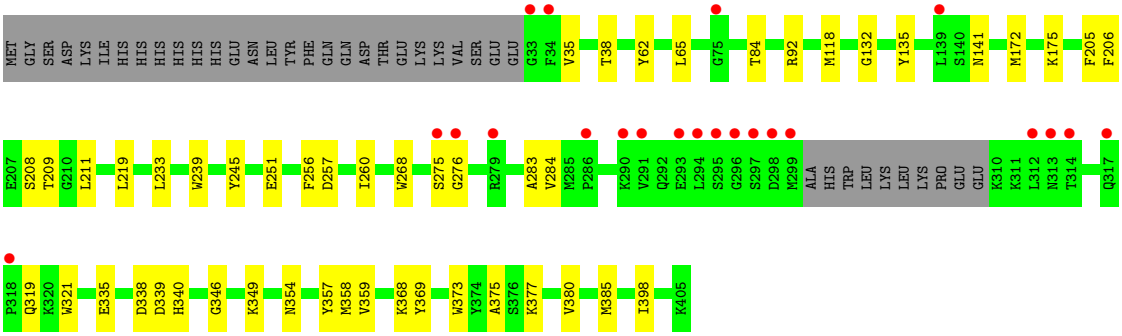
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	97	97	97	0	0
4	B	97	97	97	0	0
4	C	45	45	45	0	0
4	D	49	49	49	0	0
4	E	137	137	137	0	0
4	F	133	133	133	0	0

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.

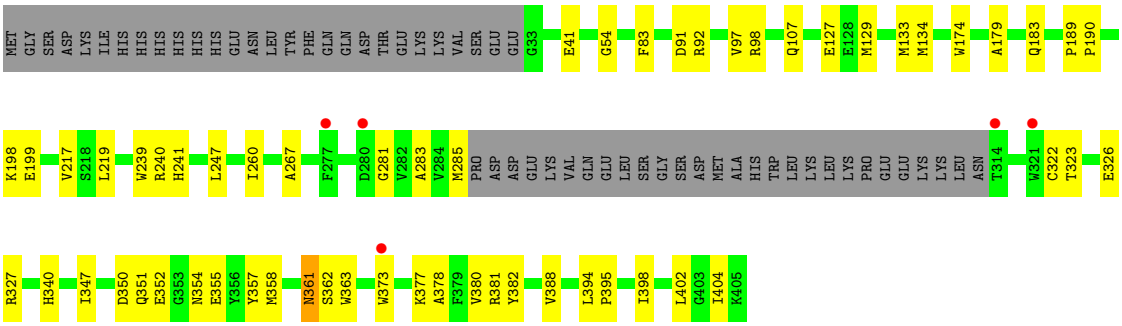
• Molecule 1: Aminopeptidase C

Chain A:



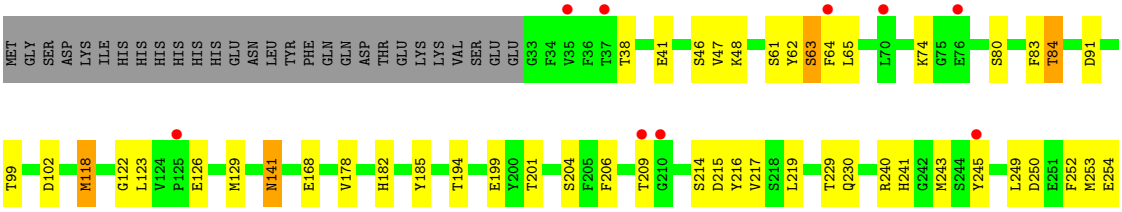
• Molecule 1: Aminopeptidase C

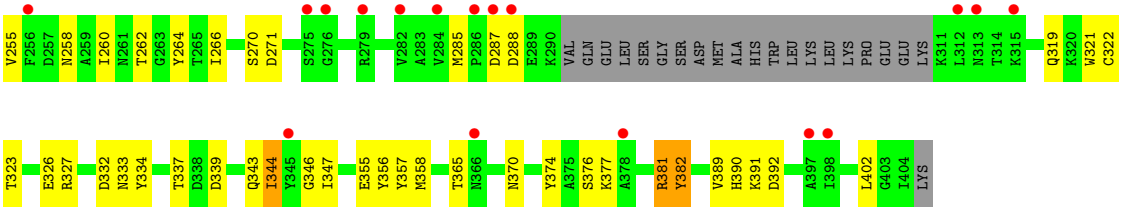
Chain B:



• Molecule 1: Aminopeptidase C

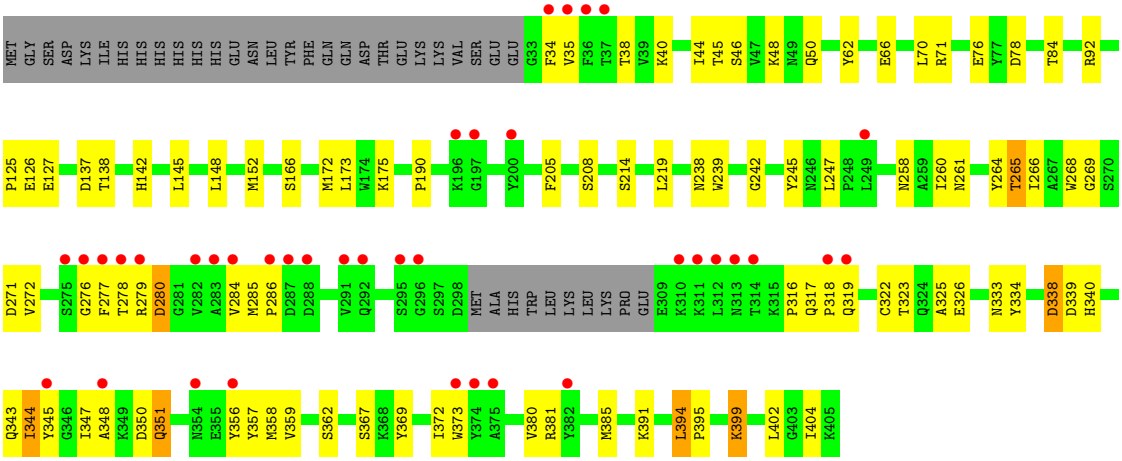
Chain C:





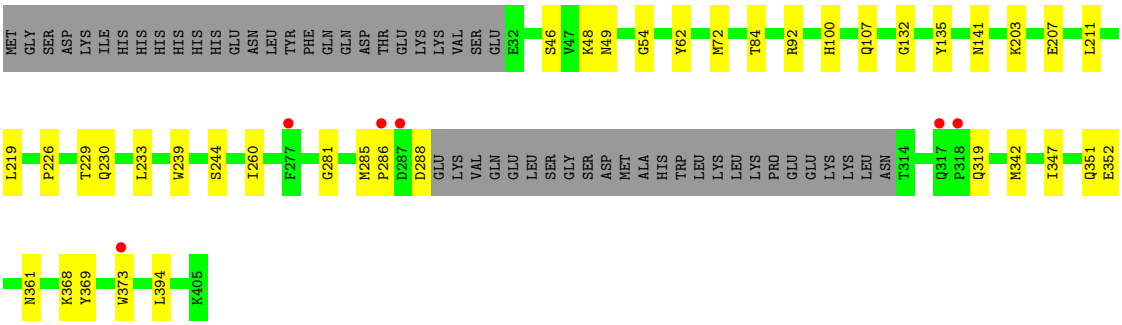
• Molecule 1: Aminopeptidase C

Chain D:



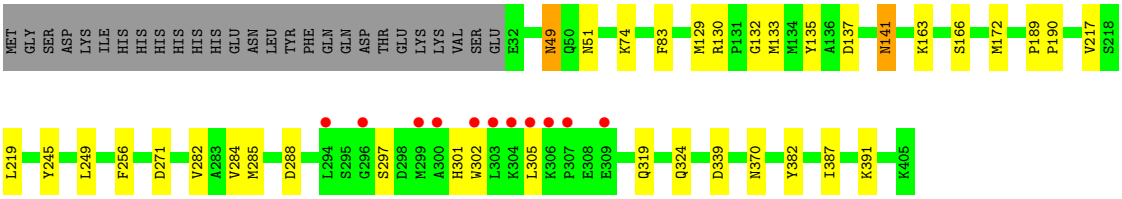
• Molecule 1: Aminopeptidase C

Chain E:



• Molecule 1: Aminopeptidase C

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	103.91Å 136.97Å 208.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.10 – 2.36 50.12 – 2.36	Depositor EDS
% Data completeness (in resolution range)	99.0 (50.10-2.36) 99.0 (50.12-2.36)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	0.14	Depositor
$< I/\sigma(I) >$ [1]	2.23 (at 2.37Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.186 , 0.231 0.188 , 0.231	Depositor DCC
R_{free} test set	6069 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	46.0	Xtriage
Anisotropy	0.089	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 41.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	17403	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.10% 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: T1O, K

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	0.45	0/2897	0.57	0/3935
1	B	0.44	0/2793	0.59	0/3790
1	C	0.45	0/2786	0.60	0/3792
1	D	0.45	0/2846	0.60	0/3873
1	E	0.47	0/2812	0.61	0/3817
1	F	0.52	0/3024	0.64	0/4104
All	All	0.47	0/17158	0.60	0/23311

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	2821	0	2601	30	0
1	B	2721	0	2543	41	0
1	C	2715	0	2480	82	0
1	D	2775	0	2518	124	0
1	E	2739	0	2556	26	0
1	F	2943	0	2751	26	0
2	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
3	A	20	0	0	0	0
3	B	20	0	0	0	0
3	C	20	0	0	0	0
3	D	20	0	0	0	0
3	E	20	0	0	0	0
3	F	20	0	0	0	0
4	A	97	0	0	0	0
4	B	97	0	0	1	0
4	C	45	0	0	0	0
4	D	49	0	0	1	0
4	E	137	0	0	2	0
4	F	133	0	0	1	0
All	All	17403	0	15449	325	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 (325) 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:D:394:LEU:HB3	1:D:399:LYS:CE	1.29	1.61
1:D:394:LEU:HB3	1:D:399:LYS:NZ	1.11	1.40
1:D:394:LEU:CB	1:D:399:LYS:CE	2.04	1.35
1:D:345:TYR:CE2	1:D:372:ILE:HD11	1.62	1.33
1:D:266:ILE:HB	1:D:344:ILE:CG2	1.58	1.32
1:D:394:LEU:CB	1:D:399:LYS:NZ	1.94	1.30
1:D:265:THR:CG2	1:D:343:GLN:HE21	1.51	1.21
1:D:394:LEU:CB	1:D:399:LYS:HZ1	1.51	1.19
1:D:265:THR:HG21	1:D:343:GLN:NE2	1.62	1.12
1:D:265:THR:HG21	1:D:343:GLN:HE21	1.02	1.09
1:D:394:LEU:HB3	1:D:399:LYS:HE2	1.36	1.01
1:D:345:TYR:HE2	1:D:372:ILE:HD11	0.87	1.00
1:C:64:PHE:HA	1:C:343:GLN:NE2	1.80	0.97
1:D:344:ILE:HD12	1:D:357:TYR:HB3	1.48	0.95
1:D:345:TYR:HE2	1:D:372:ILE:CD1	1.79	0.95
1:D:266:ILE:HB	1:D:344:ILE:HG23	1.49	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:281:GLY:O	1:E:373:TRP:HB2	1.71	0.91
1:D:266:ILE:HB	1:D:344:ILE:HG21	1.50	0.89
1:D:394:LEU:CG	1:D:399:LYS:NZ	2.34	0.89
1:D:238:ASN:HD21	1:D:242:GLY:H	1.16	0.89
1:D:347:ILE:O	1:D:358:MET:HE1	1.73	0.88
1:D:344:ILE:CD1	1:D:357:TYR:HB3	2.03	0.88
1:C:260:ILE:HD11	1:C:344:ILE:CD1	2.03	0.88
1:C:64:PHE:N	1:C:343:GLN:HE21	1.71	0.88
1:D:394:LEU:CB	1:D:399:LYS:HE2	1.92	0.88
1:D:278:THR:HG22	1:D:280:ASP:H	1.41	0.86
1:D:394:LEU:HB2	1:D:399:LYS:CE	2.05	0.86
1:D:394:LEU:CB	1:D:399:LYS:HE3	2.03	0.86
1:C:63:SER:C	1:C:343:GLN:NE2	2.33	0.82
1:C:64:PHE:CA	1:C:343:GLN:NE2	2.43	0.81
1:D:265:THR:HG23	1:D:343:GLN:HE21	1.45	0.81
1:D:345:TYR:CE2	1:D:372:ILE:CD1	2.57	0.80
1:D:278:THR:HG21	1:D:280:ASP:OD2	1.81	0.80
1:D:344:ILE:HD11	1:D:357:TYR:CD1	2.16	0.79
1:C:260:ILE:HD11	1:C:344:ILE:HD13	1.63	0.79
1:D:347:ILE:HG22	1:D:348:ALA:N	1.99	0.78
1:F:285:MET:H	1:F:319:GLN:HE22	1.32	0.77
1:D:271:ASP:OD1	1:D:338:ASP:OD2	2.03	0.77
1:D:265:THR:CG2	1:D:343:GLN:NE2	2.33	0.76
1:D:394:LEU:HB3	1:D:399:LYS:HZ1	0.93	0.76
1:C:64:PHE:CA	1:C:343:GLN:HE21	1.98	0.76
1:D:394:LEU:HB2	1:D:399:LYS:HE3	1.67	0.75
1:D:284:VAL:HG22	1:D:319:GLN:HE22	1.51	0.74
1:D:339:ASP:H	1:D:385:MET:HE1	1.49	0.74
1:D:347:ILE:O	1:D:358:MET:CE	2.35	0.74
1:D:345:TYR:CZ	1:D:372:ILE:HD11	2.22	0.73
1:C:64:PHE:N	1:C:343:GLN:NE2	2.36	0.73
1:D:394:LEU:CG	1:D:399:LYS:HZ2	2.03	0.72
1:D:35:VAL:N	1:D:351:GLN:OE1	2.21	0.72
1:D:266:ILE:HB	1:D:344:ILE:HG22	1.68	0.72
1:D:166:SER:HB3	1:D:172:MET:HE1	1.72	0.71
1:D:394:LEU:CG	1:D:399:LYS:HZ1	2.01	0.71
1:B:340:HIS:HE2	1:B:363:TRP:HZ2	1.36	0.71
1:C:46:SER:O	1:C:48:LYS:NZ	2.24	0.70
1:E:54:GLY:H	1:E:107:GLN:NE2	1.89	0.70
1:C:358:MET:HG2	1:C:374:TYR:HE1	1.55	0.69
1:B:395:PRO:HG2	1:B:398:ILE:HD12	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:71:ARG:CZ	1:D:264:TYR:HE1	2.05	0.69
1:C:258:ASN:O	1:C:262:THR:HG22	1.92	0.69
1:C:214:SER:O	1:C:391:LYS:HE2	1.92	0.69
1:B:361:ASN:ND2	1:B:362:SER:H	1.92	0.68
1:D:266:ILE:CB	1:D:344:ILE:CG2	2.55	0.68
1:A:346:GLY:HA3	1:A:358:MET:HE3	1.75	0.68
1:C:358:MET:HG2	1:C:374:TYR:CE1	2.30	0.67
1:C:201:THR:CG2	1:C:204:SER:H	2.08	0.67
1:B:361:ASN:HD22	1:B:362:SER:H	1.42	0.67
1:B:41:GLU:HB3	1:B:358:MET:CE	2.25	0.67
1:C:260:ILE:HG21	1:C:347:ILE:HG13	1.75	0.66
1:A:206:PHE:O	1:A:209:THR:OG1	2.11	0.66
1:A:257:ASP:OD1	1:A:357:TYR:OH	2.07	0.65
1:E:285:MET:H	1:E:319:GLN:HE22	1.44	0.65
1:B:129:MET:HE2	1:B:190:PRO:HD3	1.78	0.64
1:B:83:PHE:HB2	1:B:129:MET:HE3	1.79	0.64
1:F:297:SER:HB2	1:F:301:HIS:HB2	1.79	0.64
1:C:230:GLN:HB3	1:C:243:MET:HG2	1.79	0.64
1:D:347:ILE:CG2	1:D:348:ALA:N	2.62	0.63
1:C:262:THR:HG23	1:C:264:TYR:CD1	2.32	0.63
1:D:219:LEU:HD23	1:D:245:TYR:HB2	1.81	0.63
1:C:91:ASP:OD2	1:C:240:ARG:NH2	2.31	0.62
1:F:249:LEU:H	1:F:324:GLN:HE22	1.47	0.62
1:C:62:TYR:OH	1:C:84:THR:HG21	1.99	0.62
1:C:118:MET:HB2	1:C:123:LEU:HD21	1.80	0.62
1:C:201:THR:HG23	1:C:204:SER:H	1.63	0.62
1:C:321:TRP:CH2	1:C:377:LYS:HB2	2.34	0.62
1:B:247:LEU:HD21	1:B:402:LEU:HD11	1.80	0.62
1:C:390:HIS:HD2	1:C:392:ASP:H	1.45	0.62
1:D:40:LYS:NZ	1:D:261:ASN:O	2.33	0.61
1:C:63:SER:O	1:C:343:GLN:NE2	2.31	0.61
1:D:323:THR:HG22	1:D:326:GLU:HG3	1.81	0.61
1:D:316:PRO:HG2	1:D:351:GLN:HE22	1.65	0.61
1:B:285:MET:HE1	1:B:382:TYR:HB2	1.83	0.61
1:A:118:MET:HG3	1:A:206:PHE:CE1	2.36	0.60
1:D:344:ILE:HG23	1:D:344:ILE:O	1.99	0.60
1:C:266:ILE:HB	1:C:344:ILE:CG2	2.31	0.60
1:A:38:THR:HG23	1:A:358:MET:HE1	1.84	0.60
1:D:322:CYS:O	1:D:381:ARG:NH2	2.31	0.60
1:E:203:LYS:O	1:E:207:GLU:HG3	2.00	0.60
1:C:357:TYR:CE2	1:C:377:LYS:HD3	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:394:LEU:HG	1:D:399:LYS:NZ	2.15	0.59
1:F:285:MET:H	1:F:319:GLN:NE2	1.98	0.59
1:A:209:THR:HB	1:A:211:LEU:HG	1.85	0.59
1:C:249:LEU:HD11	1:C:381:ARG:HG3	1.85	0.59
1:D:344:ILE:HD11	1:D:357:TYR:CG	2.37	0.59
1:B:281:GLY:O	1:B:373:TRP:HB2	2.03	0.58
1:C:250:ASP:O	1:C:254:GLU:HG3	2.03	0.58
1:D:316:PRO:O	1:D:317:GLN:HG3	2.03	0.58
1:D:268:TRP:CZ2	1:D:380:VAL:HG22	2.37	0.58
1:C:322:CYS:O	1:C:381:ARG:NH2	2.34	0.58
1:C:83:PHE:HD2	1:C:84:THR:HG22	1.68	0.57
1:D:284:VAL:HG13	1:D:286:PRO:HD3	1.86	0.57
1:D:214:SER:O	1:D:391:LYS:HE3	2.04	0.57
1:D:345:TYR:OH	1:D:372:ILE:CD1	2.53	0.57
1:C:262:THR:HG23	1:C:264:TYR:HD1	1.68	0.57
1:B:54:GLY:H	1:B:107:GLN:NE2	2.02	0.57
1:C:219:LEU:HD13	1:C:245:TYR:HB2	1.87	0.57
1:D:92:ARG:HG3	1:D:239:TRP:CE2	2.40	0.56
1:D:44:ILE:HD12	1:D:45:THR:O	2.05	0.56
1:D:345:TYR:OH	1:D:372:ILE:HG12	2.05	0.56
1:B:323:THR:OG1	1:B:326:GLU:HG3	2.06	0.56
1:D:316:PRO:HG2	1:D:351:GLN:NE2	2.21	0.56
1:D:238:ASN:ND2	1:D:242:GLY:H	1.97	0.56
1:D:247:LEU:HD21	1:D:402:LEU:HD21	1.87	0.56
1:D:148:LEU:O	1:D:152:MET:HG3	2.06	0.55
1:F:83:PHE:HD1	1:F:129:MET:HE1	1.71	0.55
1:A:283:ALA:HB3	1:A:375:ALA:HA	1.88	0.55
1:A:92:ARG:HB2	1:A:239:TRP:CZ2	2.41	0.55
1:A:205:PHE:O	1:A:208:SER:HB3	2.07	0.55
1:C:206:PHE:O	1:C:209:THR:HG22	2.06	0.55
1:D:344:ILE:CD1	1:D:357:TYR:CB	2.82	0.55
1:E:219:LEU:HD11	1:E:394:LEU:HD21	1.88	0.55
1:B:217:VAL:HG11	1:B:404:ILE:HD13	1.87	0.55
1:D:46:SER:O	1:D:48:LYS:HE2	2.07	0.54
1:A:256:PHE:O	1:A:260:ILE:HG22	2.06	0.54
1:A:260:ILE:HD11	1:A:346:GLY:CA	2.37	0.54
1:B:267:ALA:HB3	1:B:388:VAL:HB	1.90	0.54
1:C:178:VAL:O	1:C:182:HIS:HD2	1.90	0.54
1:D:78:ASP:OD2	1:D:126:GLU:HG3	2.07	0.54
1:D:369:TYR:HB2	1:D:372:ILE:HG22	1.89	0.54
1:E:62:TYR:HH	1:E:84:THR:HG1	1.56	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:394:LEU:HD23	1:D:399:LYS:HZ2	1.72	0.54
1:E:342:MET:CE	1:E:373:TRP:HE1	2.21	0.54
1:D:166:SER:HB3	1:D:172:MET:CE	2.38	0.54
1:C:260:ILE:HD12	1:C:346:GLY:HA2	1.91	0.53
1:C:285:MET:H	1:C:319:GLN:HE22	1.55	0.53
1:A:284:VAL:HB	1:A:319:GLN:HE22	1.73	0.53
1:C:41:GLU:HG2	1:C:358:MET:CE	2.38	0.53
1:C:287:ASP:OD1	1:C:288:ASP:N	2.41	0.53
1:C:327:ARG:HA	1:C:382:TYR:HE1	1.74	0.53
1:D:394:LEU:CD2	1:D:399:LYS:HZ2	2.21	0.52
1:C:47:VAL:HB	1:C:365:THR:HG22	1.90	0.52
1:A:65:LEU:HD22	1:A:118:MET:HE1	1.92	0.52
1:C:365:THR:O	1:C:370:ASN:HA	2.09	0.52
1:D:137:ASP:OD1	1:D:138:THR:N	2.43	0.52
1:F:249:LEU:H	1:F:324:GLN:NE2	2.08	0.52
1:C:229:THR:HG22	1:C:230:GLN:H	1.75	0.52
1:D:50:GLN:HG2	1:D:362:SER:O	2.10	0.51
1:C:355:GLU:HB3	1:C:377:LYS:HE2	1.92	0.51
1:F:83:PHE:HB2	1:F:129:MET:HE3	1.93	0.51
1:D:71:ARG:NE	1:D:264:TYR:CE1	2.79	0.51
1:D:344:ILE:CD1	1:D:357:TYR:CG	2.94	0.51
1:E:226:PRO:O	1:E:229:THR:OG1	2.28	0.51
1:A:172:MET:HB2	1:A:175:LYS:HG3	1.93	0.51
1:C:217:VAL:HG23	1:C:219:LEU:HD21	1.93	0.51
1:D:172:MET:HB2	1:D:175:LYS:HG3	1.91	0.51
1:D:219:LEU:HD11	1:D:394:LEU:HD11	1.91	0.51
1:F:129:MET:HE2	1:F:190:PRO:HD3	1.92	0.51
1:B:98:ARG:NH1	1:C:332:ASP:OD1	2.34	0.51
1:C:215:ASP:O	1:C:391:LYS:HG3	2.11	0.51
1:D:266:ILE:CB	1:D:344:ILE:HG21	2.34	0.51
1:D:34:PHE:HE1	1:D:356:TYR:HH	1.59	0.50
1:B:357:TYR:CE2	1:B:377:LYS:HD2	2.47	0.50
1:C:219:LEU:CD1	1:C:245:TYR:HB2	2.41	0.50
1:F:370:ASN:ND2	4:F:607:HOH:O	2.45	0.50
1:D:62:TYR:OH	1:D:84:THR:OG1	2.17	0.50
1:D:142:HIS:HB3	1:D:145:LEU:HD23	1.94	0.50
1:C:41:GLU:HG2	1:C:358:MET:HE1	1.94	0.50
1:D:238:ASN:ND2	4:D:601:HOH:O	2.35	0.50
1:D:271:ASP:HA	1:D:338:ASP:OD2	2.12	0.50
1:D:394:LEU:C	1:D:399:LYS:HE2	2.32	0.50
1:A:359:VAL:CG1	1:A:373:TRP:HB2	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:344:ILE:HD11	1:D:357:TYR:HB3	1.90	0.50
1:C:252:PHE:O	1:C:255:VAL:HG12	2.10	0.50
1:D:260:ILE:HG21	1:D:347:ILE:HG13	1.93	0.49
1:E:48:LYS:HD2	4:E:733:HOH:O	2.12	0.49
1:B:91:ASP:OD2	1:B:240:ARG:NH2	2.45	0.49
1:C:323:THR:OG1	1:C:326:GLU:HG3	2.12	0.49
1:C:83:PHE:CD2	1:C:84:THR:HG22	2.47	0.49
1:D:278:THR:HG22	1:D:279:ARG:N	2.28	0.49
1:D:323:THR:CG2	1:D:326:GLU:H	2.26	0.48
1:E:54:GLY:H	1:E:107:GLN:HE21	1.59	0.48
1:D:339:ASP:N	1:D:385:MET:HE1	2.26	0.48
1:F:282:VAL:HG13	1:F:284:VAL:HG13	1.95	0.48
1:A:219:LEU:HD23	1:A:245:TYR:HB2	1.96	0.47
1:C:122:GLY:O	1:C:123:LEU:HD23	2.13	0.47
1:B:198:LYS:HD2	1:B:199:GLU:H	1.79	0.47
1:B:41:GLU:HB3	1:B:358:MET:HE1	1.94	0.47
1:A:132:GLY:HA2	1:A:135:TYR:CZ	2.48	0.47
1:B:355:GLU:HB3	1:B:377:LYS:HG2	1.96	0.47
1:C:253:MET:HG3	1:C:381:ARG:HB2	1.97	0.47
1:E:351:GLN:HG2	1:E:352:GLU:HG2	1.96	0.47
1:A:251:GLU:HB3	1:A:398:ILE:HD11	1.95	0.47
1:C:266:ILE:HG23	1:C:389:VAL:HG13	1.96	0.47
1:C:356:TYR:O	1:C:377:LYS:NZ	2.46	0.47
1:D:284:VAL:HG22	1:D:319:GLN:NE2	2.26	0.47
1:D:125:PRO:HG3	1:D:205:PHE:CZ	2.49	0.47
1:D:323:THR:HG23	1:D:325:ALA:H	1.80	0.47
1:E:132:GLY:HA2	1:E:135:TYR:CE1	2.50	0.47
1:B:219:LEU:HD11	1:B:394:LEU:HD21	1.97	0.47
1:E:368:LYS:HD3	1:E:369:TYR:CZ	2.50	0.47
1:F:49:ASN:ND2	1:F:51:ASN:H	2.12	0.47
1:B:355:GLU:HB3	1:B:377:LYS:CG	2.45	0.46
1:A:268:TRP:CZ2	1:A:380:VAL:HG22	2.51	0.46
1:B:283:ALA:HB2	1:B:373:TRP:HZ3	1.81	0.46
1:C:38:THR:HG21	1:C:41:GLU:HG3	1.97	0.46
1:B:357:TYR:CZ	1:B:377:LYS:HE3	2.50	0.46
1:D:71:ARG:NE	1:D:264:TYR:HE1	2.14	0.46
1:D:394:LEU:HG	1:D:399:LYS:HZ2	1.77	0.46
1:A:276:GLY:HA3	1:A:284:VAL:O	2.15	0.46
1:B:285:MET:HE2	1:B:378:ALA:HB1	1.98	0.46
1:A:260:ILE:HD11	1:A:346:GLY:HA2	1.98	0.46
1:B:92:ARG:HG3	1:B:239:TRP:CE2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:61:SER:O	1:C:65:LEU:HG	2.16	0.46
1:D:391:LYS:HD3	1:D:404:ILE:CG2	2.46	0.46
1:E:132:GLY:HA2	1:E:135:TYR:CZ	2.51	0.46
1:C:327:ARG:HA	1:C:382:TYR:CE1	2.51	0.46
1:D:351:GLN:CD	1:D:351:GLN:H	2.19	0.46
1:A:62:TYR:HH	1:A:84:THR:HG1	1.64	0.45
1:D:323:THR:HG23	1:D:325:ALA:N	2.31	0.45
1:B:127:GLU:CD	1:B:127:GLU:H	2.20	0.45
1:C:214:SER:O	1:C:391:LYS:CE	2.63	0.45
1:E:260:ILE:HG21	1:E:347:ILE:HG13	1.98	0.45
1:D:278:THR:CG2	1:D:280:ASP:H	2.23	0.45
1:C:83:PHE:HA	1:C:129:MET:SD	2.57	0.45
1:F:132:GLY:HA2	1:F:135:TYR:CE1	2.52	0.45
1:C:333:ASN:O	1:C:334:TYR:HB2	2.16	0.45
1:D:258:ASN:HD22	1:D:395:PRO:HG3	1.82	0.45
1:E:342:MET:HE1	1:E:373:TRP:NE1	2.31	0.45
1:A:62:TYR:OH	1:A:84:THR:OG1	2.35	0.45
1:D:127:GLU:CD	1:D:127:GLU:H	2.21	0.45
1:B:133:MET:HG3	1:B:134:MET:HE3	1.98	0.44
1:D:38:THR:HG23	1:D:358:MET:HE1	1.99	0.44
1:A:368:LYS:HG2	1:A:369:TYR:CE1	2.51	0.44
1:D:285:MET:O	1:D:319:GLN:HB2	2.16	0.44
1:D:345:TYR:CD1	1:D:345:TYR:O	2.70	0.44
1:E:342:MET:HE2	1:E:361:ASN:CB	2.47	0.44
1:F:129:MET:HE2	1:F:129:MET:HB2	1.86	0.44
1:F:130:ARG:H	1:F:133:MET:HE3	1.83	0.44
1:C:168:GLU:OE1	1:C:168:GLU:N	2.49	0.44
1:D:333:ASN:O	1:D:334:TYR:HB2	2.18	0.44
1:F:141:ASN:C	1:F:141:ASN:HD22	2.21	0.44
1:F:256:PHE:CZ	1:F:387:ILE:HG21	2.53	0.44
1:D:70:LEU:HD21	1:D:76:GLU:HA	1.99	0.44
1:F:130:ARG:H	1:F:133:MET:CE	2.31	0.44
1:F:271:ASP:HA	1:F:339:ASP:HB2	1.99	0.44
1:B:260:ILE:HG21	1:B:347:ILE:HG12	2.00	0.44
1:B:322:CYS:SG	1:B:381:ARG:HG2	2.57	0.44
1:D:71:ARG:NH2	1:D:264:TYR:HE1	2.16	0.44
1:D:238:ASN:HD21	1:D:242:GLY:N	1.98	0.44
1:E:92:ARG:HB2	1:E:239:TRP:CZ2	2.52	0.44
1:C:230:GLN:HB3	1:C:243:MET:CG	2.46	0.43
1:E:233:LEU:HD23	1:E:233:LEU:HA	1.86	0.43
1:F:217:VAL:HG13	1:F:391:LYS:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:337:THR:OG1	1:C:339:ASP:OD1	2.36	0.43
1:D:339:ASP:H	1:D:385:MET:CE	2.24	0.43
1:A:335:GLU:OE2	1:F:163:LYS:HD2	2.19	0.43
1:C:194:THR:HA	1:C:199:GLU:HA	1.99	0.43
1:E:46:SER:OG	1:E:48:LYS:HE3	2.18	0.43
1:D:359:VAL:HG23	1:D:373:TRP:HB2	1.99	0.43
1:C:356:TYR:C	1:C:377:LYS:NZ	2.71	0.43
1:F:302:TRP:HA	1:F:305:LEU:HD22	2.00	0.43
1:C:141:ASN:C	1:C:141:ASN:HD22	2.21	0.43
1:E:230:GLN:HA	1:E:244:SER:O	2.18	0.43
1:A:349:LYS:HA	1:A:354:ASN:O	2.18	0.43
1:D:316:PRO:HB3	1:D:350:ASP:OD2	2.19	0.43
1:B:241:HIS:CE1	1:C:241:HIS:NE2	2.86	0.42
1:B:285:MET:CE	1:B:382:TYR:HB2	2.46	0.42
1:D:284:VAL:CG2	1:D:319:GLN:HE22	2.27	0.42
1:B:129:MET:CE	1:B:189:PRO:HA	2.49	0.42
1:D:62:TYR:O	1:D:66:GLU:HG3	2.18	0.42
1:D:316:PRO:CG	1:D:351:GLN:HE22	2.31	0.42
1:A:233:LEU:HD23	1:A:233:LEU:HA	1.90	0.42
1:A:338:ASP:O	1:A:340:HIS:N	2.52	0.42
1:C:216:TYR:CE1	1:C:390:HIS:HB2	2.54	0.42
1:C:402:LEU:HA	1:C:402:LEU:HD22	1.78	0.42
1:E:342:MET:HE3	1:E:373:TRP:HE1	1.84	0.42
1:A:377:LYS:HB2	1:A:377:LYS:HE2	1.74	0.42
1:C:185:TYR:CD2	1:D:173:LEU:HD23	2.55	0.42
1:C:260:ILE:HD12	1:C:346:GLY:CA	2.49	0.42
1:B:285:MET:HE1	1:B:378:ALA:O	2.20	0.42
1:F:166:SER:HB3	1:F:172:MET:HE1	2.02	0.42
1:D:345:TYR:OH	1:D:372:ILE:CG1	2.67	0.42
1:B:179:ALA:O	1:B:183:GLN:HG3	2.19	0.42
1:D:269:GLY:HA2	1:D:340:HIS:O	2.20	0.42
1:F:129:MET:CE	1:F:189:PRO:HA	2.50	0.42
1:D:78:ASP:CG	1:D:126:GLU:HG3	2.41	0.41
1:B:350:ASP:OD2	1:B:354:ASN:HB2	2.21	0.41
1:B:361:ASN:HD22	1:B:362:SER:N	2.13	0.41
1:B:361:ASN:HB3	4:B:640:HOH:O	2.20	0.41
1:C:63:SER:C	1:C:343:GLN:HE21	2.04	0.41
1:C:356:TYR:HA	1:C:376:SER:HA	2.02	0.41
1:D:272:VAL:HB	1:D:277:PHE:CD2	2.55	0.41
1:B:357:TYR:HD2	1:B:380:VAL:HG21	1.85	0.41
1:C:229:THR:HG22	1:C:230:GLN:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:71:ARG:CZ	1:D:264:TYR:CE1	2.95	0.41
1:B:351:GLN:HG2	1:B:352:GLU:HG3	2.02	0.41
1:C:260:ILE:HG23	1:C:346:GLY:HA2	2.01	0.41
1:E:285:MET:H	1:E:319:GLN:NE2	2.13	0.41
1:C:358:MET:HB2	1:C:358:MET:HE2	1.80	0.41
1:C:390:HIS:CD2	1:C:392:ASP:H	2.32	0.41
1:D:344:ILE:HD11	1:D:357:TYR:CB	2.48	0.41
1:B:97:VAL:HG21	1:B:174:TRP:CH2	2.55	0.41
1:C:80:SER:HB2	1:C:126:GLU:HA	2.02	0.41
1:D:92:ARG:HG3	1:D:239:TRP:NE1	2.36	0.41
1:D:276:GLY:HA3	1:D:284:VAL:O	2.20	0.41
1:C:99:THR:HB	1:C:102:ASP:HB2	2.03	0.41
1:C:344:ILE:HG13	1:C:357:TYR:HB3	2.03	0.41
1:E:100:HIS:HD2	4:E:663:HOH:O	2.03	0.41
1:E:286:PRO:HB2	1:E:288:ASP:O	2.20	0.41
1:E:72:MET:HE1	1:E:211:LEU:HD23	2.02	0.40
1:F:130:ARG:HB2	1:F:133:MET:HE3	2.02	0.40
1:C:270:SER:OG	1:C:271:ASP:N	2.54	0.40
1:D:317:GLN:HB3	1:D:318:PRO:HD2	2.02	0.40
1:F:189:PRO:HA	1:F:190:PRO:HD3	1.95	0.40
1:F:219:LEU:HD23	1:F:245:TYR:HB2	2.01	0.40
1:A:357:TYR:OH	1:A:377:LYS:HD3	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	360/401 (90%)	342 (95%)	16 (4%)	2 (1%)	25 27
1	B	341/401 (85%)	333 (98%)	8 (2%)	0	100 100
1	C	348/401 (87%)	338 (97%)	10 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	359/401 (90%)	347 (97%)	12 (3%)	0	100	100
1	E	345/401 (86%)	336 (97%)	9 (3%)	0	100	100
1	F	373/401 (93%)	367 (98%)	6 (2%)	0	100	100
All	All	2126/2406 (88%)	2063 (97%)	61 (3%)	2 (0%)	100	63

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	339[A]	ASP
1	A	339[B]	ASP

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	288/346 (83%)	283 (98%)	5 (2%)	60	72
1	B	284/346 (82%)	282 (99%)	2 (1%)	84	91
1	C	274/346 (79%)	266 (97%)	8 (3%)	42	52
1	D	278/346 (80%)	268 (96%)	10 (4%)	35	43
1	E	284/346 (82%)	282 (99%)	2 (1%)	84	91
1	F	306/346 (88%)	300 (98%)	6 (2%)	55	66
All	All	1714/2076 (83%)	1681 (98%)	33 (2%)	57	68

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	VAL
1	A	141	ASN
1	A	275	SER
1	A	321	TRP
1	A	385	MET
1	B	327	ARG

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Mol	Chain	Res	Type
1	B	361	ASN
1	C	63	SER
1	C	74	LYS
1	C	84	THR
1	C	118	MET
1	C	141	ASN
1	C	344	ILE
1	C	381	ARG
1	C	382	TYR
1	D	190	PRO
1	D	208	SER
1	D	265	THR
1	D	280	ASP
1	D	338	ASP
1	D	344	ILE
1	D	351	GLN
1	D	367	SER
1	D	394	LEU
1	D	399	LYS
1	E	49	ASN
1	E	141	ASN
1	F	49	ASN
1	F	74	LYS
1	F	137	ASP
1	F	141	ASN
1	F	288	ASP
1	F	382	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	141	ASN
1	A	170	ASN
1	A	343	GLN
1	B	107	GLN
1	B	183	GLN
1	B	241	HIS
1	B	361	ASN
1	C	42	ASN
1	C	141	ASN
1	C	182	HIS
1	C	183	GLN

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Mol	Chain	Res	Type
1	C	343	GLN
1	C	390	HIS
1	D	238	ASN
1	D	343	GLN
1	E	42	ASN
1	E	49	ASN
1	E	51	ASN
1	E	107	GLN
1	E	141	ASN
1	E	236	GLN
1	E	319	GLN
1	E	366	ASN
1	F	42	ASN
1	F	49	ASN
1	F	141	ASN
1	F	319	GLN
1	F	324	GLN
1	F	370	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 17 ligands modelled in this entry, 11 are monoatomic - leaving 6 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	$\#\|Z\| > 2$
3	T1O	A	503	1	21,21,21	6.38	13 (61%)	27,28,28	3.05	11 (40%)
3	T1O	B	502	1	21,21,21	6.28	13 (61%)	27,28,28	3.57	15 (55%)
3	T1O	F	503	1	21,21,21	6.37	13 (61%)	27,28,28	2.94	10 (37%)
3	T1O	C	503	1	21,21,21	6.29	12 (57%)	27,28,28	3.17	11 (40%)
3	T1O	E	503	1	21,21,21	6.28	13 (61%)	27,28,28	3.82	14 (51%)
3	T1O	D	503	1	21,21,21	6.35	12 (57%)	27,28,28	2.84	13 (48%)

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	T1O	A	503	1	-	9/12/33/33	0/2/2/2
3	T1O	B	502	1	-	6/12/33/33	0/2/2/2
3	T1O	F	503	1	-	8/12/33/33	0/2/2/2
3	T1O	C	503	1	-	7/12/33/33	0/2/2/2
3	T1O	E	503	1	-	7/12/33/33	0/2/2/2
3	T1O	D	503	1	-	6/12/33/33	0/2/2/2

All (76) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	503	T1O	C02-N08	15.57	1.61	1.35
3	D	503	T1O	C02-N08	15.48	1.61	1.35
3	C	503	T1O	C02-N08	15.44	1.61	1.35
3	A	503	T1O	C02-N08	15.40	1.60	1.35
3	F	503	T1O	C02-N08	15.23	1.60	1.35
3	B	502	T1O	C02-N08	15.20	1.60	1.35
3	E	503	T1O	C05-N08	-12.10	1.27	1.46
3	A	503	T1O	C05-N08	-11.99	1.27	1.46
3	B	502	T1O	C05-N08	-11.97	1.27	1.46
3	D	503	T1O	C05-N08	-11.93	1.27	1.46
3	C	503	T1O	C05-N08	-11.91	1.27	1.46
3	F	503	T1O	C05-N08	-11.78	1.28	1.46
3	B	502	T1O	C06-S07	-11.59	1.47	1.81
3	C	503	T1O	C06-S07	-11.54	1.47	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	503	T1O	C06-S07	-11.51	1.47	1.81
3	D	503	T1O	C06-S07	-11.49	1.47	1.81
3	A	503	T1O	C06-S07	-11.47	1.47	1.81
3	F	503	T1O	C06-S07	-11.47	1.47	1.81
3	D	503	T1O	C02-N03	9.57	1.51	1.35
3	F	503	T1O	C02-N03	9.49	1.51	1.35
3	C	503	T1O	C02-N03	9.11	1.50	1.35
3	B	502	T1O	C02-N03	9.10	1.50	1.35
3	F	503	T1O	C06-C05	8.99	1.69	1.53
3	B	502	T1O	C06-C05	8.97	1.69	1.53
3	D	503	T1O	C06-C05	8.96	1.69	1.53
3	A	503	T1O	C02-N03	8.92	1.50	1.35
3	A	503	T1O	C06-C05	8.87	1.69	1.53
3	C	503	T1O	C06-C05	8.85	1.69	1.53
3	E	503	T1O	C06-C05	8.71	1.68	1.53
3	E	503	T1O	C02-N03	8.59	1.49	1.35
3	F	503	T1O	C14-N15	7.44	1.50	1.33
3	A	503	T1O	C14-N15	7.14	1.49	1.33
3	D	503	T1O	C14-N15	6.50	1.48	1.33
3	E	503	T1O	C04-N03	-6.37	1.34	1.45
3	A	503	T1O	C04-N03	-6.35	1.34	1.45
3	C	503	T1O	C14-N15	6.35	1.47	1.33
3	B	502	T1O	C04-N03	-6.25	1.34	1.45
3	D	503	T1O	C04-N03	-6.16	1.34	1.45
3	F	503	T1O	C04-N03	-6.11	1.35	1.45
3	C	503	T1O	C04-N03	-6.10	1.35	1.45
3	B	502	T1O	C14-N15	5.97	1.47	1.33
3	E	503	T1O	C14-N15	5.85	1.46	1.33
3	D	503	T1O	C05-C04	5.01	1.69	1.55
3	F	503	T1O	C05-C04	4.97	1.69	1.55
3	C	503	T1O	C05-C04	4.90	1.69	1.55
3	A	503	T1O	C05-C04	4.88	1.69	1.55
3	B	502	T1O	C05-C04	4.69	1.68	1.55
3	E	503	T1O	C05-C04	4.64	1.68	1.55
3	D	503	T1O	C09-S07	-3.96	1.76	1.82
3	A	503	T1O	C09-S07	-3.95	1.76	1.82
3	F	503	T1O	C09-S07	-3.85	1.76	1.82
3	C	503	T1O	C09-S07	-3.82	1.76	1.82
3	B	502	T1O	C09-S07	-3.79	1.76	1.82
3	E	503	T1O	C09-S07	-3.76	1.76	1.82
3	B	502	T1O	C09-C04	-3.58	1.45	1.53
3	E	503	T1O	C09-C04	-3.47	1.46	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	503	T1O	C10-C09	3.35	1.60	1.52
3	D	503	T1O	C10-C09	3.32	1.60	1.52
3	C	503	T1O	C09-C04	-3.19	1.46	1.53
3	A	503	T1O	C16-C17	3.11	1.56	1.51
3	A	503	T1O	C09-C04	-3.10	1.46	1.53
3	C	503	T1O	C10-C09	3.05	1.59	1.52
3	F	503	T1O	C10-C09	3.05	1.59	1.52
3	F	503	T1O	C09-C04	-3.04	1.47	1.53
3	E	503	T1O	C10-C09	3.03	1.59	1.52
3	D	503	T1O	C09-C04	-3.00	1.47	1.53
3	F	503	T1O	C13-C14	2.89	1.56	1.51
3	F	503	T1O	C16-C17	2.83	1.55	1.51
3	B	502	T1O	C10-C09	2.76	1.59	1.52
3	A	503	T1O	C13-C14	2.72	1.56	1.51
3	E	503	T1O	C16-C17	2.70	1.55	1.51
3	B	502	T1O	C16-C17	2.69	1.55	1.51
3	E	503	T1O	O20-C14	-2.49	1.18	1.23
3	B	502	T1O	O20-C14	-2.46	1.18	1.23
3	D	503	T1O	C13-C14	2.29	1.55	1.51
3	C	503	T1O	C16-C17	2.27	1.55	1.51

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	503	T1O	C09-C04-N03	-9.77	104.37	113.13
3	E	503	T1O	C06-S07-C09	9.08	108.53	89.89
3	C	503	T1O	C06-S07-C09	8.78	107.93	89.89
3	F	503	T1O	C06-S07-C09	8.58	107.52	89.89
3	B	502	T1O	C06-S07-C09	7.97	106.27	89.89
3	A	503	T1O	C06-S07-C09	7.88	106.07	89.89
3	B	502	T1O	C09-C04-N03	-7.23	106.65	113.13
3	D	503	T1O	C06-S07-C09	6.86	103.98	89.89
3	E	503	T1O	C05-C04-N03	6.39	109.54	102.67
3	A	503	T1O	C09-C04-N03	-6.36	107.43	113.13
3	E	503	T1O	C04-N03-C02	-6.03	107.00	112.62
3	C	503	T1O	C04-N03-C02	-5.79	107.22	112.62
3	D	503	T1O	C04-C05-N08	5.75	108.54	102.43
3	B	502	T1O	C05-C04-N03	5.72	108.82	102.67
3	C	503	T1O	C05-C04-N03	5.64	108.73	102.67
3	A	503	T1O	C04-N03-C02	-5.58	107.42	112.62
3	B	502	T1O	C04-N03-C02	-5.54	107.46	112.62
3	A	503	T1O	C05-C04-N03	5.50	108.59	102.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	503	T1O	C04-C05-N08	5.50	108.28	102.43
3	A	503	T1O	C04-C05-N08	5.31	108.07	102.43
3	F	503	T1O	C04-N03-C02	-5.28	107.70	112.62
3	C	503	T1O	C04-C05-N08	5.21	107.97	102.43
3	F	503	T1O	C05-C04-N03	5.13	108.19	102.67
3	D	503	T1O	C04-N03-C02	-5.12	107.85	112.62
3	B	502	T1O	C13-C14-N15	5.02	124.88	116.42
3	D	503	T1O	C05-C04-N03	5.00	108.04	102.67
3	B	502	T1O	C04-C09-S07	4.90	109.87	105.20
3	B	502	T1O	C04-C05-N08	4.88	107.62	102.43
3	E	503	T1O	C18-C17-C16	4.68	122.60	115.34
3	E	503	T1O	C04-C09-S07	4.50	109.49	105.20
3	E	503	T1O	C04-C05-N08	4.41	107.11	102.43
3	C	503	T1O	C09-C04-N03	-4.39	109.20	113.13
3	B	502	T1O	C18-C17-C16	4.24	121.92	115.34
3	E	503	T1O	O19-C17-C16	-4.17	118.32	121.35
3	C	503	T1O	C04-C09-S07	4.10	109.11	105.20
3	F	503	T1O	C09-C04-N03	-4.09	109.47	113.13
3	B	502	T1O	C12-C13-C14	-4.01	102.00	113.26
3	C	503	T1O	C18-C17-C16	3.93	121.44	115.34
3	E	503	T1O	C13-C14-N15	3.77	122.76	116.42
3	A	503	T1O	C18-C17-C16	3.70	121.08	115.34
3	A	503	T1O	C05-N08-C02	-3.54	107.85	112.46
3	D	503	T1O	C05-N08-C02	-3.48	107.93	112.46
3	D	503	T1O	C13-C14-N15	3.42	122.18	116.42
3	C	503	T1O	C05-N08-C02	-3.41	108.01	112.46
3	F	503	T1O	C05-N08-C02	-3.36	108.08	112.46
3	B	502	T1O	C09-C04-C05	-3.35	105.05	108.94
3	F	503	T1O	C04-C09-S07	3.31	108.36	105.20
3	D	503	T1O	C06-C05-C04	-3.18	105.90	108.66
3	E	503	T1O	C12-C13-C14	-3.14	104.44	113.26
3	D	503	T1O	C09-C04-C05	-3.13	105.31	108.94
3	D	503	T1O	C05-C06-S07	-3.10	103.65	106.31
3	C	503	T1O	O19-C17-C16	-3.02	119.16	121.35
3	E	503	T1O	C05-N08-C02	-3.02	108.53	112.46
3	B	502	T1O	C05-N08-C02	-2.99	108.56	112.46
3	D	503	T1O	C09-C04-N03	-2.99	110.45	113.13
3	D	503	T1O	C18-C17-C16	2.86	119.78	115.34
3	F	503	T1O	C18-C17-C16	2.84	119.75	115.34
3	A	503	T1O	C09-C04-C05	-2.78	105.71	108.94
3	B	502	T1O	O20-C14-C13	-2.78	116.94	122.02
3	B	502	T1O	C11-C10-C09	-2.75	108.28	113.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	502	T1O	O20-C14-N15	-2.58	118.15	123.01
3	F	503	T1O	C13-C14-N15	2.54	120.69	116.42
3	C	503	T1O	C12-C13-C14	-2.50	106.25	113.26
3	E	503	T1O	C09-C04-C05	-2.47	106.07	108.94
3	E	503	T1O	O20-C14-N15	-2.44	118.40	123.01
3	E	503	T1O	C10-C09-C04	-2.29	108.06	114.73
3	D	503	T1O	O19-C17-C16	-2.22	119.73	121.35
3	D	503	T1O	O20-C14-N15	-2.21	118.85	123.01
3	A	503	T1O	C04-C09-S07	2.18	107.28	105.20
3	A	503	T1O	C06-C05-C04	-2.15	106.79	108.66
3	A	503	T1O	C13-C14-N15	2.15	120.04	116.42
3	C	503	T1O	C13-C14-N15	2.07	119.90	116.42
3	F	503	T1O	C06-C05-C04	-2.06	106.88	108.66
3	B	502	T1O	C10-C09-C04	-2.03	108.83	114.73

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	503	T1O	C04-C09-C10-C11
3	A	503	T1O	S07-C09-C10-C11
3	A	503	T1O	C09-C10-C11-C12
3	A	503	T1O	C17-C16-N15-C14
3	A	503	T1O	N15-C16-C17-C18
3	B	502	T1O	N15-C16-C17-C18
3	B	502	T1O	N15-C16-C17-O19
3	C	503	T1O	N15-C16-C17-C18
3	C	503	T1O	N15-C16-C17-O19
3	D	503	T1O	C04-C09-C10-C11
3	D	503	T1O	S07-C09-C10-C11
3	E	503	T1O	N15-C16-C17-C18
3	E	503	T1O	N15-C16-C17-O19
3	F	503	T1O	C04-C09-C10-C11
3	F	503	T1O	S07-C09-C10-C11
3	F	503	T1O	N15-C16-C17-C18
3	B	502	T1O	C13-C14-N15-C16
3	C	503	T1O	C13-C14-N15-C16
3	D	503	T1O	C13-C14-N15-C16
3	E	503	T1O	C13-C14-N15-C16
3	E	503	T1O	C11-C12-C13-C14
3	F	503	T1O	C11-C12-C13-C14
3	B	502	T1O	O20-C14-N15-C16

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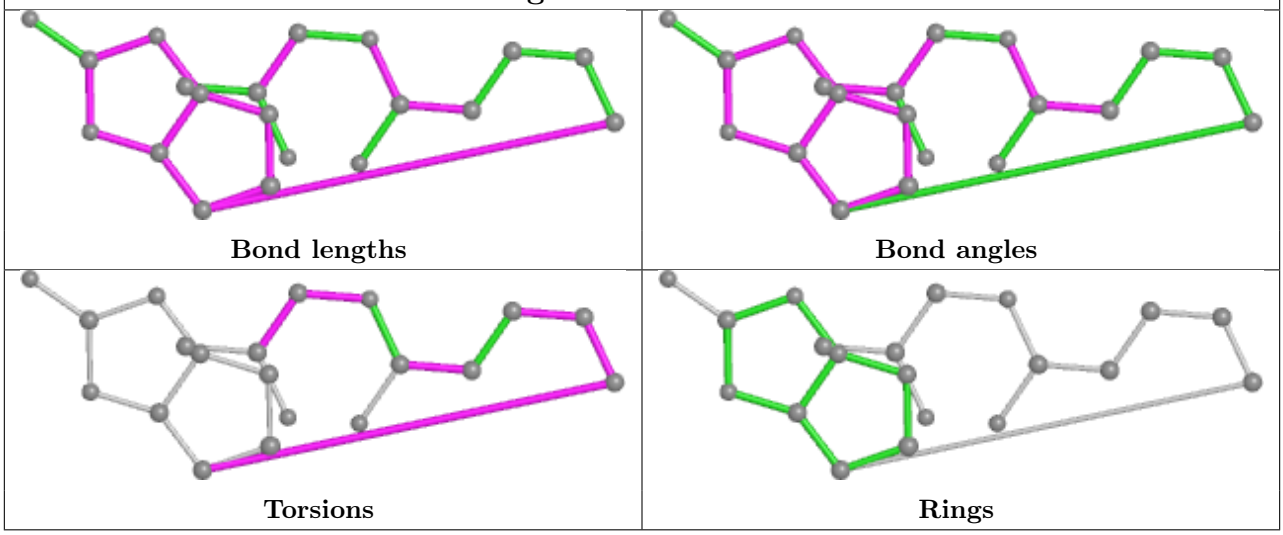
Mol	Chain	Res	Type	Atoms
3	C	503	T1O	O20-C14-N15-C16
3	D	503	T1O	O20-C14-N15-C16
3	E	503	T1O	O20-C14-N15-C16
3	C	503	T1O	C11-C12-C13-C14
3	F	503	T1O	C12-C13-C14-O20
3	F	503	T1O	C12-C13-C14-N15
3	A	503	T1O	C12-C13-C14-O20
3	C	503	T1O	C09-C10-C11-C12
3	E	503	T1O	C09-C10-C11-C12
3	A	503	T1O	C10-C11-C12-C13
3	A	503	T1O	C12-C13-C14-N15
3	B	502	T1O	C10-C11-C12-C13
3	E	503	T1O	C10-C11-C12-C13
3	C	503	T1O	C10-C11-C12-C13
3	D	503	T1O	N15-C16-C17-O19
3	D	503	T1O	C09-C10-C11-C12
3	F	503	T1O	C10-C11-C12-C13
3	B	502	T1O	C09-C10-C11-C12
3	F	503	T1O	C09-C10-C11-C12
3	A	503	T1O	N15-C16-C17-O19

There are no ring outliers.

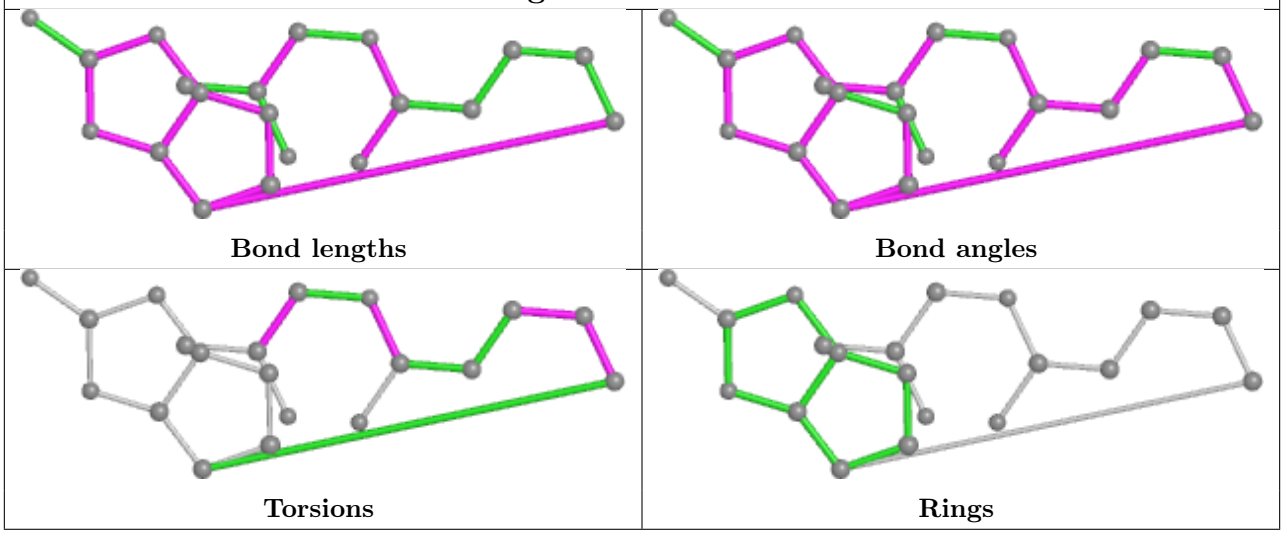
No monomer is involved in short contacts.

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.

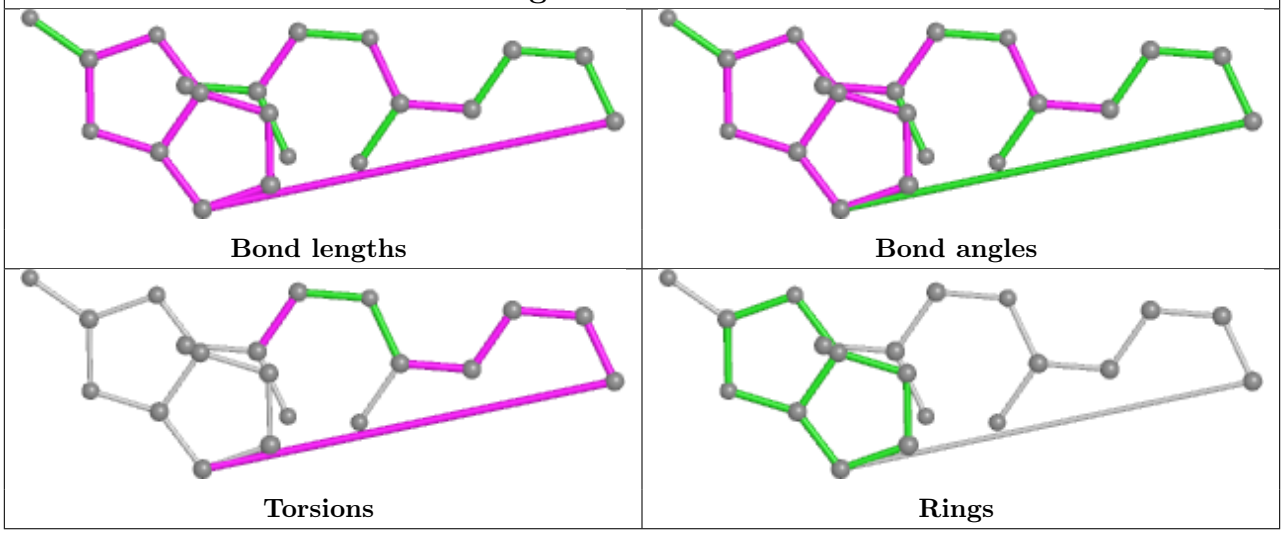
Ligand T1O A 503



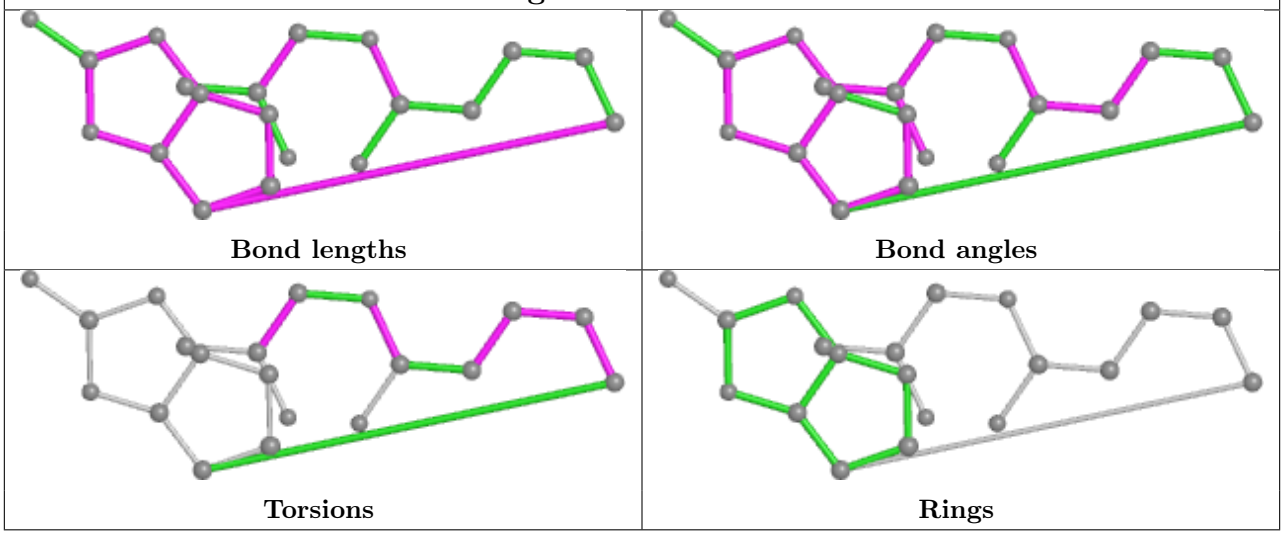
Ligand T1O B 502



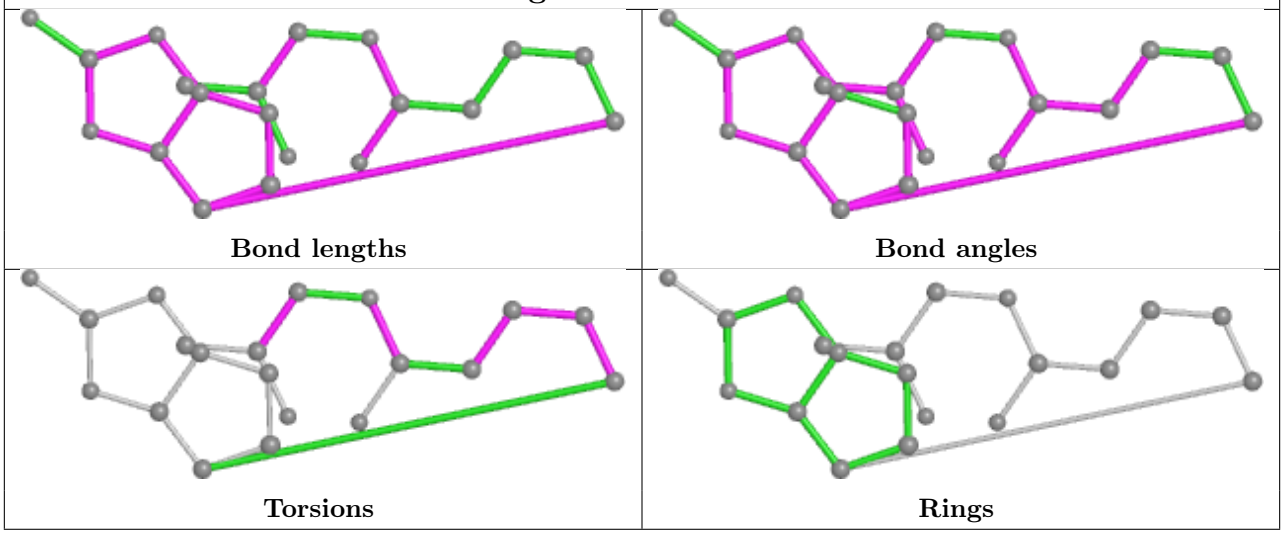
Ligand T1O F 503



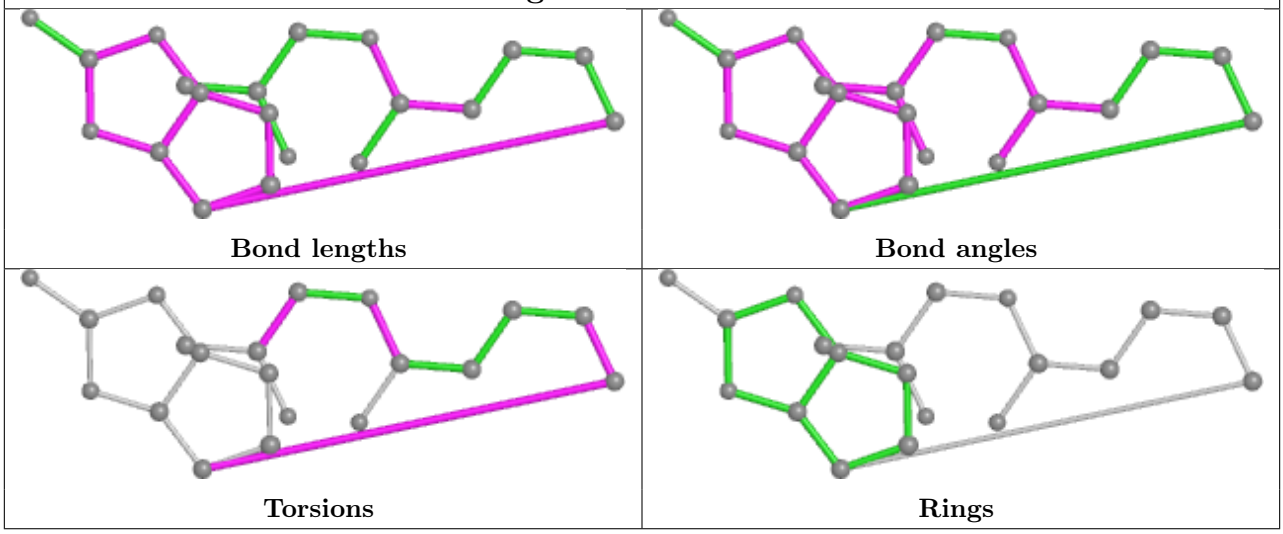
Ligand T1O C 503



Ligand T1O E 503



Ligand T1O D 503



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	363/401 (90%)	0.14	22 (6%)	21	31	33, 60, 99, 147	0
1	B	345/401 (86%)	-0.08	5 (1%)	75	83	36, 56, 81, 116	0
1	C	352/401 (87%)	0.37	26 (7%)	14	22	42, 78, 107, 151	0
1	D	363/401 (90%)	0.54	38 (10%)	6	9	37, 72, 112, 148	0
1	E	349/401 (87%)	-0.15	6 (1%)	70	78	33, 44, 77, 125	0
1	F	374/401 (93%)	0.04	11 (2%)	51	62	30, 42, 85, 146	0
All	All	2146/2406 (89%)	0.14	108 (5%)	28	41	30, 56, 103, 151	0

All (108) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	286	PRO	7.8
1	A	276	GLY	7.0
1	C	312	LEU	6.7
1	F	300	ALA	6.0
1	D	286	PRO	6.0
1	D	291	VAL	5.9
1	A	299	MET	5.8
1	F	304	LYS	5.7
1	D	36	PHE	5.4
1	C	245	TYR	5.3
1	F	305	LEU	5.3
1	A	318	PRO	4.9
1	D	314	THR	4.8
1	D	312	LEU	4.6
1	D	275	SER	4.5
1	C	378	ALA	4.4
1	D	292	GLN	4.4
1	D	375	ALA	4.4
1	D	295	SER	4.3

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Mol	Chain	Res	Type	RSRZ
1	D	34	PHE	4.2
1	A	312	LEU	4.2
1	D	374	TYR	4.1
1	C	398	ILE	4.0
1	C	288	ASP	3.9
1	D	296	GLY	3.9
1	A	295	SER	3.9
1	D	283	ALA	3.9
1	C	286	PRO	3.9
1	B	280	ASP	3.7
1	C	210	GLY	3.7
1	C	70	LEU	3.7
1	D	354	ASN	3.6
1	D	277	PHE	3.6
1	A	291	VAL	3.6
1	F	302	TRP	3.6
1	E	287	ASP	3.5
1	C	256	PHE	3.4
1	D	318	PRO	3.4
1	A	296	GLY	3.4
1	C	276	GLY	3.4
1	D	282	VAL	3.3
1	A	298	ASP	3.2
1	D	348	ALA	3.2
1	A	279	ARG	3.2
1	D	284	VAL	3.1
1	F	299	MET	3.1
1	B	314	THR	3.1
1	B	373	TRP	3.1
1	D	287	ASP	3.1
1	D	313	ASN	3.0
1	A	290	LYS	3.0
1	A	313	ASN	3.0
1	D	356	TYR	3.0
1	C	275	SER	2.9
1	D	276	GLY	2.9
1	D	35	VAL	2.9
1	D	197	GLY	2.9
1	C	35	VAL	2.9
1	B	321	TRP	2.9
1	D	319	GLN	2.9
1	C	125	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	37	THR	2.8
1	C	313	ASN	2.8
1	E	317	GLN	2.7
1	D	196	LYS	2.6
1	D	200	TYR	2.6
1	D	249	LEU	2.6
1	C	284	VAL	2.6
1	C	366	ASN	2.6
1	A	294	LEU	2.6
1	D	382	TYR	2.6
1	A	297	SER	2.5
1	A	286	PRO	2.5
1	D	345	TYR	2.5
1	D	278	THR	2.5
1	F	294	LEU	2.5
1	D	310	LYS	2.5
1	D	373	TRP	2.5
1	A	75	GLY	2.5
1	F	296	GLY	2.4
1	C	76	GLU	2.4
1	C	287	ASP	2.4
1	D	311	LYS	2.4
1	A	275	SER	2.4
1	A	314	THR	2.3
1	C	64	PHE	2.3
1	C	37	THR	2.3
1	B	277	PHE	2.3
1	C	209	THR	2.3
1	A	33	GLY	2.3
1	A	34	PHE	2.3
1	E	277	PHE	2.3
1	E	318	PRO	2.3
1	A	317	GLN	2.3
1	E	373	TRP	2.2
1	F	307	PRO	2.2
1	C	345	TYR	2.2
1	F	303	LEU	2.2
1	D	288	ASP	2.2
1	C	279	ARG	2.1
1	F	306	LYS	2.1
1	F	309	GLU	2.1
1	D	279	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	282	VAL	2.1
1	A	139	LEU	2.1
1	A	293	GLU	2.1
1	C	397	ALA	2.1
1	C	315	LYS	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)

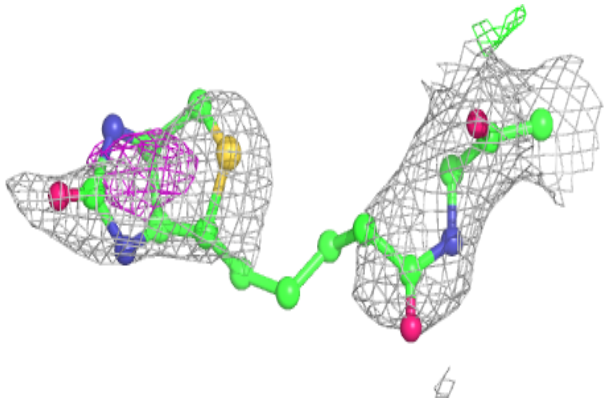
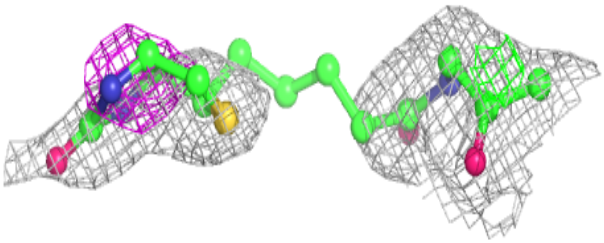
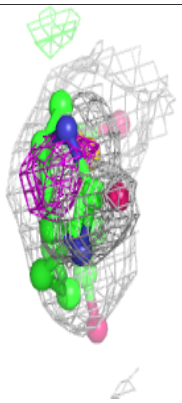
There are no monosaccharides in this entry.

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.

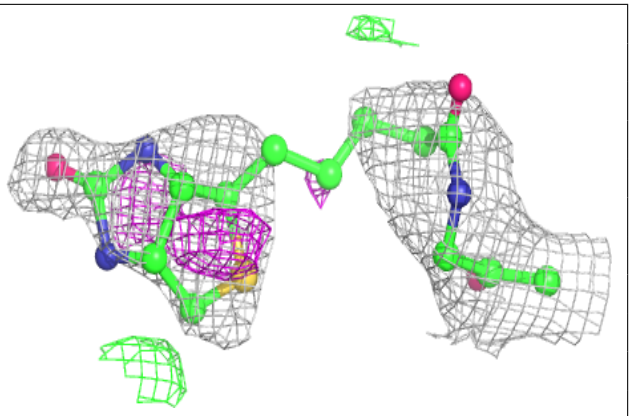
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	K	C	501	1/1	0.21	0.11	116,116,116,116	0
2	K	E	502	1/1	0.64	0.14	116,116,116,116	0
3	T1O	C	503	20/20	0.79	0.32	54,100,109,110	0
3	T1O	D	503	20/20	0.79	0.28	51,100,118,122	0
2	K	D	501	1/1	0.82	0.23	100,100,100,100	0
2	K	D	502	1/1	0.83	0.12	123,123,123,123	0
3	T1O	A	503	20/20	0.88	0.33	47,91,104,109	0
3	T1O	B	502	20/20	0.88	0.26	39,82,92,93	0
2	K	C	502	1/1	0.89	0.16	83,83,83,83	0
2	K	A	501	1/1	0.89	0.15	94,94,94,94	0
3	T1O	F	503	20/20	0.89	0.28	39,82,106,106	0
2	K	F	501	1/1	0.91	0.17	67,67,67,67	0
3	T1O	E	503	20/20	0.92	0.14	38,67,77,78	0
2	K	A	502	1/1	0.93	0.10	58,58,58,58	0
2	K	B	501	1/1	0.98	0.16	56,56,56,56	0
2	K	E	501	1/1	0.98	0.16	41,41,41,41	0
2	K	F	502	1/1	0.99	0.16	45,45,45,45	0

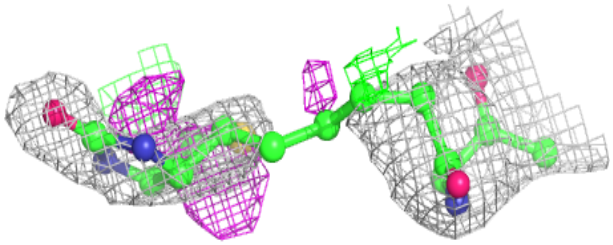
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

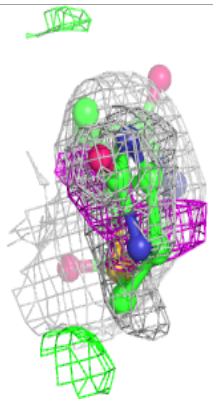
Electron density around T1O C 503: $2mF_o$-DF_c (at 0.7 rmsd) in gray mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)	
	

Electron density around T1O D 503:

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

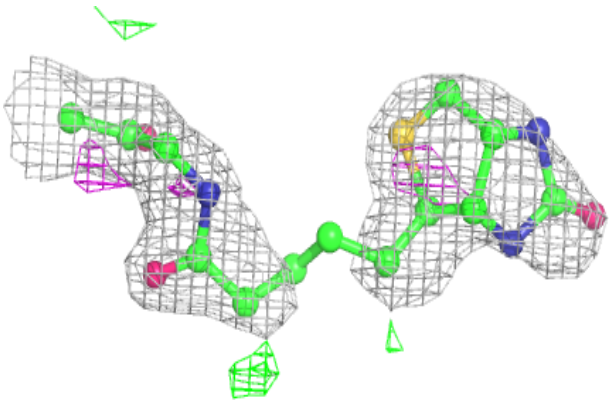


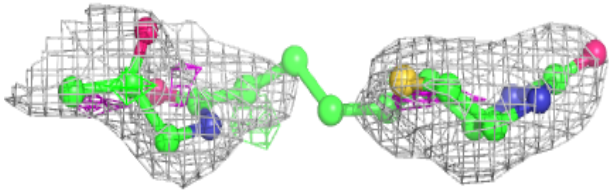


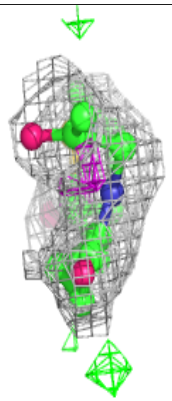


Electron density around T1O A 503:

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

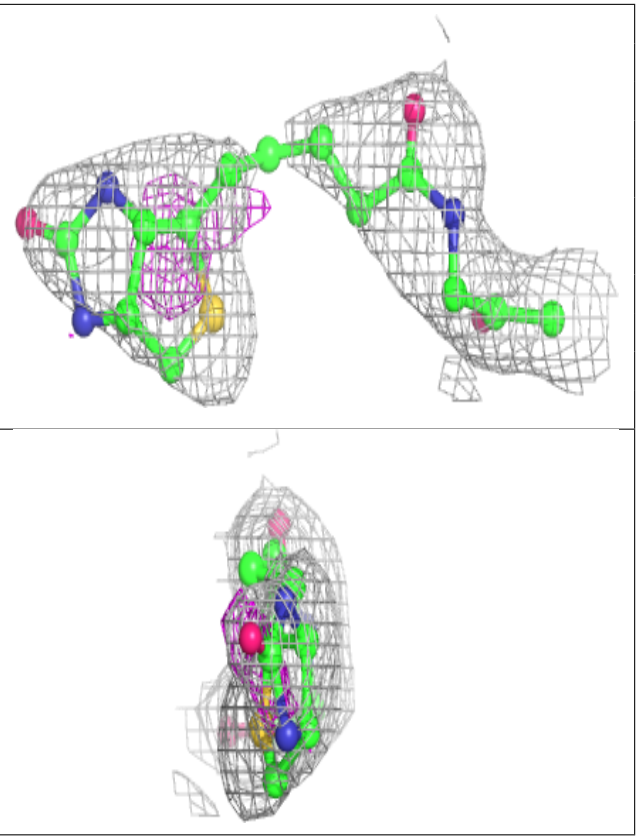






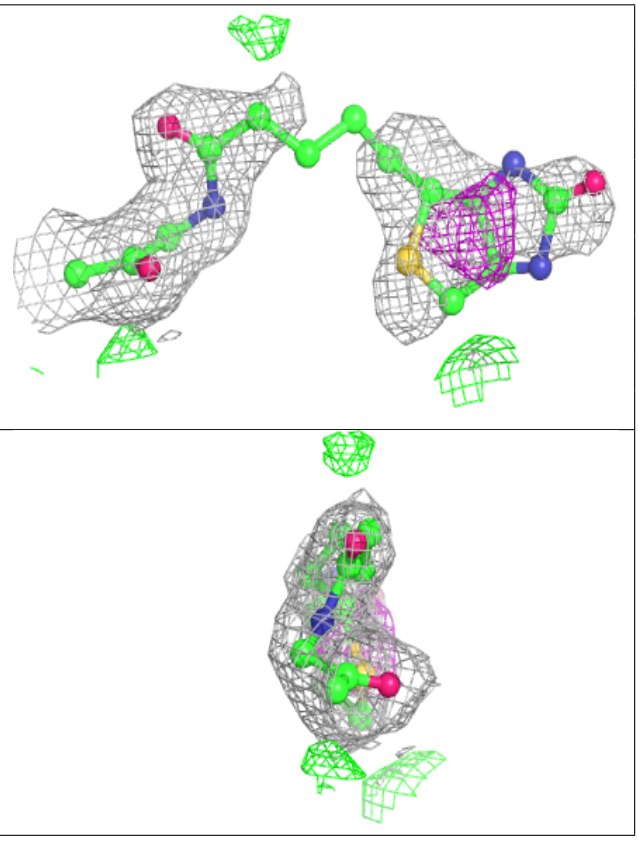
Electron density around T1O B 502:

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



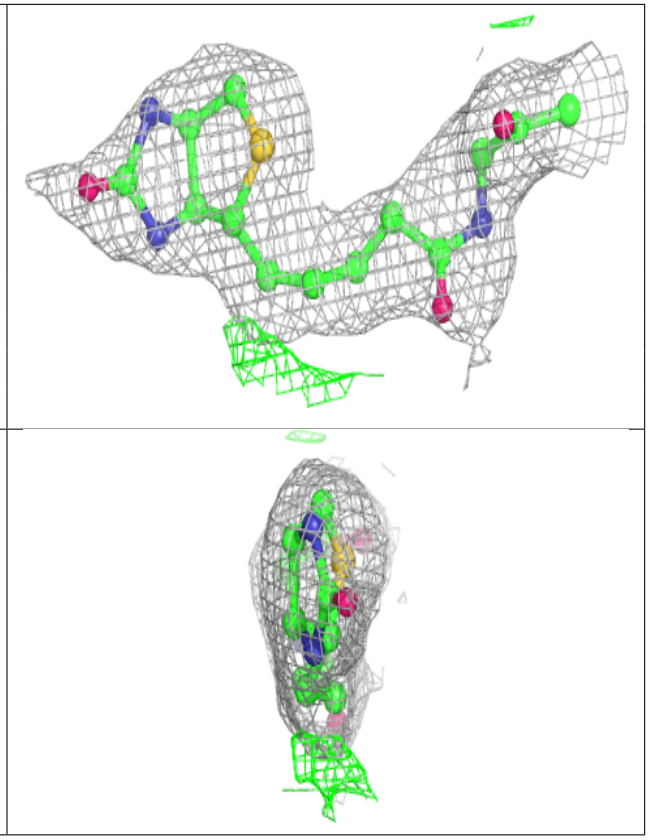
Electron density around T1O F 503:

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



Electron density around T1O E 503:

$2mF_o$-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.