Full wwPDB X-ray Structure Validation Report (i)

Aug 26, 2023 – 11:02 PM EDT

PDB ID	:	3G42
Title	:	Crystal Structure of TACE with Tryptophan Sulfonamide Derivative Inhibitor
Authors	:	Xu, W.; Park, K.; Gopalsamy, A.; Aplasca, A.; Zhang, Y.H.; Levin, J.I.
Deposited on	:	2009-02-03
Resolution	:	2.10 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:

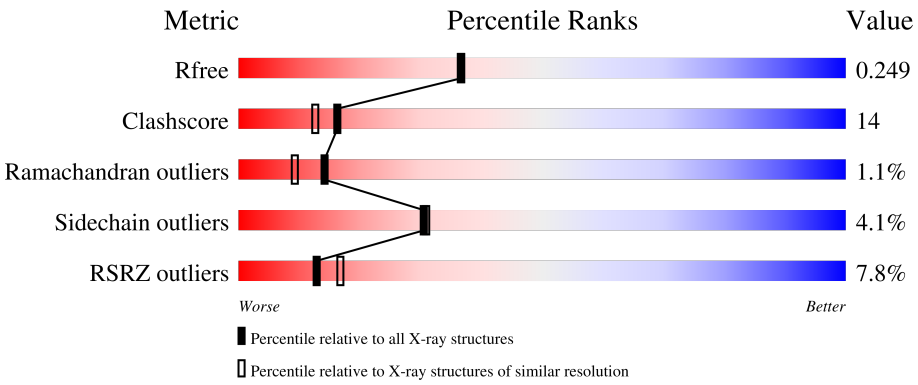
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 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 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	288	7%, 67%, 19%, •, 12%
1	B	288	11%, 62%, 24%, •, 12%
1	C	288	4%, 69%, 18%, •, 11%
1	D	288	5%, 66%, 18%, •, 12%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 8642 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 ADAM 17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	254	2016	1268	341	394	13	0	0	0
1	B	254	2016	1268	341	394	13	0	0	0
1	C	256	2031	1277	343	398	13	0	0	0
1	D	254	2017	1270	341	393	13	0	0	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	266	ALA	SER	engineered mutation	UNP P78536
A	452	GLN	ASN	acetylation	UNP P78536
A	493	SER	-	expression tag	UNP P78536
A	494	HIS	-	expression tag	UNP P78536
A	495	HIS	-	expression tag	UNP P78536
A	496	HIS	-	expression tag	UNP P78536
A	497	HIS	-	expression tag	UNP P78536
A	498	HIS	-	expression tag	UNP P78536
A	499	HIS	-	expression tag	UNP P78536
B	266	ALA	SER	engineered mutation	UNP P78536
B	452	GLN	ASN	engineered mutation	UNP P78536
B	493	SER	-	expression tag	UNP P78536
B	494	HIS	-	expression tag	UNP P78536
B	495	HIS	-	expression tag	UNP P78536
B	496	HIS	-	expression tag	UNP P78536
B	497	HIS	-	expression tag	UNP P78536
B	498	HIS	-	expression tag	UNP P78536
B	499	HIS	-	expression tag	UNP P78536
C	266	ALA	SER	engineered mutation	UNP P78536
C	452	GLN	ASN	engineered mutation	UNP P78536
C	493	SER	-	expression tag	UNP P78536

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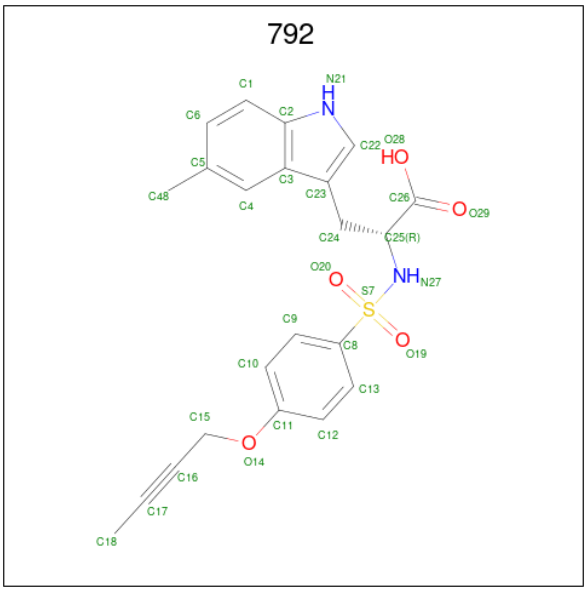
Chain	Residue	Modelled	Actual	Comment	Reference
C	494	HIS	-	expression tag	UNP P78536
C	495	HIS	-	expression tag	UNP P78536
C	496	HIS	-	expression tag	UNP P78536
C	497	HIS	-	expression tag	UNP P78536
C	498	HIS	-	expression tag	UNP P78536
C	499	HIS	-	expression tag	UNP P78536
D	266	ALA	SER	engineered mutation	UNP P78536
D	452	GLN	ASN	engineered mutation	UNP P78536
D	493	SER	-	expression tag	UNP P78536
D	494	HIS	-	expression tag	UNP P78536
D	495	HIS	-	expression tag	UNP P78536
D	496	HIS	-	expression tag	UNP P78536
D	497	HIS	-	expression tag	UNP P78536
D	498	HIS	-	expression tag	UNP P78536
D	499	HIS	-	expression tag	UNP P78536

- Molecule 2 is N-{[4-(but-2-yn-1-yloxy)phenyl]sulfonyl}-5-methyl-D-tryptophan (three-letter code: 792) (formula: $C_{22}H_{22}N_2O_5S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
2	A	1	29	21	2	5	1	0	0
			Total	C	N	O	S		
2	B	1	30	22	2	5	1	0	0
			Total	C	N	O	S		
2	C	1	30	22	2	5	1	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
2	D	1	30	22	2	5	1	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
3	A	1	1	1	0	0
			Total	Zn		
3	B	1	1	1	0	0
			Total	Zn		
3	C	1	1	1	0	0
			Total	Zn		
3	D	1	1	1	0	0

- Molecule 4 is water.

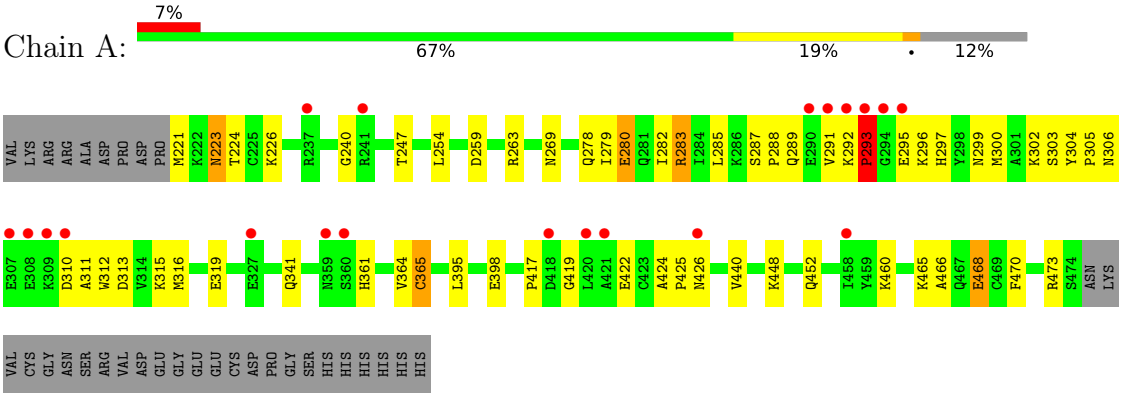
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	105	105	105	0	0
			Total	O		
4	B	97	97	97	0	0
			Total	O		
4	C	122	122	122	0	0
			Total	O		
4	D	115	115	115	0	0

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.

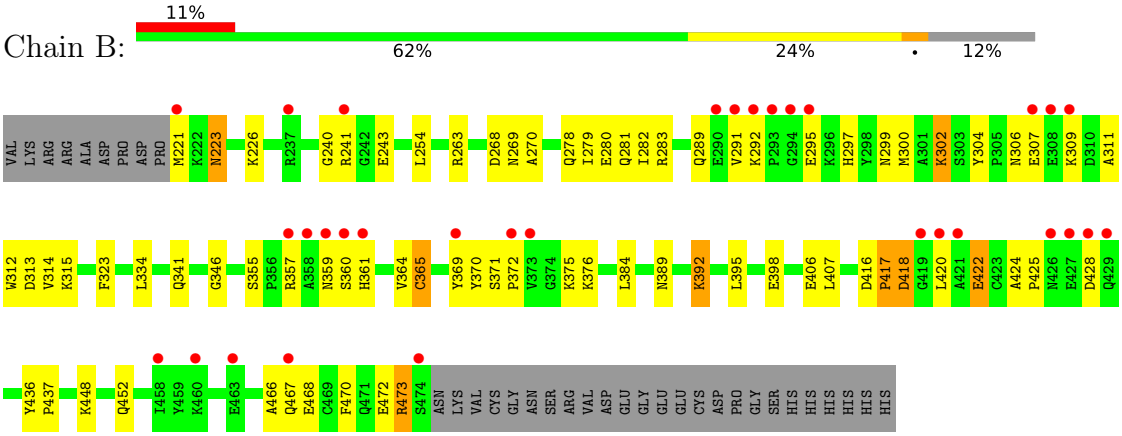
- Molecule 1: ADAM 17

Chain A:



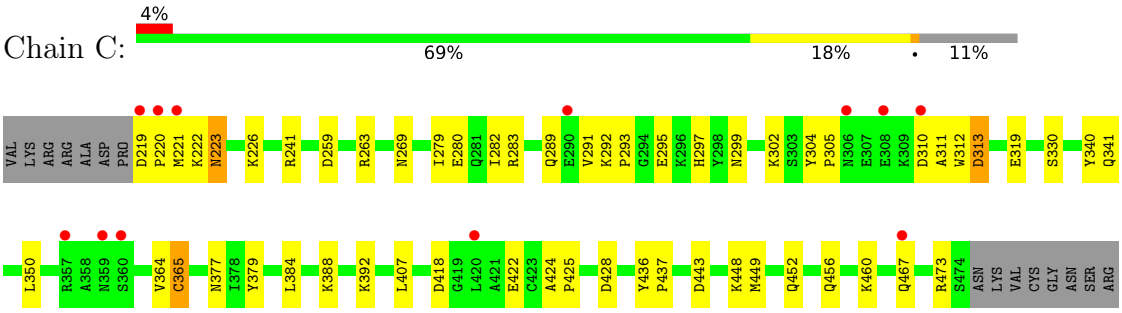
- Molecule 1: ADAM 17

Chain B:



- Molecule 1: ADAM 17

Chain C:



VAL ASP GLU GLY GLU GLU CYS ASP PRO GLY SER HIS HIS HIS HIS HIS HIS

• Molecule 1: ADAM 17

Chain D:

VAL LYS ARG ARG ALA ASP PRO ASP P220 M221 K222 N223 K226 G240 T247 L254 N269 K273 I279 E280 Q281 I282 R283 I284 V291 K292 E295 K296 H297 Y298 N299 M300 A301 K302 S303 Y304 A311 W312 D313 F323 E327 S330 Q341 A358 N359

S360 H361 V364 C365 P366 K367 A368 Y369 P372 V373 G374 K375 Y379 L380 L395 T396 K397 E398 L401 V402 T403 L407 P417 D418 E422 C423 A424 P425 N426 E427 D428 Q429 Y436 P437 M449 Q452 K465 E472 R473 SER ASN LYS VAL CYS GLY ASN SER

ARG VAL ASP GLU GLY GLU GLU CYS ASP PRO GLY SER HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	163.85Å 51.33Å 132.74Å 90.00° 102.64° 90.00°	Depositor
Resolution (Å)	20.00 – 2.10 19.98 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.5 (20.00-2.10) 98.4 (19.98-2.10)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	6.22 (at 2.09Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.218 , 0.257 0.211 , 0.249	Depositor DCC
R_{free} test set	3153 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	27.1	Xtriage
Anisotropy	0.218	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 49.3	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	0.94	EDS
Total number of atoms	8642	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 61.98 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.2067e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 792

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	0.34	0/2061	0.62	1/2780 (0.0%)
1	B	0.32	0/2061	0.58	0/2780
1	C	0.34	0/2077	0.62	1/2803 (0.0%)
1	D	0.34	0/2063	0.61	1/2783 (0.0%)
All	All	0.33	0/8262	0.61	3/11146 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	313	ASP	N-CA-C	-5.95	94.94	111.00
1	C	313	ASP	N-CA-C	-5.53	96.07	111.00
1	D	313	ASP	N-CA-C	-5.50	96.14	111.00

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	2016	0	1932	54	0
1	B	2016	0	1932	74	0
1	C	2031	0	1943	51	0
1	D	2017	0	1935	63	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	29	0	18	0	0
2	B	30	0	21	0	0
2	C	30	0	21	0	0
2	D	30	0	21	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	105	0	0	6	0
4	B	97	0	0	5	0
4	C	122	0	0	8	0
4	D	115	0	0	2	0
All	All	8642	0	7823	231	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 14.

All (231) 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:C:291:VAL:HG22	1:C:295:GLU:HG3	1.29	1.11
1:B:311:ALA:HB2	1:B:341:GLN:HB2	1.46	0.98
1:D:291:VAL:HG13	1:D:295:GLU:HG3	1.46	0.98
1:B:263:ARG:HD3	1:B:473:ARG:HH21	1.35	0.89
1:A:263:ARG:HE	1:A:473:ARG:HH21	1.22	0.87
1:B:311:ALA:HB1	1:B:341:GLN:HE21	1.40	0.86
1:D:269:ASN:HD21	1:D:452:GLN:HE22	1.20	0.85
1:B:312:TRP:H	1:B:341:GLN:NE2	1.75	0.84
1:A:263:ARG:NE	1:A:473:ARG:HH21	1.75	0.83
1:B:291:VAL:CG2	1:B:295:GLU:HG3	2.11	0.81
1:D:426:ASN:HB2	1:D:429:GLN:HE22	1.45	0.79
1:D:472:GLU:O	1:D:473:ARG:HB2	1.82	0.79
1:D:283:ARG:HH11	1:D:283:ARG:HB3	1.49	0.78
1:A:291:VAL:HG13	1:A:295:GLU:HG3	1.65	0.78
1:D:426:ASN:HB2	1:D:429:GLN:NE2	2.00	0.77
1:C:377:ASN:ND2	1:D:327:GLU:HG2	2.01	0.76
1:C:449:MET:HG2	4:C:153:HOH:O	1.85	0.75
1:C:319:GLU:HG2	4:C:530:HOH:O	1.87	0.74
1:A:283:ARG:HH11	1:A:283:ARG:HB3	1.51	0.74
1:C:259:ASP:OD2	1:C:473:ARG:NH2	2.20	0.73
1:B:417:PRO:HG2	1:B:420:LEU:HD23	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:417:PRO:O	1:D:418:ASP:HB2	1.88	0.73
1:B:241:ARG:HH12	1:C:241:ARG:HG3	1.55	0.72
1:B:417:PRO:O	1:B:418:ASP:HB2	1.89	0.72
1:B:223:ASN:H	1:B:223:ASN:HD22	1.38	0.71
1:D:223:ASN:H	1:D:223:ASN:HD22	1.37	0.71
1:A:291:VAL:CG1	1:A:295:GLU:HG3	2.20	0.71
1:C:291:VAL:HG22	1:C:295:GLU:CG	2.16	0.71
1:B:311:ALA:CB	1:B:341:GLN:HB2	2.21	0.70
1:D:311:ALA:HB2	1:D:341:GLN:HB2	1.74	0.70
1:C:269:ASN:HD21	1:C:452:GLN:HE22	1.39	0.69
1:D:291:VAL:HG11	1:D:295:GLU:O	1.91	0.69
1:C:263:ARG:HD3	1:C:473:ARG:NH2	2.08	0.68
1:A:223:ASN:HD22	1:A:223:ASN:H	1.41	0.67
1:B:306:ASN:HB3	1:B:309:LYS:HG2	1.76	0.67
1:B:357:ARG:HB2	1:B:360:SER:HB2	1.76	0.67
1:A:269:ASN:HD21	1:A:452:GLN:HE22	1.43	0.67
1:A:303:SER:OG	1:A:310:ASP:HA	1.94	0.67
1:A:283:ARG:HB3	1:A:283:ARG:NH1	2.09	0.66
1:B:243:GLU:OE2	1:C:241:ARG:NH1	2.28	0.66
1:B:263:ARG:HD3	1:B:473:ARG:NH2	2.11	0.65
1:B:263:ARG:NH2	1:C:443:ASP:HB3	2.12	0.64
1:C:297:HIS:CD2	1:C:299:ASN:H	2.16	0.64
1:C:223:ASN:HD22	1:C:223:ASN:H	1.45	0.64
1:D:359:ASN:HA	1:D:367:LYS:HE2	1.79	0.64
1:D:417:PRO:O	1:D:418:ASP:CB	2.46	0.64
1:B:291:VAL:HG23	1:B:295:GLU:HG3	1.79	0.63
1:D:428:ASP:N	1:D:428:ASP:OD2	2.29	0.63
1:D:323:PHE:HE2	1:D:374:GLY:HA3	1.64	0.62
1:B:269:ASN:HD21	1:B:452:GLN:HE22	1.44	0.62
1:D:283:ARG:HH11	1:D:283:ARG:CB	2.11	0.62
1:A:297:HIS:CD2	1:A:299:ASN:H	2.17	0.62
1:D:311:ALA:HB1	1:D:341:GLN:HE21	1.64	0.62
1:A:259:ASP:OD2	1:A:473:ARG:NH2	2.33	0.61
1:C:297:HIS:HD2	1:C:299:ASN:H	1.49	0.60
1:C:456:GLN:O	1:C:460:LYS:HD3	2.03	0.59
1:D:297:HIS:CD2	1:D:299:ASN:H	2.21	0.59
1:D:297:HIS:HD2	1:D:299:ASN:H	1.50	0.59
1:A:289:GLN:O	1:A:291:VAL:HG23	2.03	0.59
1:C:279:ILE:HG21	1:C:282:ILE:HG13	1.83	0.59
1:D:449:MET:HG2	4:D:82:HOH:O	2.02	0.59
1:B:241:ARG:NH1	1:C:241:ARG:NH2	2.51	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:312:TRP:H	1:B:341:GLN:HE21	1.52	0.58
1:B:417:PRO:O	1:B:418:ASP:CB	2.51	0.58
1:D:223:ASN:H	1:D:223:ASN:ND2	2.01	0.58
1:D:365:CYS:SG	1:D:465:LYS:HB3	2.43	0.58
1:A:263:ARG:CZ	1:A:473:ARG:HE	2.17	0.57
1:D:426:ASN:HD22	1:D:429:GLN:HE22	1.51	0.57
1:B:323:PHE:CE2	1:B:376:LYS:HE2	2.39	0.57
1:B:278:GLN:NE2	1:B:473:ARG:HD2	2.20	0.56
1:B:223:ASN:H	1:B:223:ASN:ND2	2.02	0.56
1:B:281:GLN:NE2	1:B:283:ARG:HH22	2.04	0.56
1:D:279:ILE:HG21	1:D:282:ILE:HG13	1.87	0.56
1:D:330:SER:HB3	1:D:379:TYR:CE1	2.40	0.56
1:B:226:LYS:HB3	1:B:280:GLU:HB2	1.88	0.55
1:A:287:SER:HB2	1:A:288:PRO:HD2	1.88	0.55
1:C:377:ASN:HD22	1:D:327:GLU:CD	2.09	0.55
1:D:473:ARG:HG3	1:D:473:ARG:HH11	1.71	0.55
1:A:291:VAL:HG12	1:A:292:LYS:N	2.20	0.55
1:B:269:ASN:HD21	1:B:452:GLN:NE2	2.03	0.55
1:B:395:LEU:HB2	1:B:398:GLU:HG3	1.88	0.54
1:D:292:LYS:HG2	1:D:295:GLU:CD	2.27	0.54
1:D:372:PRO:O	1:D:375:LYS:HD3	2.08	0.54
1:B:371:SER:O	1:B:375:LYS:N	2.40	0.54
1:B:359:ASN:HB2	4:B:512:HOH:O	2.07	0.54
1:C:263:ARG:HD3	1:C:473:ARG:CZ	2.38	0.54
1:B:297:HIS:CD2	1:B:299:ASN:H	2.27	0.53
1:C:292:LYS:HB3	1:C:293:PRO:HD2	1.89	0.53
1:D:428:ASP:HB2	1:D:429:GLN:HE21	1.74	0.53
1:C:377:ASN:HD22	1:D:327:GLU:HG2	1.73	0.53
1:B:223:ASN:HD22	1:B:223:ASN:N	2.02	0.53
1:B:292:LYS:HG2	1:B:295:GLU:CD	2.30	0.53
1:C:279:ILE:HG21	1:C:282:ILE:CG1	2.38	0.52
1:A:292:LYS:HG2	1:A:295:GLU:HG2	1.91	0.52
1:A:316:MET:HE2	4:A:515:HOH:O	2.09	0.52
1:B:357:ARG:NH1	1:B:357:ARG:HB3	2.24	0.52
1:A:440:VAL:HG13	4:A:162:HOH:O	2.09	0.52
1:D:472:GLU:O	1:D:473:ARG:CB	2.57	0.52
1:D:312:TRP:H	1:D:341:GLN:NE2	2.08	0.51
1:B:311:ALA:HB1	1:B:341:GLN:NE2	2.16	0.51
1:D:291:VAL:HG13	1:D:295:GLU:CG	2.29	0.51
1:C:289:GLN:HG2	1:C:297:HIS:CG	2.46	0.51
1:C:467:GLN:HB2	4:C:194:HOH:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:302:LYS:NZ	1:B:302:LYS:HB3	2.26	0.51
1:B:221:MET:O	1:B:472:GLU:HA	2.11	0.51
1:B:314:VAL:HG13	1:B:315:LYS:N	2.26	0.51
1:B:357:ARG:HB3	1:B:357:ARG:HH11	1.76	0.51
1:B:241:ARG:CZ	1:C:241:ARG:NH2	2.73	0.51
1:A:312:TRP:H	1:A:341:GLN:NE2	2.09	0.50
1:B:291:VAL:HG21	1:B:295:GLU:O	2.11	0.50
1:D:364:VAL:O	1:D:365:CYS:HB2	2.11	0.50
1:B:361:HIS:N	1:B:361:HIS:CD2	2.79	0.50
1:A:263:ARG:CZ	1:A:473:ARG:HH21	2.24	0.50
1:B:268:ASP:OD2	1:B:270:ALA:HB3	2.10	0.50
1:B:289:GLN:HG2	1:B:297:HIS:CG	2.46	0.50
1:D:254:LEU:C	1:D:254:LEU:HD23	2.31	0.50
1:B:424:ALA:N	1:B:425:PRO:HD3	2.27	0.50
1:D:223:ASN:HD22	1:D:223:ASN:N	2.00	0.49
1:B:392:LYS:HE3	4:B:197:HOH:O	2.11	0.49
1:A:291:VAL:HG12	1:A:292:LYS:O	2.12	0.49
1:A:292:LYS:CG	1:A:295:GLU:HG2	2.41	0.49
1:B:263:ARG:HH21	1:C:443:ASP:HB3	1.76	0.49
1:C:219:ASP:O	1:C:222:LYS:N	2.46	0.49
1:C:377:ASN:HD22	1:D:327:GLU:CG	2.25	0.49
1:C:436:TYR:CD1	1:C:437:PRO:HD2	2.47	0.49
1:A:426:ASN:HB3	4:A:520:HOH:O	2.13	0.49
1:B:420:LEU:HD11	1:B:422:GLU:HB2	1.94	0.49
1:C:364:VAL:O	1:C:365:CYS:HB2	2.13	0.49
1:C:311:ALA:HB2	1:C:341:GLN:HB3	1.94	0.49
1:A:395:LEU:HB2	1:A:398:GLU:HG3	1.95	0.48
1:A:283:ARG:HH12	1:A:285:LEU:HD21	1.79	0.48
1:A:279:ILE:HG21	1:A:282:ILE:CG1	2.43	0.48
1:B:221:MET:HG3	1:B:472:GLU:HG2	1.95	0.48
1:A:226:LYS:HG2	4:A:33:HOH:O	2.13	0.48
1:D:361:HIS:O	1:D:380:LEU:HD12	2.14	0.48
1:B:384:LEU:HD12	1:B:384:LEU:C	2.33	0.48
1:C:377:ASN:ND2	1:D:327:GLU:CG	2.75	0.48
1:C:223:ASN:HD22	1:C:223:ASN:N	2.07	0.47
1:D:422:GLU:OE1	1:D:452:GLN:HG3	2.13	0.47
1:A:364:VAL:O	1:A:365:CYS:HB2	2.14	0.47
1:C:330:SER:HB3	1:C:379:TYR:CE1	2.49	0.47
1:C:428:ASP:HB3	4:C:83:HOH:O	2.15	0.47
1:B:312:TRP:H	1:B:341:GLN:HE22	1.56	0.47
1:C:448:LYS:HD2	4:C:567:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:240:GLY:HA3	1:D:247:THR:OG1	2.14	0.47
1:B:297:HIS:HE1	4:B:531:HOH:O	1.98	0.47
1:D:279:ILE:HD13	1:D:282:ILE:HD11	1.96	0.47
1:A:292:LYS:HG2	1:A:295:GLU:OE2	2.15	0.47
1:B:370:TYR:O	1:B:372:PRO:HD3	2.15	0.47
1:A:304:TYR:CD1	1:A:305:PRO:HA	2.50	0.46
1:D:279:ILE:HG21	1:D:282:ILE:CG1	2.45	0.46
1:C:226:LYS:HB3	1:C:280:GLU:HB2	1.96	0.46
1:A:296:LYS:NZ	4:A:515:HOH:O	2.47	0.46
1:A:223:ASN:H	1:A:223:ASN:ND2	2.09	0.46
1:A:279:ILE:HG21	1:A:282:ILE:HG12	1.98	0.45
1:B:355:SER:HB3	1:B:360:SER:OG	2.16	0.45
1:A:223:ASN:HD22	1:A:223:ASN:N	2.05	0.45
1:A:240:GLY:HA3	1:A:247:THR:OG1	2.17	0.45
1:A:466:ALA:O	1:A:470:PHE:HB2	2.16	0.45
1:C:340:TYR:CE2	1:C:388:LYS:HD2	2.51	0.45
1:D:395:LEU:HB2	1:D:398:GLU:HG3	1.98	0.45
1:C:312:TRP:H	1:C:341:GLN:NE2	2.15	0.45
1:A:224:THR:HG23	1:A:263:ARG:NH2	2.32	0.45
1:D:302:LYS:HG2	4:D:206:HOH:O	2.17	0.45
1:D:473:ARG:HG3	1:D:473:ARG:NH1	2.31	0.45
1:A:424:ALA:N	1:A:425:PRO:HD3	2.32	0.45
1:D:221:MET:O	1:D:472:GLU:HA	2.17	0.45
1:D:403:THR:HG22	1:D:407:LEU:HD22	1.99	0.44
1:A:226:LYS:HB3	1:A:280:GLU:HB2	1.99	0.44
1:B:315:LYS:HD3	4:B:508:HOH:O	2.17	0.44
1:B:364:VAL:O	1:B:365:CYS:HB2	2.17	0.44
1:D:424:ALA:N	1:D:425:PRO:HD3	2.32	0.44
1:B:297:HIS:HD2	1:B:299:ASN:H	1.65	0.44
1:C:384:LEU:C	1:C:384:LEU:HD12	2.37	0.44
1:A:361:HIS:HE1	4:A:506:HOH:O	1.99	0.44
1:D:397:LYS:O	1:D:401:LEU:HG	2.17	0.44
1:B:417:PRO:HB2	1:B:420:LEU:HB3	1.99	0.44
1:A:417:PRO:C	1:A:419:GLY:H	2.21	0.44
1:B:291:VAL:HG22	1:B:295:GLU:HG3	1.96	0.44
1:D:297:HIS:O	1:D:300:MET:HG2	2.18	0.43
1:A:303:SER:OG	1:A:310:ASP:CA	2.64	0.43
1:D:226:LYS:HB3	1:D:280:GLU:HB2	2.01	0.43
1:A:291:VAL:CG1	1:A:292:LYS:N	2.81	0.43
1:B:254:LEU:C	1:B:254:LEU:HD23	2.39	0.43
1:B:281:GLN:NE2	1:B:283:ARG:NH2	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:312:TRP:H	1:D:341:GLN:HE21	1.66	0.43
1:C:283:ARG:NE	4:C:533:HOH:O	2.49	0.43
1:A:278:GLN:NE2	1:A:473:ARG:NH1	2.66	0.43
1:C:350:LEU:HD12	4:C:565:HOH:O	2.18	0.43
1:D:300:MET:CE	1:D:304:TYR:HB2	2.48	0.42
1:D:398:GLU:O	1:D:402:VAL:HG23	2.19	0.42
1:C:311:ALA:CB	1:C:341:GLN:HB3	2.49	0.42
1:A:300:MET:HG3	1:A:302:LYS:O	2.19	0.42
1:C:292:LYS:O	1:C:295:GLU:HG2	2.19	0.42
1:C:302:LYS:HE2	1:C:302:LYS:HB3	1.85	0.42
1:C:424:ALA:N	1:C:425:PRO:HD3	2.35	0.42
1:B:384:LEU:HD12	1:B:384:LEU:O	2.20	0.42
1:C:219:ASP:O	1:C:221:MET:N	2.53	0.42
1:A:254:LEU:C	1:A:254:LEU:HD23	2.39	0.42
1:A:292:LYS:HD3	1:A:293:PRO:HD2	2.00	0.42
1:B:279:ILE:HG21	1:B:282:ILE:CG1	2.50	0.42
1:B:346:GLY:HA2	1:B:389:ASN:OD1	2.19	0.42
1:C:223:ASN:H	1:C:223:ASN:ND2	2.16	0.42
1:B:240:GLY:O	1:B:241:ARG:HB2	2.20	0.41
1:B:452:GLN:NE2	1:B:452:GLN:HA	2.35	0.41
1:D:311:ALA:CB	1:D:341:GLN:HB2	2.46	0.41
1:A:302:LYS:HE2	1:A:302:LYS:HB3	1.85	0.41
1:A:448:LYS:HE3	1:A:448:LYS:HB3	1.97	0.41
1:B:223:ASN:ND2	1:B:223:ASN:N	2.62	0.41
1:B:334:LEU:HD21	1:B:364:VAL:HA	2.03	0.41
1:C:241:ARG:HG3	1:C:241:ARG:NH2	2.35	0.41
1:A:311:ALA:HA	1:A:341:GLN:HE21	1.86	0.41
1:D:281:GLN:HE21	1:D:282:ILE:N	2.18	0.41
1:B:406:GLU:HA	1:B:406:GLU:OE1	2.20	0.41
1:C:304:TYR:CD1	1:C:305:PRO:HA	2.55	0.41
1:B:466:ALA:O	1:B:470:PHE:HB2	2.20	0.41
1:D:361:HIS:O	1:D:380:LEU:HB2	2.19	0.41
1:D:273:LYS:NZ	1:D:273:LYS:HB2	2.35	0.41
1:D:436:TYR:CD1	1:D:437:PRO:HD2	2.56	0.41
1:A:465:LYS:HA	1:A:468:GLU:HB2	2.02	0.41
1:B:369:TYR:CD1	1:B:369:TYR:C	2.93	0.41
1:B:416:ASP:O	1:B:417:PRO:C	2.58	0.41
1:B:448:LYS:HE3	4:B:181:HOH:O	2.20	0.41
1:D:247:THR:HG21	1:D:284:ILE:HD12	2.03	0.41
1:B:300:MET:CE	1:B:304:TYR:HB2	2.50	0.41
1:C:302:LYS:HD2	4:C:102:HOH:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:HIS:HD2	1:A:299:ASN:H	1.65	0.40
1:A:305:PRO:HG2	1:A:306:ASN:OD1	2.21	0.40
1:A:315:LYS:O	1:A:319:GLU:HG3	2.21	0.40
1:B:436:TYR:CD1	1:B:437:PRO:HD2	2.57	0.40
1:D:247:THR:CG2	1:D:284:ILE:HD12	2.52	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	252/288 (88%)	237 (94%)	13 (5%)	2 (1%)	19 15
1	B	252/288 (88%)	240 (95%)	9 (4%)	3 (1%)	13 8
1	C	254/288 (88%)	244 (96%)	8 (3%)	2 (1%)	19 15
1	D	252/288 (88%)	244 (97%)	4 (2%)	4 (2%)	9 5
All	All	1010/1152 (88%)	965 (96%)	34 (3%)	11 (1%)	14 9

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	293	PRO
1	B	417	PRO
1	D	417	PRO
1	B	418	ASP
1	D	418	ASP
1	C	220	PRO
1	A	365	CYS
1	B	365	CYS
1	C	365	CYS
1	D	365	CYS

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Mol	Chain	Res	Type
1	D	368	ALA

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	217/247 (88%)	209 (96%)	8 (4%)	34	35
1	B	217/247 (88%)	206 (95%)	11 (5%)	24	22
1	C	219/247 (89%)	212 (97%)	7 (3%)	39	41
1	D	217/247 (88%)	207 (95%)	10 (5%)	27	26
All	All	870/988 (88%)	834 (96%)	36 (4%)	30	31

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	221	MET
1	A	223	ASN
1	A	280	GLU
1	A	283	ARG
1	A	293	PRO
1	A	422	GLU
1	A	460	LYS
1	A	468	GLU
1	B	223	ASN
1	B	302	LYS
1	B	307	GLU
1	B	313	ASP
1	B	392	LYS
1	B	407	LEU
1	B	422	GLU
1	B	428	ASP
1	B	467	GLN
1	B	468	GLU
1	B	473	ARG
1	C	223	ASN

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Mol	Chain	Res	Type
1	C	310	ASP
1	C	313	ASP
1	C	392	LYS
1	C	407	LEU
1	C	418	ASP
1	C	422	GLU
1	D	223	ASN
1	D	273	LYS
1	D	281	GLN
1	D	283	ARG
1	D	296	LYS
1	D	313	ASP
1	D	359	ASN
1	D	407	LEU
1	D	428	ASP
1	D	429	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	223	ASN
1	A	297	HIS
1	A	320	GLN
1	A	341	GLN
1	A	359	ASN
1	A	361	HIS
1	A	426	ASN
1	A	452	GLN
1	A	456	GLN
1	A	471	GLN
1	B	223	ASN
1	B	281	GLN
1	B	297	HIS
1	B	341	GLN
1	B	452	GLN
1	B	456	GLN
1	B	471	GLN
1	C	223	ASN
1	C	297	HIS
1	C	306	ASN
1	C	341	GLN
1	C	361	HIS

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Mol	Chain	Res	Type
1	C	452	GLN
1	C	471	GLN
1	D	223	ASN
1	D	281	GLN
1	D	297	HIS
1	D	341	GLN
1	D	361	HIS
1	D	429	GLN
1	D	452	GLN
1	D	456	GLN
1	D	471	GLN

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 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
2	792	C	3	3	31,32,32	1.86	10 (32%)	39,45,45	1.18	3 (7%)
2	792	D	4	3	31,32,32	1.82	9 (29%)	39,45,45	1.02	3 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	792	B	2	3	31,32,32	1.88	11 (35%)	39,45,45	1.04	2 (5%)
2	792	A	1	3	30,31,32	1.96	10 (33%)	39,44,45	1.08	3 (7%)

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	792	C	3	3	-	3/22/24/24	0/3/3/3
2	792	D	4	3	-	3/22/24/24	0/3/3/3
2	792	B	2	3	-	5/22/24/24	0/3/3/3
2	792	A	1	3	-	4/22/23/24	0/3/3/3

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	792	C13-C8	3.73	1.44	1.38
2	B	2	792	C12-C11	3.54	1.45	1.38
2	D	4	792	C12-C11	3.53	1.45	1.38
2	C	3	792	C12-C11	3.50	1.45	1.38
2	B	2	792	C1-C6	3.49	1.44	1.36
2	D	4	792	C13-C8	3.47	1.44	1.38
2	C	3	792	C1-C6	3.45	1.43	1.36
2	B	2	792	C9-C8	3.43	1.44	1.38
2	C	3	792	C13-C8	3.43	1.44	1.38
2	A	1	792	C12-C11	3.41	1.45	1.38
2	D	4	792	C1-C6	3.39	1.43	1.36
2	B	2	792	C13-C8	3.36	1.44	1.38
2	C	3	792	C4-C5	3.31	1.43	1.37
2	A	1	792	S7-N27	3.30	1.67	1.61
2	A	1	792	C4-C5	3.29	1.43	1.37
2	B	2	792	C4-C5	3.22	1.43	1.37
2	D	4	792	C9-C8	3.12	1.43	1.38
2	A	1	792	C1-C6	3.12	1.43	1.36
2	C	3	792	C9-C8	3.07	1.43	1.38
2	A	1	792	C9-C8	3.06	1.43	1.38
2	B	2	792	C13-C12	3.01	1.44	1.38
2	D	4	792	C13-C12	3.00	1.44	1.38
2	C	3	792	C13-C12	2.97	1.44	1.38
2	D	4	792	C4-C5	2.86	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	792	C13-C12	2.86	1.44	1.38
2	B	2	792	C10-C11	2.55	1.43	1.38
2	A	1	792	C10-C9	2.50	1.43	1.38
2	D	4	792	C10-C11	2.47	1.43	1.38
2	D	4	792	C10-C9	2.45	1.43	1.38
2	C	3	792	C10-C9	2.45	1.43	1.38
2	B	2	792	C10-C9	2.43	1.43	1.38
2	A	1	792	C10-C11	2.37	1.43	1.38
2	C	3	792	S7-N27	2.33	1.65	1.61
2	A	1	792	O28-C26	-2.26	1.23	1.30
2	C	3	792	O28-C26	-2.26	1.23	1.30
2	C	3	792	C10-C11	2.21	1.43	1.38
2	B	2	792	O14-C11	2.12	1.42	1.37
2	B	2	792	S7-N27	2.05	1.65	1.61
2	D	4	792	O28-C26	-2.04	1.23	1.30
2	B	2	792	O28-C26	-2.04	1.23	1.30

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	3	792	C8-S7-N27	3.77	113.00	107.78
2	A	1	792	O20-S7-O19	-3.49	115.26	119.55
2	C	3	792	O20-S7-O19	-3.42	115.34	119.55
2	D	4	792	O20-S7-O19	-3.29	115.50	119.55
2	B	2	792	O20-S7-O19	-3.18	115.64	119.55
2	B	2	792	C6-C5-C4	2.38	121.33	118.40
2	A	1	792	C6-C5-C4	2.33	121.27	118.40
2	C	3	792	C6-C5-C4	2.24	121.16	118.40
2	D	4	792	C6-C5-C4	2.15	121.05	118.40
2	D	4	792	C8-S7-N27	2.07	110.64	107.78
2	A	1	792	C5-C4-C3	-2.02	119.36	121.64

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1	792	C10-C11-O14-C15
2	A	1	792	C12-C11-O14-C15
2	C	3	792	C10-C11-O14-C15
2	C	3	792	C12-C11-O14-C15
2	B	2	792	C10-C11-O14-C15
2	D	4	792	C10-C11-O14-C15

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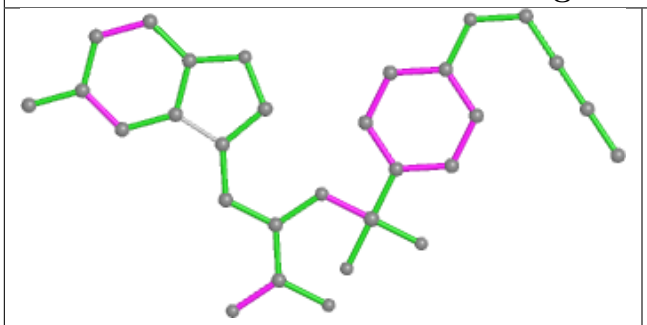
Mol	Chain	Res	Type	Atoms
2	B	2	792	C12-C11-O14-C15
2	D	4	792	C12-C11-O14-C15
2	B	2	792	N27-C25-C26-O29
2	C	3	792	O14-C15-C16-C17
2	B	2	792	O14-C15-C16-C17
2	D	4	792	O14-C15-C16-C17
2	A	1	792	N27-C25-C26-O29
2	B	2	792	N27-C25-C26-O28
2	A	1	792	O14-C15-C16-C17

There are no ring outliers.

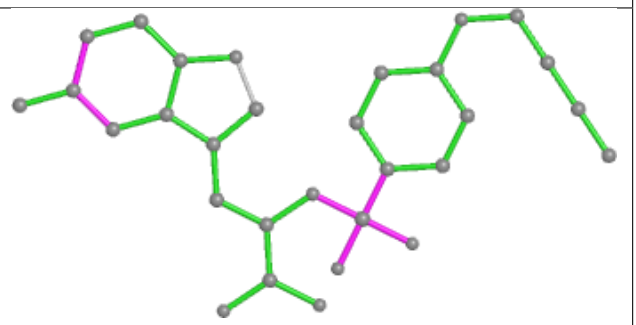
No monomer is involved in short contacts.

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.

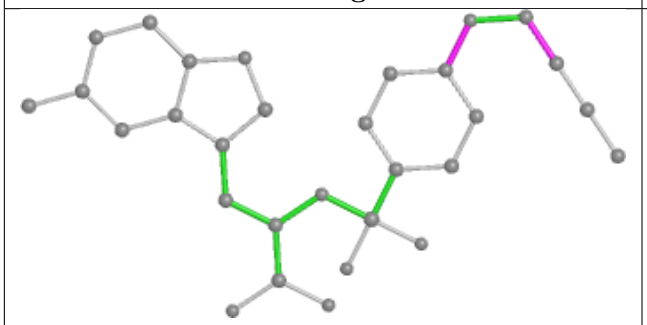
Ligand 792 C 3



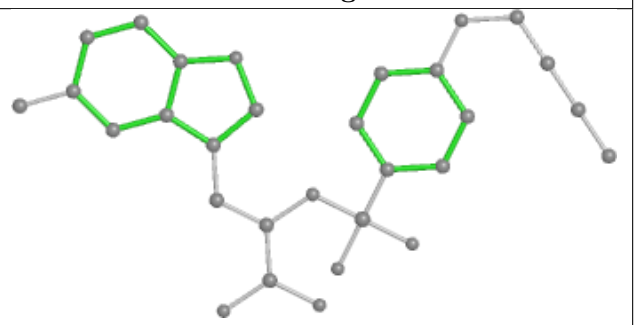
Bond lengths



Bond angles

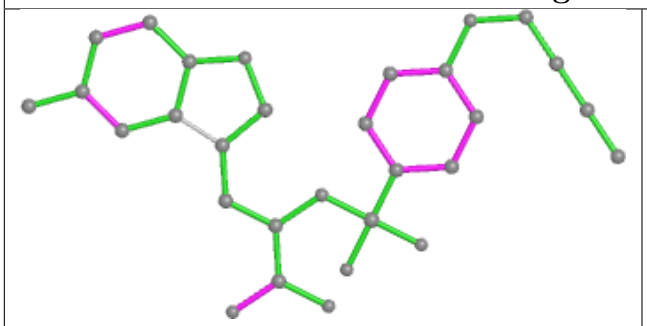


Torsions

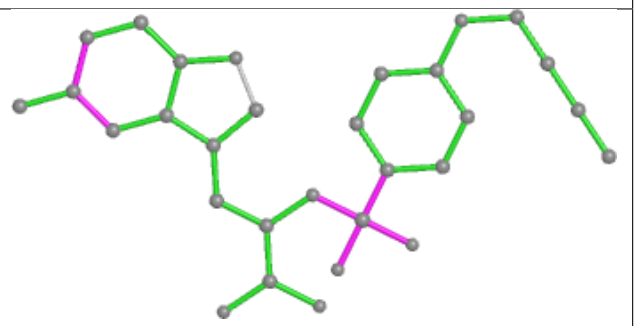


Rings

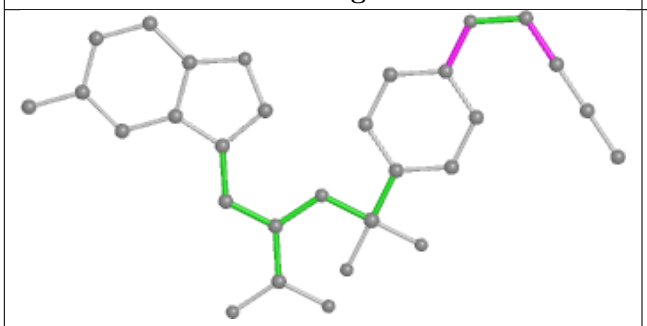
Ligand 792 D 4



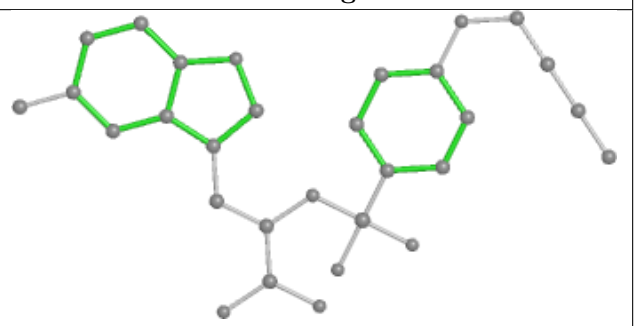
Bond lengths



Bond angles

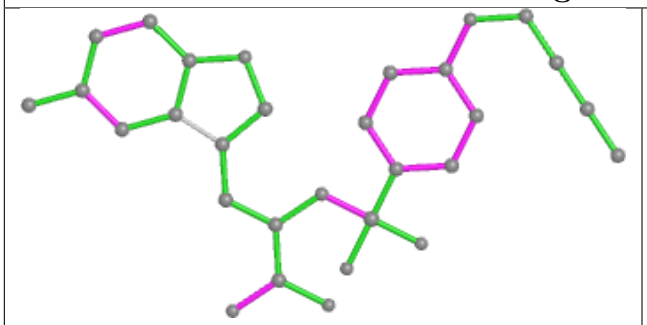


Torsions

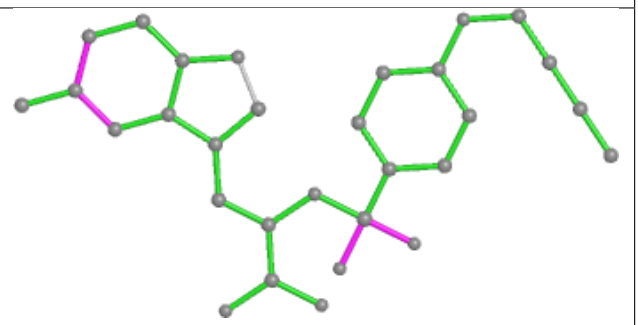


Rings

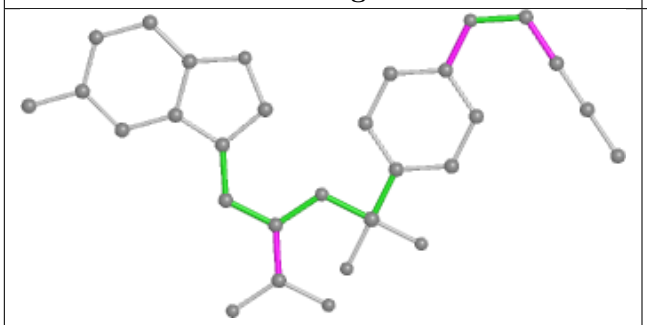
Ligand 792 B 2



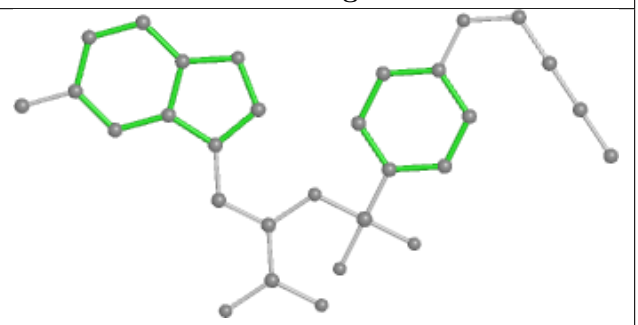
Bond lengths



Bond angles

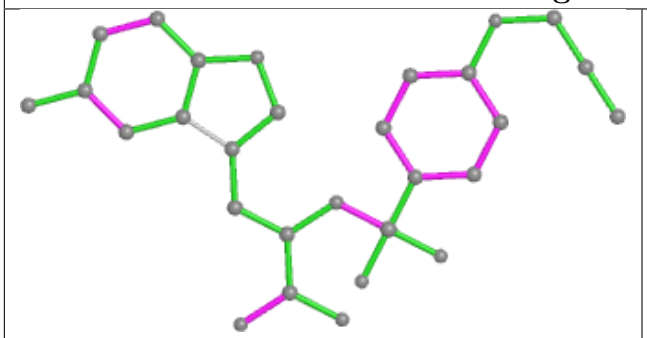


Torsions

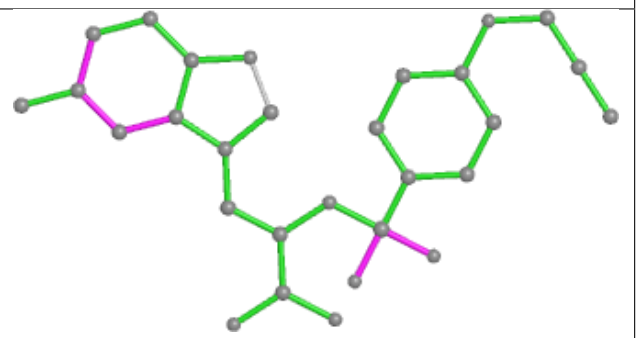


Rings

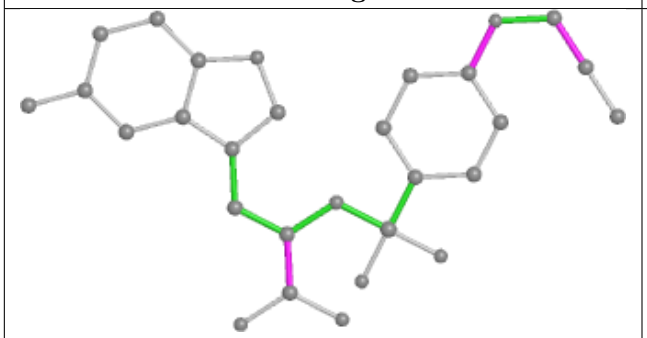
Ligand 792 A 1



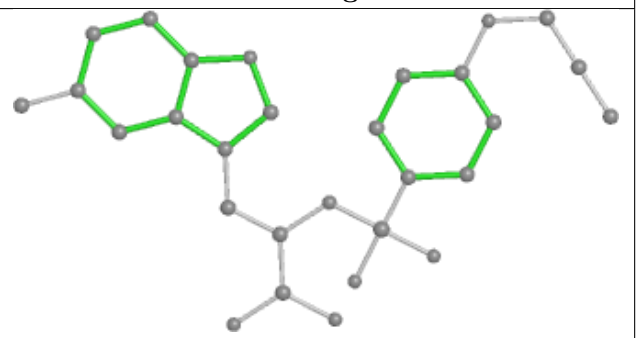
Bond lengths



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 (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	254/288 (88%)	0.41	20 (7%)	12	16	17, 29, 50, 56	0
1	B	254/288 (88%)	0.59	32 (12%)	3	5	19, 34, 53, 59	0
1	C	256/288 (88%)	0.32	12 (4%)	31	37	17, 27, 47, 61	0
1	D	254/288 (88%)	0.35	15 (5%)	22	27	17, 29, 49, 56	0
All	All	1018/1152 (88%)	0.42	79 (7%)	13	17	17, 29, 50, 61	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	219	ASP	8.4
1	C	221	MET	5.4
1	B	359	ASN	5.0
1	D	221	MET	5.0
1	C	310	ASP	4.8
1	A	420	LEU	4.5
1	C	220	PRO	4.5
1	D	373	VAL	4.4
1	B	221	MET	4.4
1	B	419	GLY	4.1
1	A	293	PRO	4.0
1	C	420	LEU	4.0
1	B	360	SER	3.8
1	D	372	PRO	3.7
1	B	426	ASN	3.7
1	B	428	ASP	3.6
1	A	294	GLY	3.6
1	D	220	PRO	3.6
1	A	290	GLU	3.5
1	D	473	ARG	3.5
1	B	294	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	359	ASN	3.5
1	B	421	ALA	3.4
1	D	366	PRO	3.4
1	A	421	ALA	3.3
1	C	359	ASN	3.3
1	B	429	GLN	3.1
1	B	308	GLU	3.1
1	D	358	ALA	3.1
1	A	241	ARG	3.1
1	A	426	ASN	3.0
1	D	369	TYR	3.0
1	B	467	GLN	3.0
1	B	292	LYS	3.0
1	A	291	VAL	2.9
1	D	428	ASP	2.8
1	C	467	GLN	2.8
1	A	418	ASP	2.8
1	A	310	ASP	2.8
1	B	369	TYR	2.8
1	A	360	SER	2.7
1	A	292	LYS	2.7
1	C	290	GLU	2.7
1	B	420	LEU	2.7
1	A	359	ASN	2.7
1	C	360	SER	2.6
1	D	375	LYS	2.6
1	B	307	GLU	2.6
1	C	306	ASN	2.6
1	B	357	ARG	2.5
1	B	373	VAL	2.5
1	B	372	PRO	2.5
1	B	291	VAL	2.5
1	D	426	ASN	2.5
1	A	237	ARG	2.5
1	B	361	HIS	2.5
1	B	295	GLU	2.5
1	B	427	GLU	2.4
1	B	460	LYS	2.4
1	B	458	ILE	2.4
1	B	241	ARG	2.4
1	D	364	VAL	2.3
1	B	290	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	293	PRO	2.3
1	B	309	LYS	2.3
1	B	358	ALA	2.3
1	A	295	GLU	2.3
1	A	458	ILE	2.3
1	A	327	GLU	2.2
1	B	237	ARG	2.2
1	B	474	SER	2.2
1	A	307	GLU	2.2
1	A	308	GLU	2.2
1	C	357	ARG	2.1
1	A	309	LYS	2.1
1	D	281	GLN	2.1
1	D	361	HIS	2.1
1	C	308	GLU	2.1
1	B	463	GLU	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	792	A	1	29/30	0.94	0.13	20,28,33,36	0
2	792	B	2	30/30	0.94	0.11	26,32,37,38	0
2	792	C	3	30/30	0.94	0.13	26,29,33,35	0
2	792	D	4	30/30	0.95	0.12	22,30,35,39	0
3	ZN	B	500	1/1	0.99	0.04	31,31,31,31	0
3	ZN	C	500	1/1	0.99	0.06	24,24,24,24	0
3	ZN	A	500	1/1	1.00	0.04	23,23,23,23	0

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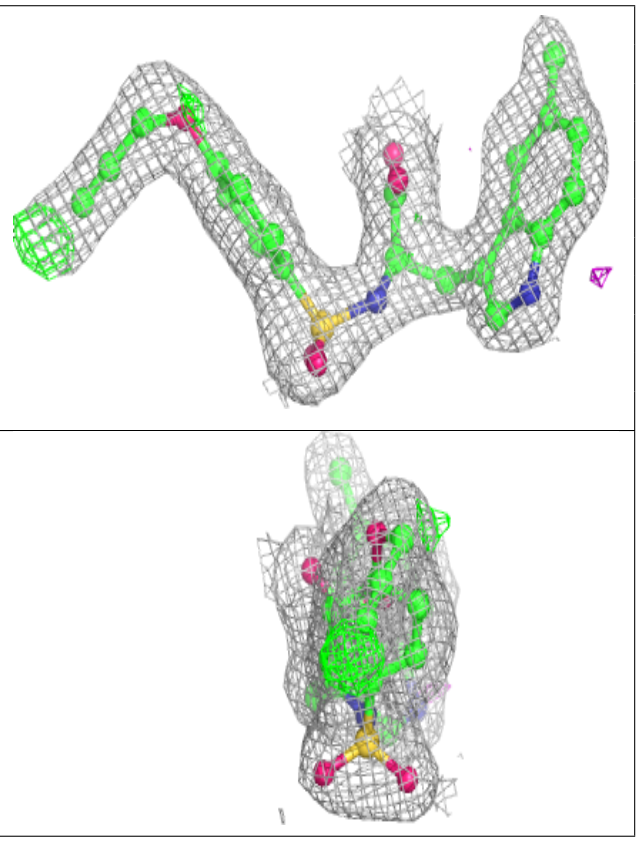
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ZN	D	500	1/1	1.00	0.06	25,25,25,25	0

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.

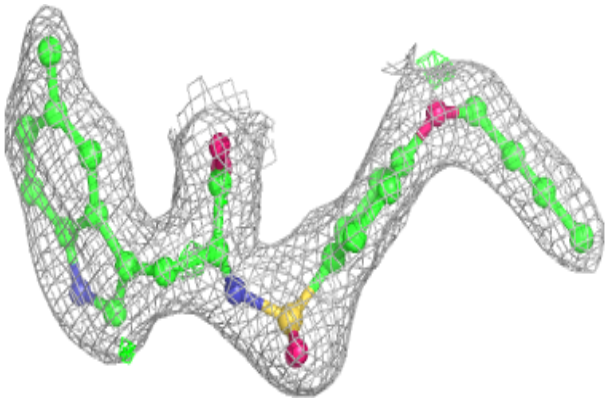
Electron density around 792 A 1:

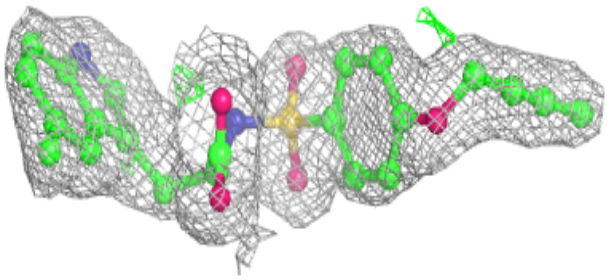
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

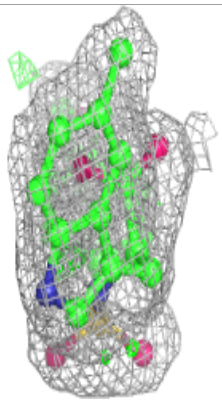


Electron density around 792 B 2:

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

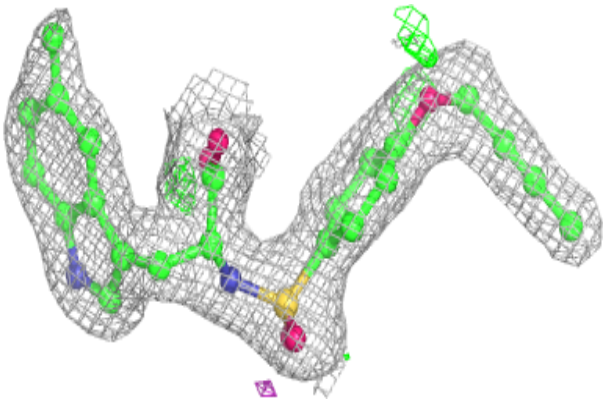


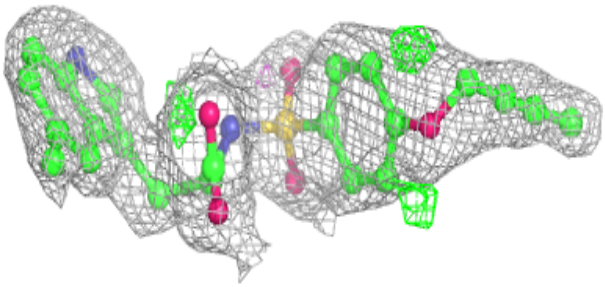


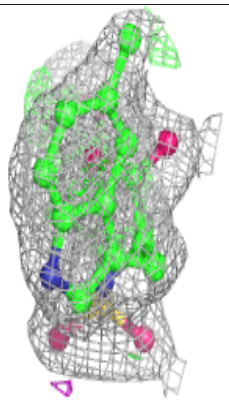


Electron density around 792 C 3:

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

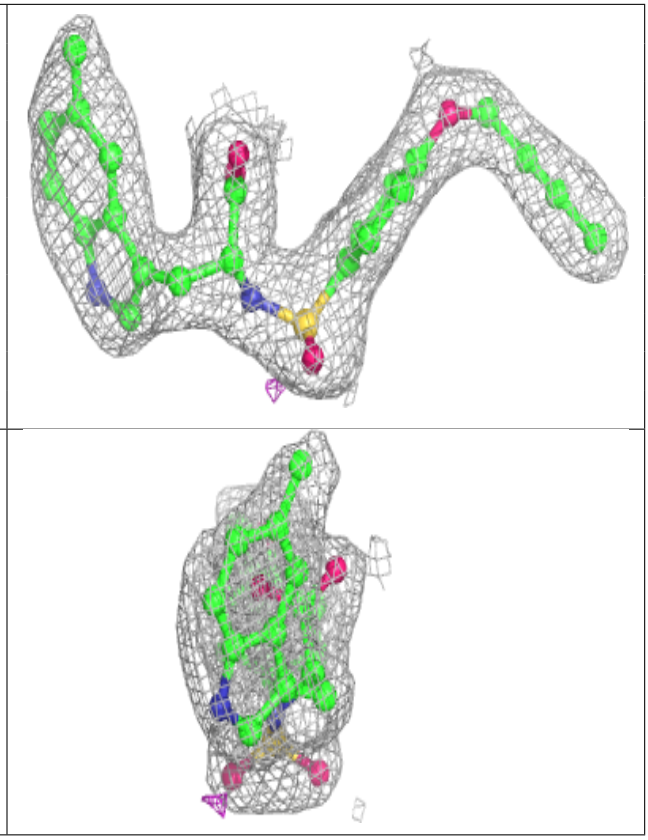






Electron density around 792 D 4:

$2mF_o$-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.