



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:38 PM UTC

PDB ID : 6FU1 / pdb_00006fu1
Title : Crystal structure of Schistosoma mansoni HDAC8 complexed with a n-alkyl hydroxamate
Authors : Marek, M.; Shaik, T.B.; Romier, C.
Deposited on : 2018-02-26
Resolution : 1.55 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

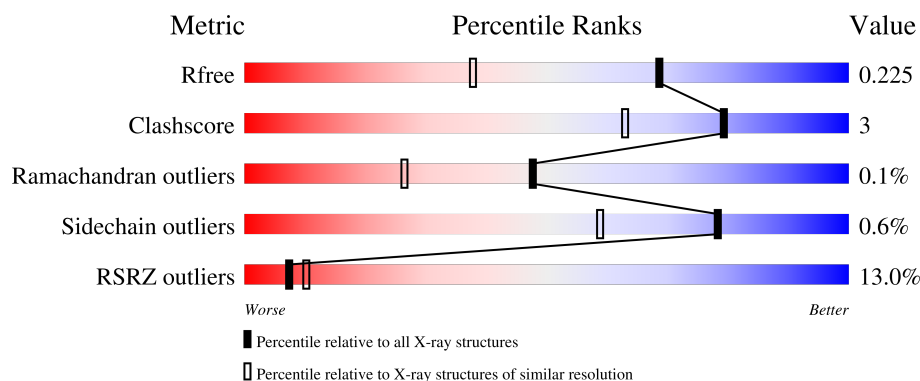
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.55 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}	180053	1003 (1.54-1.54)
Clashscore	190562	1025 (1.54-1.54)
Ramachandran outliers	187476	1007 (1.54-1.54)
Sidechain outliers	187428	1007 (1.54-1.54)
RSRZ outliers	180081	1002 (1.54-1.54)

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 $\leq 5\%$. 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	446	12% 83% 6% 11%
1	B	446	10% 84% 7% 8%
1	C	446	9% 86% 5% 9%
1	D	446	15% 85% • 11%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13624 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 Histone deacetylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	395	Total	C	N	O	S	0	6	0
			3188	2059	528	585	16			
1	B	411	Total	C	N	O	S	0	6	0
			3295	2121	551	604	19			
1	C	407	Total	C	N	O	S	0	6	0
			3265	2106	544	596	19			
1	D	396	Total	C	N	O	S	0	4	0
			3187	2059	528	584	16			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	441	GLY	-	expression tag	UNP A5H660
A	442	SER	-	expression tag	UNP A5H660
A	443	LEU	-	expression tag	UNP A5H660
A	444	VAL	-	expression tag	UNP A5H660
A	445	PRO	-	expression tag	UNP A5H660
A	446	ARG	-	expression tag	UNP A5H660
B	441	GLY	-	expression tag	UNP A5H660
B	442	SER	-	expression tag	UNP A5H660
B	443	LEU	-	expression tag	UNP A5H660
B	444	VAL	-	expression tag	UNP A5H660
B	445	PRO	-	expression tag	UNP A5H660
B	446	ARG	-	expression tag	UNP A5H660
C	441	GLY	-	expression tag	UNP A5H660
C	442	SER	-	expression tag	UNP A5H660
C	443	LEU	-	expression tag	UNP A5H660
C	444	VAL	-	expression tag	UNP A5H660
C	445	PRO	-	expression tag	UNP A5H660
C	446	ARG	-	expression tag	UNP A5H660
D	441	GLY	-	expression tag	UNP A5H660
D	442	SER	-	expression tag	UNP A5H660
D	443	LEU	-	expression tag	UNP A5H660

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Chain	Residue	Modelled	Actual	Comment	Reference
D	444	VAL	-	expression tag	UNP A5H660
D	445	PRO	-	expression tag	UNP A5H660
D	446	ARG	-	expression tag	UNP A5H660

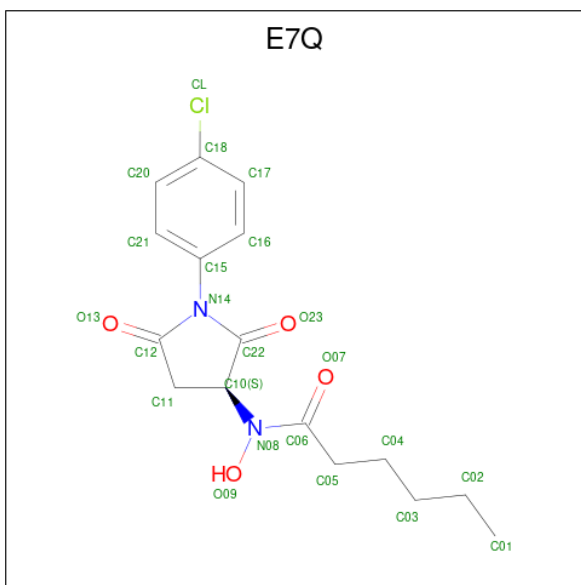
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 3 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total K 2 2	0	0
3	B	2	Total K 2 2	0	0
3	C	2	Total K 2 2	0	0
3	D	2	Total K 2 2	0	0

- Molecule 4 is {N}-[(3 {S})-1-(4-chlorophenyl)-2,5-bis(oxidanylidene)pyrrolidin-3-yl]- {N}-oxidanylidene-hexanamide (CCD ID: E7Q) (formula: C₁₆H₁₉ClN₂O₄).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	Cl	N	O	0	0
			23	16	1	2	4		
4	A	1	Total	C	Cl	N	O	0	0
			14	10	1	1	2		
4	B	1	Total	C	N	O		0	0
			9	6	1	2			
4	B	1	Total	C	Cl	N	O	0	0
			14	10	1	1	2		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0
5	C	1	Total C O 6 3 3	0	0

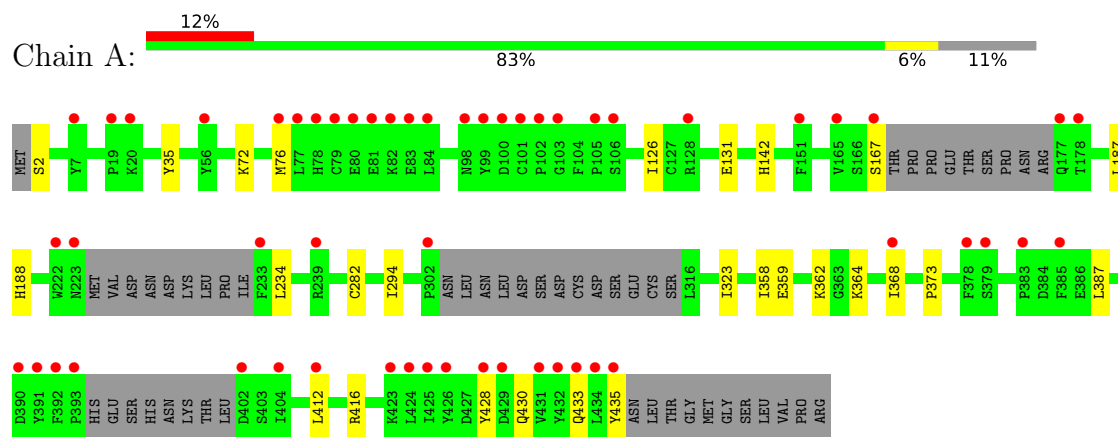
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	141	Total O 141 141	0	0
6	B	166	Total O 166 166	0	0
6	C	167	Total O 167 167	0	0
6	D	125	Total O 125 125	0	0

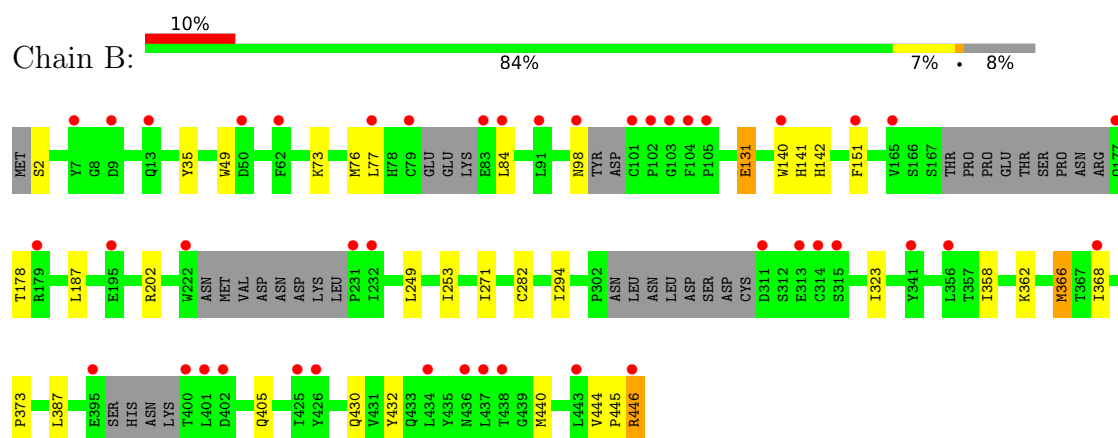
3 Residue-property plots

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.

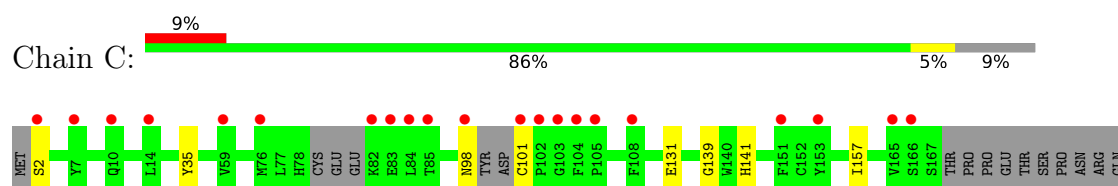
- Molecule 1: Histone deacetylase

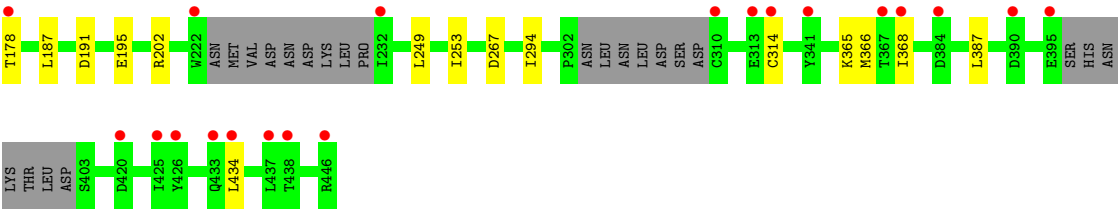


- Molecule 1: Histone deacetylase

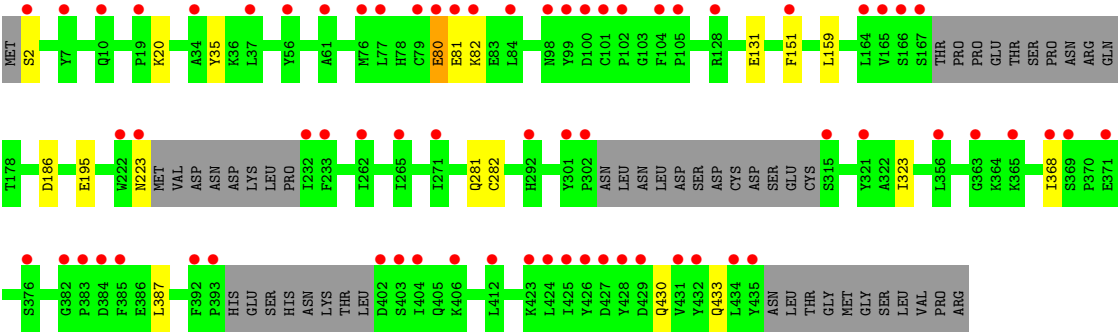
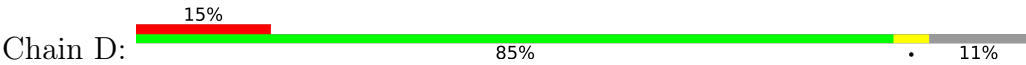


- Molecule 1: Histone deacetylase





● Molecule 1: Histone deacetylase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	70.71Å 70.69Å 99.19Å 75.33° 77.78° 84.80°	Depositor
Resolution (Å)	41.96 – 1.55 41.96 – 1.55	Depositor EDS
% Data completeness (in resolution range)	95.7 (41.96-1.55) 95.7 (41.96-1.55)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.02 (at 1.55Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.199 , 0.223 0.202 , 0.225	Depositor DCC
R_{free} test set	12654 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	22.1	Xtriage
Anisotropy	0.094	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 44.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.054 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	13624	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.87% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: GOL, ZN, E7Q, 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	0.32	0/3295	0.51	0/4479
1	B	0.34	0/3402	0.52	0/4623
1	C	0.35	0/3372	0.54	0/4581
1	D	0.31	0/3289	0.50	0/4473
All	All	0.33	0/13358	0.52	0/18156

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	3188	0	3086	19	0
1	B	3295	0	3203	25	0
1	C	3265	0	3174	13	0
1	D	3187	0	3084	11	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	37	0	0	2	0
4	B	23	0	0	5	0
5	A	6	0	8	1	0
5	B	6	0	8	0	0
5	C	6	0	8	0	0
6	A	141	0	0	0	0
6	B	166	0	0	1	0
6	C	167	0	0	0	0
6	D	125	0	0	1	0
All	All	13624	0	12571	68	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 3.

All (68) 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:80:GLU:O	1:D:82:LYS:N	2.17	0.78
1:B:142:HIS:NE2	4:B:504:E7Q:O09	2.23	0.72
1:B:35:TYR:CE1	1:B:368:ILE:HG23	2.26	0.71
1:C:35:TYR:CE1	1:C:368:ILE:HG23	2.26	0.70
1:A:35:TYR:CE1	1:A:368:ILE:HG23	2.30	0.67
1:B:141:HIS:NE2	4:B:504:E7Q:O09	2.25	0.66
1:C:267:ASP:HB3	1:C:434:LEU:HD11	1.80	0.63
1:A:234:LEU:HB2	5:A:505:GOL:H31	1.81	0.63
1:B:73:LYS:HA	1:B:76:MET:HE2	1.80	0.62
1:B:49:TRP:O	6:B:601:HOH:O	2.16	0.62
1:D:35:TYR:CE1	1:D:368:ILE:HG23	2.36	0.60
1:A:358:ILE:HG23	1:A:362:LYS:HD3	1.86	0.57
1:B:2:SER:N	1:B:131:GLU:OE1	2.37	0.57
1:B:405:GLN:HG2	1:B:440:MET:HE3	1.86	0.56
1:D:2:SER:N	1:D:131:GLU:OE1	2.38	0.56
1:C:178:THR:HB	1:C:202:ARG:HH21	1.74	0.52
1:B:366:MET:HA	1:B:366:MET:HE3	1.91	0.52
1:B:151:PHE:HD2	4:B:504:E7Q:C03	2.22	0.51
1:A:430:GLN:O	1:A:433:GLN:HG2	2.11	0.50
1:B:35:TYR:CD1	1:B:368:ILE:HG23	2.47	0.50
1:B:187:LEU:HD21	1:B:294:ILE:HD12	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:368:ILE:HG21	1:A:387:LEU:HD22	1.93	0.49
1:A:35:TYR:CD1	1:A:368:ILE:HG23	2.48	0.49
1:A:412:LEU:HD13	1:A:435:TYR:CE2	2.48	0.49
1:A:368:ILE:HG21	1:A:387:LEU:CD2	2.43	0.49
1:D:186:ASP:HB2	1:D:281:GLN:OE1	2.14	0.48
1:B:358:ILE:HG23	1:B:362:LYS:HD3	1.95	0.48
1:C:368:ILE:HG21	1:C:387:LEU:HD22	1.96	0.48
1:D:368:ILE:HG21	1:D:387:LEU:HD22	1.96	0.48
1:A:2:SER:N	1:A:131:GLU:OE2	2.47	0.47
1:C:35:TYR:CD1	1:C:368:ILE:HG23	2.49	0.47
1:C:187:LEU:HD21	1:C:294:ILE:HD12	1.96	0.47
1:C:191:ASP:O	1:C:195:GLU:HG2	2.15	0.46
1:B:271:ILE:HD13	1:B:430:GLN:HG2	1.97	0.46
1:C:368:ILE:HG21	1:C:387:LEU:CD2	2.46	0.46
1:A:126:ILE:HD13	1:A:167[B]:SER:OG	2.16	0.46
1:B:445:PRO:O	1:B:446:ARG:HB2	2.16	0.45
1:B:368:ILE:HG21	1:B:387:LEU:HD22	1.99	0.45
1:B:151:PHE:HB2	4:B:504:E7Q:C01	2.46	0.45
1:D:368:ILE:HG21	1:D:387:LEU:CD2	2.47	0.45
1:A:72:LYS:HG2	1:A:76:MET:HE3	1.99	0.45
1:B:368:ILE:HG21	1:B:387:LEU:CD2	2.47	0.44
1:D:20:LYS:HE2	1:D:151[A]:PHE:CE2	2.53	0.44
1:D:430:GLN:O	1:D:433:GLN:HG2	2.18	0.44
1:B:98:ASN:O	1:B:98:ASN:ND2	2.50	0.44
1:B:282[B]:CYS:SG	1:B:323:ILE:HD11	2.58	0.44
1:B:432:TYR:HA	1:B:444:VAL:HG21	2.00	0.43
1:C:249:LEU:HD13	1:C:253:ILE:HD13	2.00	0.43
1:A:35:TYR:CZ	1:A:373:PRO:HD3	2.53	0.43
1:D:282[B]:CYS:SG	1:D:323:ILE:HD11	2.58	0.43
1:A:187:LEU:HD21	1:A:294:ILE:HD12	2.00	0.43
1:A:188:HIS:CE1	4:A:504:E7Q:C10	3.01	0.43
1:A:368:ILE:CG2	1:A:387:LEU:HD22	2.49	0.43
1:C:2:SER:N	1:C:131:GLU:OE2	2.51	0.43
1:C:365:LYS:O	1:C:366:MET:HE2	2.18	0.43
1:A:282[B]:CYS:SG	1:A:323:ILE:HD11	2.59	0.42
1:B:178:THR:HB	1:B:202:ARG:HH21	1.84	0.42
1:D:195:GLU:OE2	6:D:601:HOH:O	2.22	0.42
1:D:159:LEU:HD23	1:D:159:LEU:HA	1.85	0.42
1:A:359:GLU:HG3	1:A:364:LYS:O	2.19	0.42
1:A:142:HIS:HD2	4:A:504:E7Q:C05	2.33	0.41
1:B:77:LEU:HD13	1:B:84:LEU:HG	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:249:LEU:HD13	1:B:253:ILE:HD13	2.02	0.41
1:C:141:HIS:CD2	1:C:141:HIS:H	2.38	0.41
1:B:140:TRP:CZ3	4:B:504:E7Q:C02	3.03	0.41
1:A:416:ARG:HD3	1:A:428:TYR:OH	2.21	0.41
1:B:35:TYR:CZ	1:B:373:PRO:HD3	2.55	0.41
1:C:139:GLY:HA2	1:C:157:ILE:HD11	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	390/446 (87%)	384 (98%)	6 (2%)	0	100	100
1	B	403/446 (90%)	398 (99%)	5 (1%)	0	100	100
1	C	399/446 (90%)	394 (99%)	5 (1%)	0	100	100
1	D	390/446 (87%)	385 (99%)	4 (1%)	1 (0%)	36	19
All	All	1582/1784 (89%)	1561 (99%)	20 (1%)	1 (0%)	48	26

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	81	GLU

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	348/391 (89%)	348 (100%)	0	100	100
1	B	362/391 (93%)	359 (99%)	3 (1%)	73	51
1	C	358/391 (92%)	354 (99%)	4 (1%)	65	38
1	D	347/391 (89%)	345 (99%)	2 (1%)	78	59
All	All	1415/1564 (90%)	1406 (99%)	9 (1%)	78	59

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	131	GLU
1	B	366	MET
1	B	446	ARG
1	C	98	ASN
1	C	101	CYS
1	C	314[A]	CYS
1	C	314[B]	CYS
1	D	80	GLU
1	D	223	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	98	ASN
1	D	33	ASN
1	D	405	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 19 ligands modelled in this entry, 12 are monoatomic - leaving 7 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
5	GOL	A	505	-	5,5,5	0.46	0	5,5,5	0.85	0
4	E7Q	B	505	-	15,15,24	0.23	0	21,21,33	0.34	0
5	GOL	C	504	-	5,5,5	0.30	0	5,5,5	0.58	0
4	E7Q	B	504	2	8,8,24	0.88	1 (12%)	7,8,33	1.62	1 (14%)
4	E7Q	A	506	-	15,15,24	0.23	0	21,21,33	0.37	0
4	E7Q	A	504	2	24,24,24	0.30	0	27,33,33	0.89	1 (3%)
5	GOL	B	506	-	5,5,5	0.35	0	5,5,5	0.47	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	A	505	-	-	4/4/4/4	-
4	E7Q	B	505	-	-	0/4/17/33	0/2/2/2
5	GOL	C	504	-	-	1/4/4/4	-
4	E7Q	B	504	2	-	5/7/7/33	-
4	E7Q	A	506	-	-	0/4/17/33	0/2/2/2
4	E7Q	A	504	2	-	9/13/33/33	0/2/2/2
5	GOL	B	506	-	-	1/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	504	E7Q	C06-N08	2.12	1.34	1.32

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	504	E7Q	C22-C10-N08	3.87	121.49	111.90
4	B	504	E7Q	O09-N08-C06	-3.83	114.13	119.79

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	504	E7Q	C05-C06-N08-C10
4	A	504	E7Q	C05-C06-N08-O09
4	A	504	E7Q	O07-C06-N08-C10
4	A	504	E7Q	O07-C06-N08-O09
4	B	504	E7Q	C05-C06-N08-O09
4	B	504	E7Q	O07-C06-N08-O09
5	A	505	GOL	O1-C1-C2-C3
4	B	504	E7Q	C03-C04-C05-C06
4	B	504	E7Q	C02-C03-C04-C05
4	A	504	E7Q	C02-C03-C04-C05
4	B	504	E7Q	C01-C02-C03-C04
5	A	505	GOL	C1-C2-C3-O3
4	A	504	E7Q	C04-C05-C06-N08
4	A	504	E7Q	C04-C05-C06-O07
5	C	504	GOL	C1-C2-C3-O3
5	A	505	GOL	O1-C1-C2-O2
5	A	505	GOL	O2-C2-C3-O3
4	A	504	E7Q	C21-C15-N14-C12
4	A	504	E7Q	C03-C04-C05-C06
5	B	506	GOL	O1-C1-C2-O2

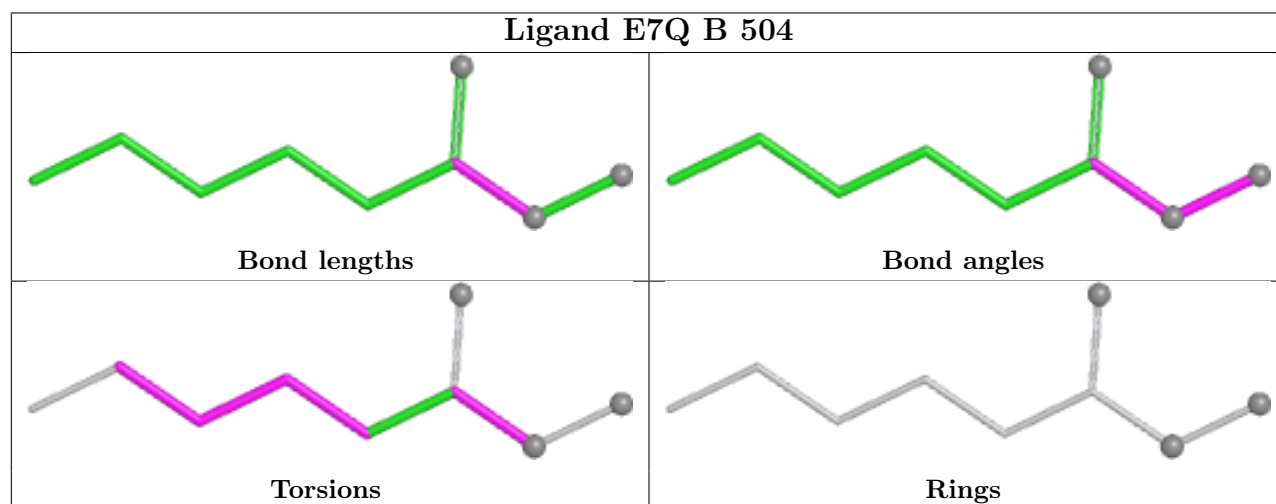
There are no ring outliers.

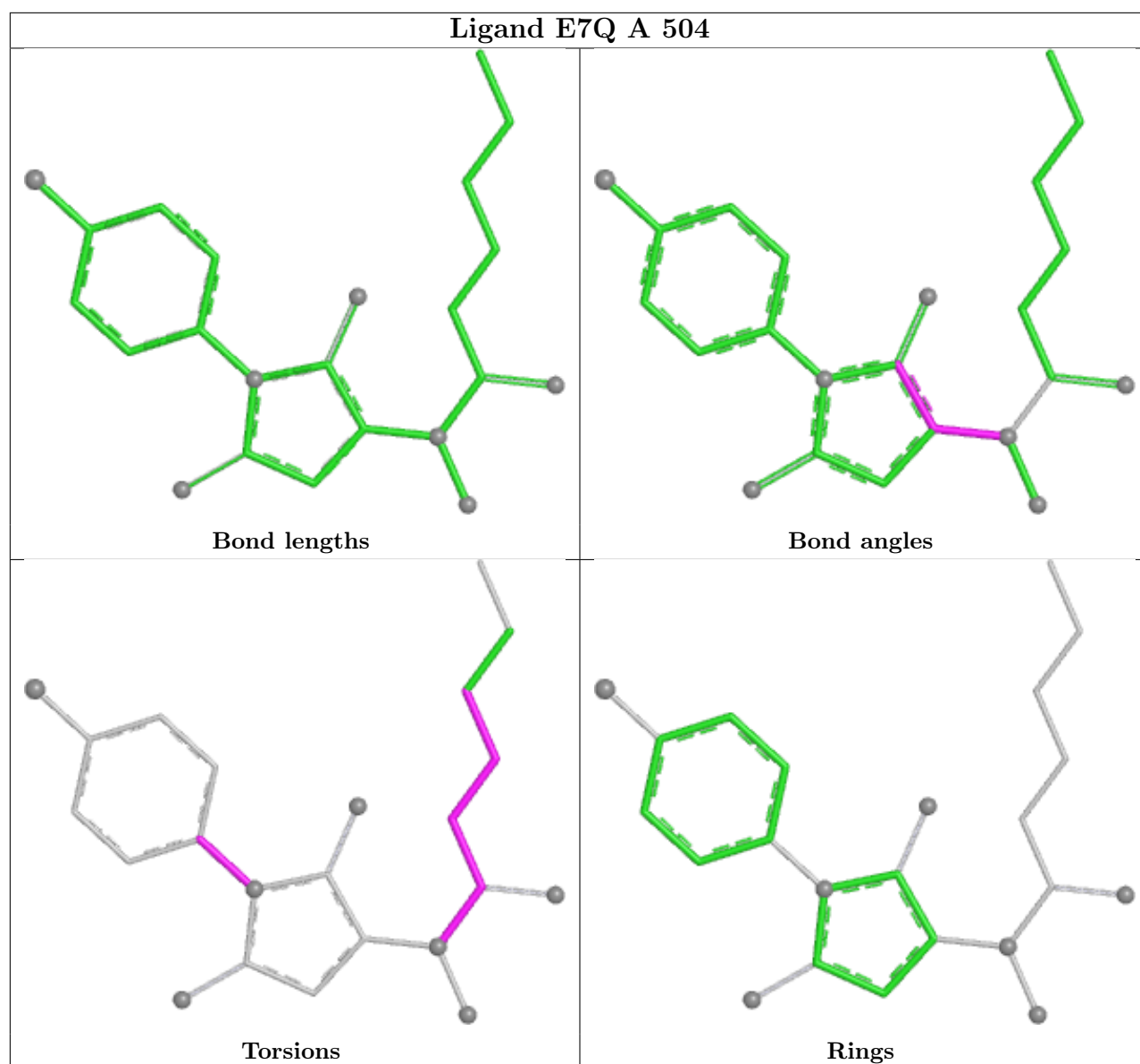
3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	505	GOL	1	0
4	B	504	E7Q	5	0
4	A	504	E7Q	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 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.





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	395/446 (88%)	1.03	55 (13%) 6 8	14, 25, 56, 96	6 (1%)
1	B	411/446 (92%)	0.88	44 (10%) 11 15	13, 24, 45, 94	6 (1%)
1	C	407/446 (91%)	0.84	41 (10%) 12 17	13, 23, 46, 99	6 (1%)
1	D	396/446 (88%)	1.20	69 (17%) 4 5	14, 27, 60, 100	4 (1%)
All	All	1609/1784 (90%)	0.99	209 (12%) 7 10	13, 25, 50, 100	22 (1%)

All (209) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	425	ILE	7.4
1	A	392	PHE	7.3
1	B	231	PRO	7.1
1	D	426	TYR	7.0
1	B	222	TRP	6.9
1	D	434	LEU	6.6
1	C	222	TRP	6.6
1	D	435	TYR	6.2
1	A	426	TYR	6.1
1	C	102	PRO	5.9
1	B	401	LEU	5.8
1	C	151[A]	PHE	5.7
1	A	428	TYR	5.7
1	A	425	ILE	5.5
1	B	400	THR	5.5
1	C	310	CYS	5.5
1	D	428	TYR	5.5
1	B	232	ILE	5.3
1	A	435	TYR	5.3
1	D	315	SER	5.0
1	A	222	TRP	4.9

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Mol	Chain	Res	Type	RSRZ
1	B	79	CYS	4.8
1	A	223	ASN	4.8
1	B	314[A]	CYS	4.8
1	B	102	PRO	4.7
1	D	392	PHE	4.7
1	A	423	LYS	4.6
1	D	223	ASN	4.6
1	C	232	ILE	4.6
1	D	165	VAL	4.6
1	A	434	LEU	4.6
1	D	232	ILE	4.4
1	A	383	PRO	4.3
1	D	368	ILE	4.3
1	D	432	TYR	4.3
1	D	383	PRO	4.2
1	D	79	CYS	4.1
1	D	101	CYS	4.1
1	D	222	TRP	4.0
1	A	100	ASP	4.0
1	A	432	TYR	4.0
1	B	98	ASN	4.0
1	A	81	GLU	4.0
1	A	79	CYS	3.9
1	D	302	PRO	3.9
1	D	99	TYR	3.9
1	A	151[A]	PHE	3.9
1	B	368	ILE	3.8
1	D	102	PRO	3.8
1	B	151	PHE	3.7
1	A	233	PHE	3.7
1	A	385	PHE	3.7
1	A	19	PRO	3.6
1	C	98	ASN	3.6
1	A	165	VAL	3.6
1	D	100	ASP	3.6
1	D	151[A]	PHE	3.6
1	A	101	CYS	3.6
1	C	314[A]	CYS	3.6
1	C	105	PRO	3.5
1	B	341	TYR	3.5
1	B	395	GLU	3.5
1	B	313	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	423	LYS	3.4
1	C	368	ILE	3.4
1	D	81	GLU	3.4
1	C	7	TYR	3.4
1	B	434	LEU	3.4
1	A	98	ASN	3.3
1	D	105	PRO	3.2
1	A	99	TYR	3.2
1	B	446	ARG	3.2
1	C	83	GLU	3.2
1	A	393	PRO	3.2
1	C	101	CYS	3.1
1	B	104	PHE	3.1
1	C	104	PHE	3.1
1	D	84	LEU	3.1
1	B	83	GLU	3.1
1	B	101	CYS	3.1
1	A	7	TYR	3.0
1	A	102	PRO	3.0
1	D	385	PHE	3.0
1	A	80	GLU	3.0
1	B	425	ILE	3.0
1	A	82	LYS	3.0
1	A	177	GLN	3.0
1	D	404	ILE	3.0
1	A	302	PRO	2.9
1	B	105	PRO	2.9
1	D	19	PRO	2.9
1	C	165	VAL	2.9
1	C	14	LEU	2.9
1	D	424	LEU	2.9
1	A	167[A]	SER	2.9
1	C	82	LYS	2.9
1	C	434	LEU	2.9
1	B	426	TYR	2.8
1	A	390	ASP	2.8
1	B	165	VAL	2.8
1	D	371	GLU	2.8
1	D	271	ILE	2.8
1	D	167	SER	2.8
1	B	103	GLY	2.8
1	B	177	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	412	LEU	2.8
1	D	406	LYS	2.8
1	A	106	SER	2.7
1	C	2	SER	2.7
1	C	395	GLU	2.7
1	A	404	ILE	2.7
1	A	84	LEU	2.7
1	D	365	LYS	2.7
1	D	393	PRO	2.7
1	C	103	GLY	2.6
1	C	420	ASP	2.6
1	C	10	GLN	2.6
1	D	382	GLY	2.6
1	C	76	MET	2.6
1	D	376	SER	2.6
1	D	321	TYR	2.6
1	A	402	ASP	2.6
1	B	438	THR	2.5
1	A	424	LEU	2.5
1	D	10	GLN	2.5
1	A	103	GLY	2.5
1	D	82	LYS	2.5
1	D	98	ASN	2.5
1	D	429	ASP	2.5
1	A	56	TYR	2.5
1	B	7	TYR	2.5
1	B	437	LEU	2.5
1	C	84	LEU	2.5
1	D	7	TYR	2.5
1	D	301	TYR	2.5
1	C	313	GLU	2.5
1	D	34	ALA	2.5
1	D	402	ASP	2.5
1	A	368	ILE	2.5
1	C	341	TYR	2.5
1	D	369	SER	2.4
1	A	105	PRO	2.4
1	C	384	ASP	2.4
1	C	85	THR	2.4
1	B	91	LEU	2.4
1	A	379	SER	2.4
1	D	2	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	233	PHE	2.4
1	D	363	GLY	2.4
1	D	37	LEU	2.4
1	D	104	PHE	2.4
1	D	166	SER	2.3
1	D	262	ILE	2.3
1	B	311	ASP	2.3
1	D	292	HIS	2.3
1	B	315	SER	2.3
1	D	427	ASP	2.3
1	C	437	LEU	2.3
1	D	128	ARG	2.3
1	D	80	GLU	2.3
1	A	431	VAL	2.3
1	D	76	MET	2.3
1	B	84	LEU	2.3
1	A	429	ASP	2.2
1	C	178	THR	2.2
1	B	356	LEU	2.2
1	D	356	LEU	2.2
1	D	56	TYR	2.2
1	B	62	PHE	2.2
1	C	166	SER	2.2
1	B	443	LEU	2.2
1	C	425	ILE	2.2
1	A	239	ARG	2.2
1	C	108	PHE	2.2
1	D	431	VAL	2.2
1	D	61	ALA	2.1
1	C	446	ARG	2.1
1	C	433	GLN	2.1
1	A	78	HIS	2.1
1	D	412	LEU	2.1
1	A	178	THR	2.1
1	C	367	THR	2.1
1	A	20	LYS	2.1
1	B	179[A]	ARG	2.1
1	B	13	GLN	2.1
1	A	83	GLU	2.1
1	A	378	PHE	2.1
1	D	403	SER	2.1
1	B	402	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	77	LEU	2.1
1	B	77	LEU	2.1
1	D	77	LEU	2.1
1	A	433	GLN	2.1
1	B	140	TRP	2.1
1	B	9	ASP	2.1
1	B	50	ASP	2.1
1	D	384	ASP	2.1
1	C	59	VAL	2.0
1	A	128	ARG	2.0
1	B	195	GLU	2.0
1	C	153	TYR	2.0
1	C	426	TYR	2.0
1	D	265	ILE	2.0
1	A	76	MET	2.0
1	C	438	THR	2.0
1	D	164	LEU	2.0
1	B	436	ASN	2.0
1	C	390	ASP	2.0
1	A	391	TYR	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 oligosaccharides 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
4	E7Q	A	504	23/23	0.67	0.30	35,78,87,94	0
4	E7Q	B	504	9/23	0.77	0.27	35,45,73,75	0
5	GOL	A	505	6/6	0.82	0.18	26,34,40,46	0

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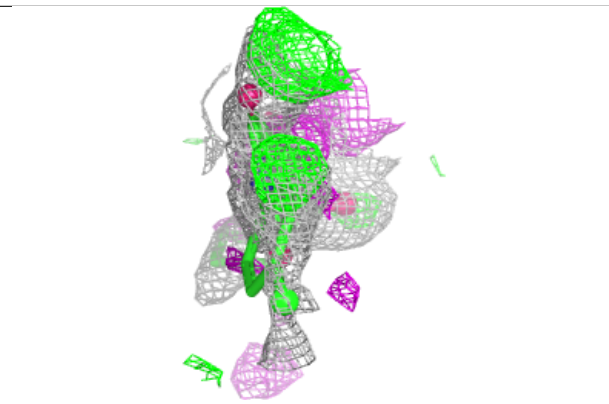
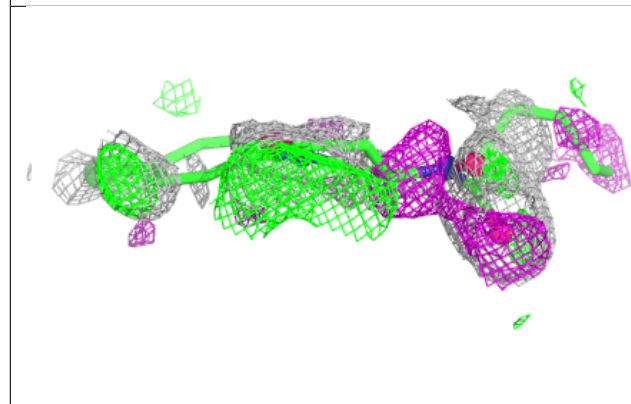
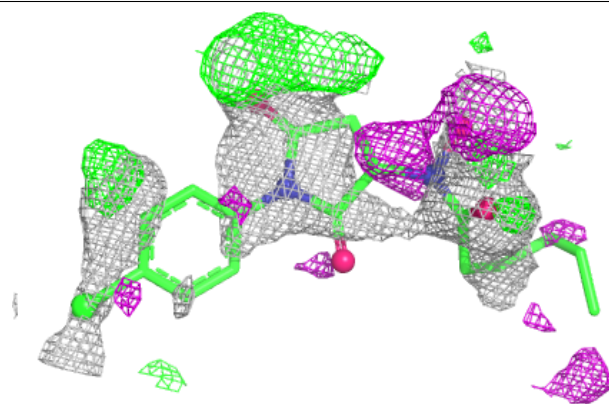
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	GOL	B	506	6/6	0.88	0.13	26,31,35,35	0
5	GOL	C	504	6/6	0.91	0.11	26,32,34,35	0
4	E7Q	B	505	14/23	0.92	0.10	22,29,33,38	0
4	E7Q	A	506	14/23	0.94	0.08	22,28,34,39	0
3	K	C	503	1/1	0.97	0.09	27,27,27,27	0
3	K	D	503	1/1	0.98	0.17	26,26,26,26	0
3	K	B	503	1/1	0.98	0.08	31,31,31,31	0
3	K	A	503	1/1	0.99	0.12	27,27,27,27	0
2	ZN	D	501	1/1	1.00	0.11	25,25,25,25	0
3	K	A	502	1/1	1.00	0.01	17,17,17,17	0
2	ZN	A	501	1/1	1.00	0.08	25,25,25,25	0
3	K	B	502	1/1	1.00	0.02	17,17,17,17	0
2	ZN	B	501	1/1	1.00	0.14	25,25,25,25	0
3	K	C	502	1/1	1.00	0.02	17,17,17,17	0
2	ZN	C	501	1/1	1.00	0.10	24,24,24,24	0
3	K	D	502	1/1	1.00	0.04	17,17,17,17	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.

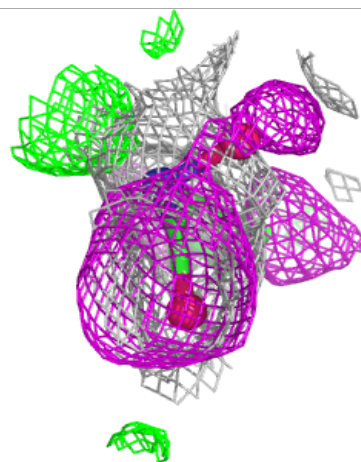
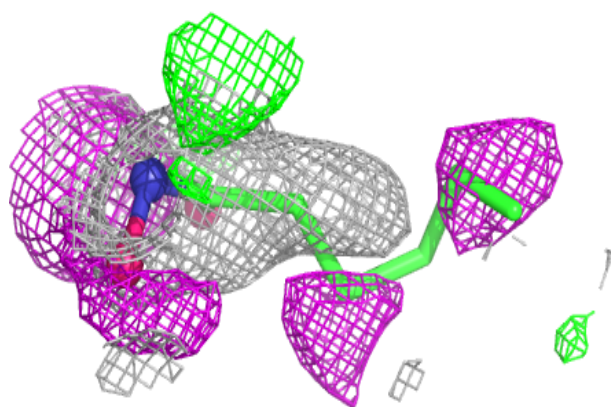
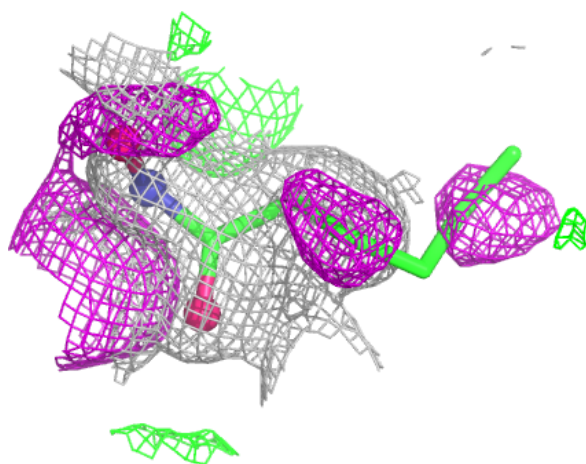
Electron density around E7Q A 504:

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 E7Q B 504:

$2mF_o-DF_c$ (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.