Full wwPDB X-ray Structure Validation Report (i)

Oct 2, 2024 – 12:09 PM EDT

PDB ID	:	9BFG
Title	:	Structure of the crosslinked PCP-E didomain of tyrocidine synthetase A
Authors	:	Heberlig, G.W.; Burkart, M.D.
Deposited on	:	2024-04-17
Resolution	:	2.18 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:

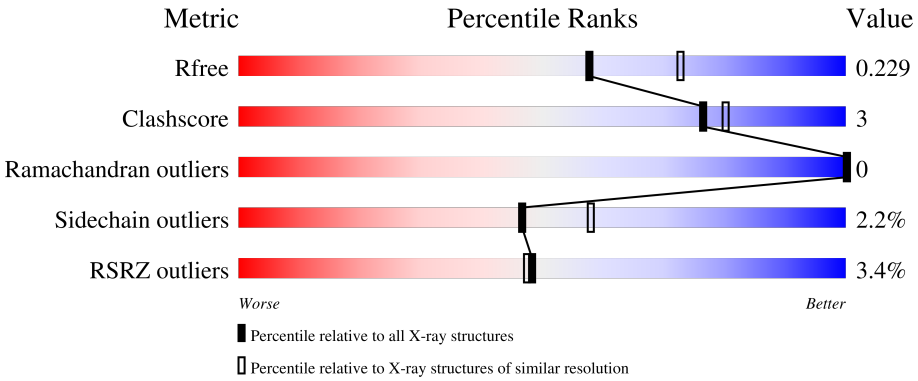
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 2.18 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}	164625	8336 (2.20-2.16)
Clashscore	180529	9404 (2.20-2.16)
Ramachandran outliers	177936	9297 (2.20-2.16)
Sidechain outliers	177891	9297 (2.20-2.16)
RSRZ outliers	164620	8337 (2.20-2.16)

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	555	4% 90% 6% ·
1	B	555	2% 88% 8% ·

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
4	GOL	A	612	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 17521 atoms, of which 8525 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 Tyrocidine synthase 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	533	Total	C	H	N	O	S	129	0	0
			8460	2706	4204	733	809	8			
1	B	532	Total	C	H	N	O	S	131	0	0
			8449	2706	4198	730	807	8			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP P09095
A	2	VAL	-	expression tag	UNP P09095
A	370	ALA	GLU	engineered mutation	UNP P09095
A	546	GLY	-	expression tag	UNP P09095
A	547	SER	-	expression tag	UNP P09095
A	548	ARG	-	expression tag	UNP P09095
A	549	SER	-	expression tag	UNP P09095
A	550	HIS	-	expression tag	UNP P09095
A	551	HIS	-	expression tag	UNP P09095
A	552	HIS	-	expression tag	UNP P09095
A	553	HIS	-	expression tag	UNP P09095
A	554	HIS	-	expression tag	UNP P09095
A	555	HIS	-	expression tag	UNP P09095
B	1	MET	-	expression tag	UNP P09095
B	2	VAL	-	expression tag	UNP P09095
B	370	ALA	GLU	engineered mutation	UNP P09095
B	546	GLY	-	expression tag	UNP P09095
B	547	SER	-	expression tag	UNP P09095
B	548	ARG	-	expression tag	UNP P09095
B	549	SER	-	expression tag	UNP P09095
B	550	HIS	-	expression tag	UNP P09095
B	551	HIS	-	expression tag	UNP P09095
B	552	HIS	-	expression tag	UNP P09095
B	553	HIS	-	expression tag	UNP P09095
B	554	HIS	-	expression tag	UNP P09095

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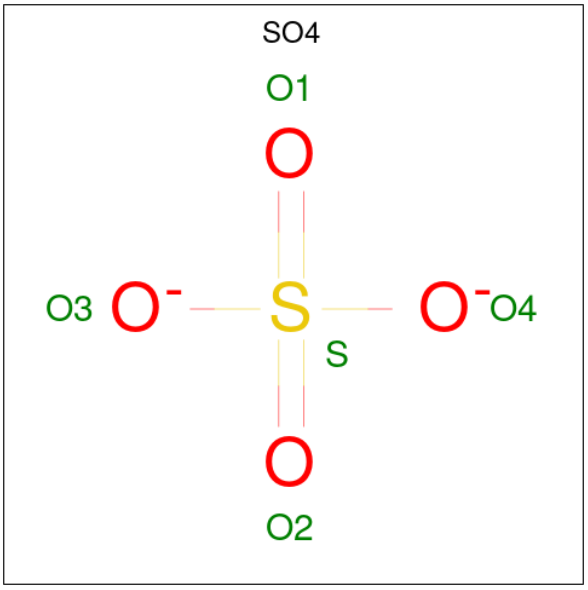
Chain	Residue	Modelled	Actual	Comment	Reference
B	555	HIS	-	expression tag	UNP P09095

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0

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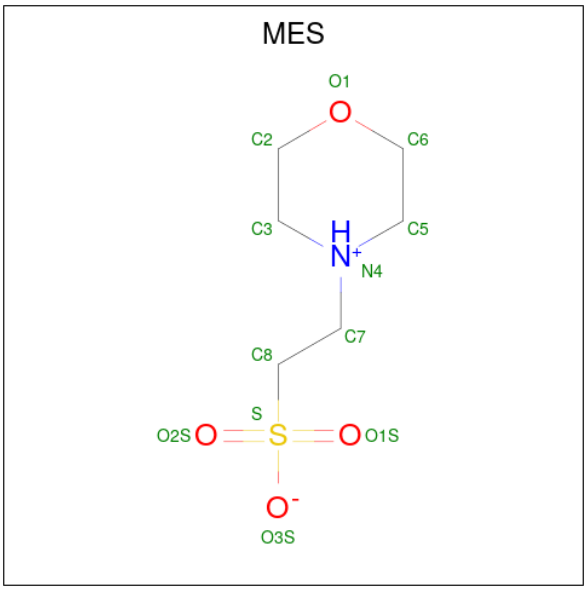
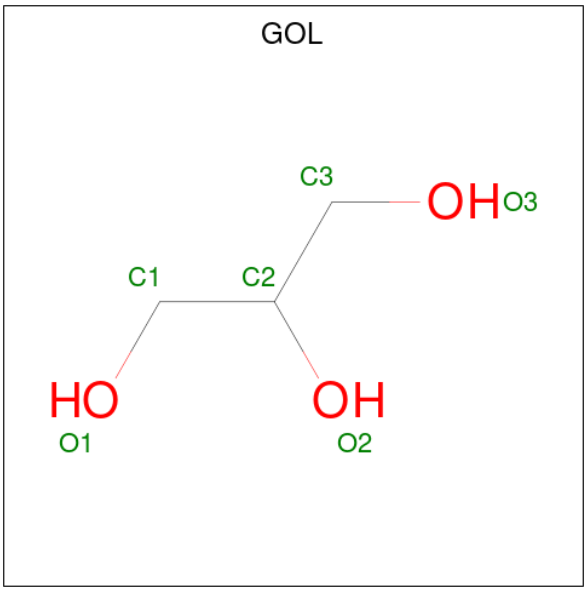
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total O S 5 4 1	0	0

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



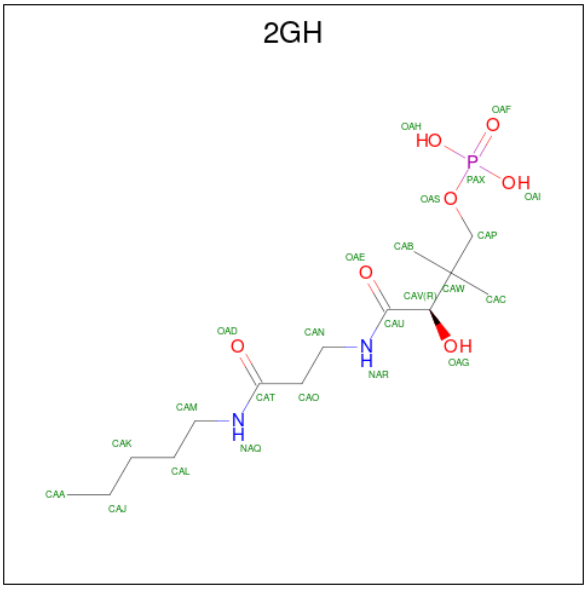
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C H N O S 25 6 13 1 4 1	0	0
3	B	1	Total C H N O S 25 6 13 1 4 1	0	0
3	B	1	Total C H N O S 25 6 13 1 4 1	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C H O 14 3 8 3	2	0
4	A	1	Total C H O 14 3 8 3	2	0
4	B	1	Total C H O 14 3 8 3	2	0
4	B	1	Total C H O 14 3 8 3	2	0

- Molecule 5 is N 3 -[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-N-pentyl-beta-alaninamide (three-letter code: 2GH) (formula: $C_{14}H_{29}N_2O_7P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	C	H	N	O	P	1	0
			49	14	26	2	6	1		
5	B	1	Total	C	H	N	O	P	1	0
			49	14	26	2	6	1		

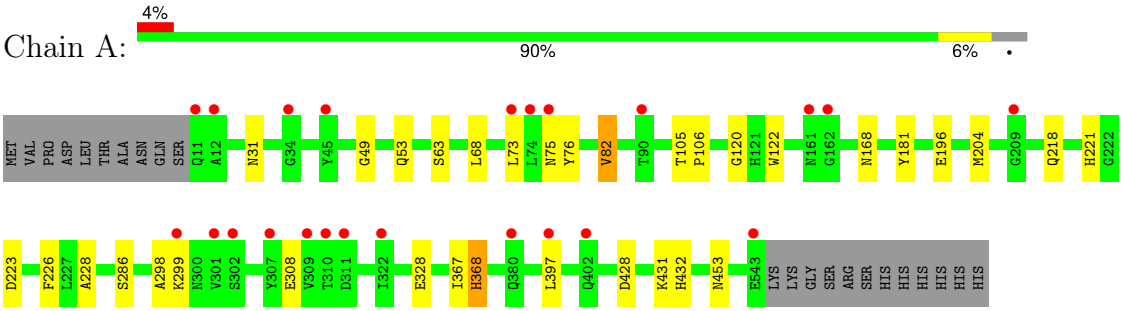
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	167	Total	O	0	0
			167	167		
6	B	156	Total	O	0	0
			156	156		

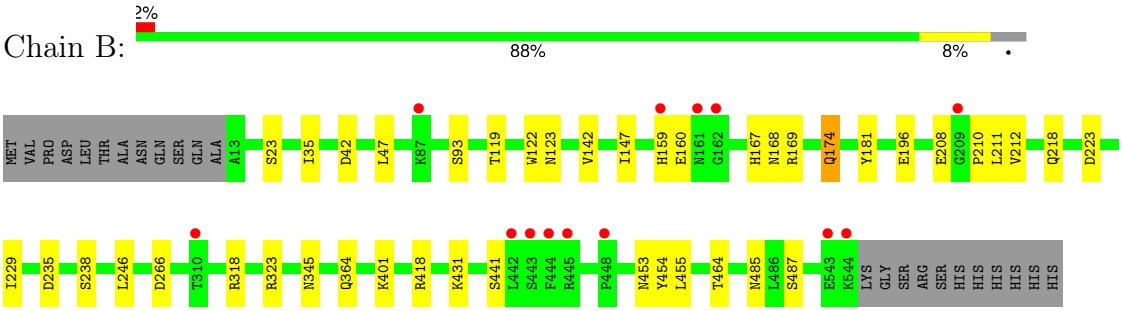
3 Residue-property plots (i)

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: Tyrocidine synthase 1



• Molecule 1: Tyrocidine synthase 1



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α, β, γ	216.38Å 216.38Å 59.76Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.85 – 2.18 46.85 – 2.18	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.85-2.18) 100.0 (46.85-2.18)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.67 (at 2.18Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.188 , 0.228 0.188 , 0.229	Depositor DCC
R_{free} test set	4242 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	36.3	Xtriage
Anisotropy	0.243	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.44 , 34.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.023 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	17521	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.80% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 2GH, GOL, MES, SO4

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	0.69	0/4352	0.81	0/5910
1	B	0.70	0/4348	0.83	0/5905
All	All	0.70	0/8700	0.82	0/11815

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

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	4256	4204	4180	22	2
1	B	4251	4198	4172	24	2
2	A	40	0	0	0	0
2	B	20	0	0	1	0
3	A	12	13	13	1	0
3	B	24	26	26	2	0
4	A	12	16	16	6	0
4	B	12	16	16	1	0
5	A	23	26	27	3	0
5	B	23	26	28	5	0
6	A	167	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	156	0	0	5	0
All	All	8996	8525	8478	48	2

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 (48) 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:A:76:TYR:CB	6:A:855:HOH:O	2.01	1.08
4:A:605:GOL:O1	5:A:610:2GH:H26	1.82	0.78
3:A:603:MES:H52	6:A:773:HOH:O	1.92	0.70
1:B:196:GLU:HG2	6:B:807:HOH:O	1.91	0.69
1:B:196:GLU:CG	6:B:807:HOH:O	2.42	0.67
1:B:345:ASN:ND2	5:B:608:2GH:H8	2.13	0.64
1:B:174:GLN:HB3	1:B:210:PRO:HG3	1.80	0.64
1:B:181:TYR:CE2	1:B:196:GLU:HG3	2.35	0.62
1:A:221:HIS:HD2	6:B:750:HOH:O	1.83	0.61
1:B:42:ASP:HB3	1:B:47:LEU:HD11	1.81	0.61
1:A:63:SER:HB3	6:A:766:HOH:O	1.99	0.61
1:A:431:LYS:NZ	4:A:612:GOL:H11	2.16	0.59
4:A:605:GOL:HO1	5:A:610:2GH:H26	1.71	0.54
1:A:308:GLU:H	1:A:308:GLU:CD	2.11	0.54
1:B:318:ARG:HD3	6:B:701:HOH:O	2.10	0.51
1:A:181:TYR:CE2	1:A:196:GLU:HG2	2.44	0.51
1:B:323:ARG:NH1	2:B:601:SO4:O3	2.42	0.51
1:B:123:ASN:O	1:B:485:ASN:HB3	2.10	0.50
1:B:431:LYS:NZ	4:B:609:GOL:H11	2.27	0.50
1:A:453:ASN:HD21	5:A:610:2GH:H20	1.78	0.49
1:A:181:TYR:CZ	1:A:196:GLU:HG2	2.49	0.48
1:B:93:SER:OG	1:B:266:ASP:OD1	2.29	0.47
1:A:73:LEU:HD12	1:A:82:VAL:HG21	1.97	0.46
1:A:431:LYS:CE	4:A:612:GOL:H11	2.45	0.46
1:B:218:GLN:HA	1:B:223:ASP:OD1	2.16	0.46
1:A:431:LYS:HZ1	4:A:612:GOL:H11	1.81	0.45
1:B:159:HIS:CE1	6:B:820:HOH:O	2.70	0.45
1:A:120:GLY:O	1:A:204:MET:HB2	2.16	0.45
1:A:226:PHE:CZ	1:A:228:ALA:HB2	2.53	0.44
1:B:453:ASN:HD21	5:B:608:2GH:H19	1.83	0.43
1:A:218:GLN:HA	1:A:223:ASP:OD1	2.19	0.43
1:B:455:LEU:HG	5:B:608:2GH:H22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:454:TYR:O	5:B:608:2GH:H15	2.18	0.43
1:B:167:HIS:NE2	3:B:605:MES:H72	2.33	0.43
1:B:169:ARG:HB3	3:B:605:MES:H62	2.00	0.43
1:A:368:HIS:HE1	6:A:817:HOH:O	2.02	0.43
1:A:431:LYS:HZ3	4:A:612:GOL:H32	1.85	0.42
1:A:105:THR:HB	1:A:106:PRO:HD2	2.02	0.41
1:B:345:ASN:HD21	5:B:608:2GH:H8	1.85	0.41
1:A:68:LEU:HD12	1:A:68:LEU:HA	1.96	0.41
1:A:49:GLY:HA2	1:A:53:GLN:OE1	2.21	0.41
1:B:142:VAL:HG11	1:B:246:LEU:HD12	2.03	0.41
1:A:298:ALA:HB2	1:A:397:LEU:HD11	2.03	0.41
1:A:432:HIS:HD2	6:A:858:HOH:O	2.02	0.41
1:B:211:LEU:O	1:B:229:ILE:HA	2.21	0.40
1:B:235:ASP:H	1:B:238:SER:HB2	1.87	0.40
1:B:147:ILE:CD1	1:B:212:VAL:HG21	2.52	0.40
1:A:221:HIS:HE1	1:B:464:THR:O	2.04	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:SER:HG	1:B:364:GLN:HE22[5_554]	1.11	0.49
1:A:75:ASN:OD1	1:B:441:SER:OG[5_554]	2.07	0.13

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	531/555 (96%)	517 (97%)	14 (3%)	0	100	100
1	B	530/555 (96%)	515 (97%)	15 (3%)	0	100	100
All	All	1061/1110 (96%)	1032 (97%)	29 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	462/484 (96%)	453 (98%)	9 (2%)	52	64
1	B	461/484 (95%)	450 (98%)	11 (2%)	44	54
All	All	923/968 (95%)	903 (98%)	20 (2%)	47	58

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	ASN
1	A	82	VAL
1	A	122	TRP
1	A	168	ASN
1	A	299	LYS
1	A	328	GLU
1	A	367	ILE
1	A	368	HIS
1	A	428	ASP
1	B	23	SER
1	B	35	ILE
1	B	119	THR
1	B	122	TRP
1	B	160	GLU
1	B	168	ASN
1	B	174	GLN
1	B	208	GLU
1	B	401	LYS
1	B	418	ARG
1	B	487	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	221	HIS
1	B	531	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

21 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	SO4	A	611	-	4,4,4	0.26	0	6,6,6	0.23	0
4	GOL	B	606	-	5,5,5	0.13	0	5,5,5	0.40	0
3	MES	B	605	-	12,12,12	0.71	0	15,16,16	0.53	0
2	SO4	A	609	-	4,4,4	0.43	0	6,6,6	0.24	0
2	SO4	B	607	-	4,4,4	0.31	0	6,6,6	0.12	0
4	GOL	A	612	-	5,5,5	0.18	0	5,5,5	0.49	0
2	SO4	B	602	-	4,4,4	0.30	0	6,6,6	0.11	0
2	SO4	B	604	-	4,4,4	0.31	0	6,6,6	0.20	0
2	SO4	A	607	-	4,4,4	0.28	0	6,6,6	0.10	0
5	2GH	B	608	1	18,22,23	0.63	0	21,28,31	1.62	5 (23%)
2	SO4	B	601	-	4,4,4	0.34	0	6,6,6	0.11	0
4	GOL	B	609	-	5,5,5	0.11	0	5,5,5	0.36	0
2	SO4	A	604	-	4,4,4	0.26	0	6,6,6	0.19	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	SO4	A	608	-	4,4,4	0.29	0	6,6,6	0.15	0
5	2GH	A	610	1	18,22,23	0.37	0	21,28,31	0.94	2 (9%)
2	SO4	A	601	-	4,4,4	0.34	0	6,6,6	0.10	0
3	MES	B	603	-	12,12,12	0.67	0	15,16,16	0.74	1 (6%)
2	SO4	A	602	-	4,4,4	0.30	0	6,6,6	0.15	0
3	MES	A	603	-	12,12,12	0.76	0	15,16,16	0.96	1 (6%)
4	GOL	A	605	-	5,5,5	0.22	0	5,5,5	0.41	0
2	SO4	A	606	-	4,4,4	0.30	0	6,6,6	0.10	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
3	MES	B	603	-	-	0/6/14/14	0/1/1/1
4	GOL	B	609	-	-	2/4/4/4	-
4	GOL	B	606	-	-	2/4/4/4	-
3	MES	B	605	-	-	3/6/14/14	0/1/1/1
5	2GH	B	608	1	-	12/26/28/29	-
5	2GH	A	610	1	-	4/26/28/29	-
3	MES	A	603	-	-	6/6/14/14	0/1/1/1
4	GOL	A	612	-	-	4/4/4/4	-
4	GOL	A	605	-	-	2/4/4/4	-

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	608	2GH	CAN-CAO-CAT	3.52	118.26	112.39
5	B	608	2GH	OAE-CAU-CAV	-3.21	111.94	120.89
5	B	608	2GH	CAB-CAW-CAP	3.08	113.31	108.22
5	B	608	2GH	CAM-NAQ-CAT	2.57	127.61	122.82
3	B	603	MES	O2S-S-C8	-2.29	103.27	106.73
3	A	603	MES	O2S-S-C8	-2.23	103.36	106.73
5	A	610	2GH	CAA-CAJ-CAK	-2.21	98.46	113.36
5	A	610	2GH	CAM-NAQ-CAT	2.16	126.85	122.82
5	B	608	2GH	CAV-CAU-NAR	2.07	120.41	116.48

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	603	MES	C8-C7-N4-C5
3	A	603	MES	N4-C7-C8-S
3	A	603	MES	C7-C8-S-O1S
3	A	603	MES	C7-C8-S-O3S
3	B	605	MES	C7-C8-S-O1S
3	B	605	MES	C7-C8-S-O2S
3	B	605	MES	C7-C8-S-O3S
4	A	612	GOL	O1-C1-C2-C3
4	A	612	GOL	C1-C2-C3-O3
4	B	606	GOL	O1-C1-C2-C3
4	B	609	GOL	O1-C1-C2-C3
5	B	608	2GH	OAS-CAP-CAW-CAB
5	B	608	2GH	OAS-CAP-CAW-CAC
5	B	608	2GH	OAS-CAP-CAW-CAV
5	B	608	2GH	CAU-CAV-CAW-CAP
5	B	608	2GH	OAG-CAV-CAW-CAB
5	B	608	2GH	CAU-CAV-CAW-CAB
5	B	608	2GH	CAU-CAV-CAW-CAC
5	B	608	2GH	CAV-CAU-NAR-CAN
5	B	608	2GH	OAE-CAU-NAR-CAN
5	A	610	2GH	CAO-CAT-NAQ-CAM
5	A	610	2GH	OAD-CAT-NAQ-CAM
5	B	608	2GH	CAK-CAL-CAM-NAQ
4	A	605	GOL	C1-C2-C3-O3
4	A	605	GOL	O2-C2-C3-O3
4	A	612	GOL	O1-C1-C2-O2
4	B	609	GOL	O1-C1-C2-O2
4	A	612	GOL	O2-C2-C3-O3
4	B	606	GOL	O1-C1-C2-O2
3	A	603	MES	C8-C7-N4-C3
5	B	608	2GH	CAJ-CAK-CAL-CAM
3	A	603	MES	C7-C8-S-O2S
5	A	610	2GH	CAJ-CAK-CAL-CAM
5	A	610	2GH	CAA-CAJ-CAK-CAL
5	B	608	2GH	OAG-CAV-CAW-CAP

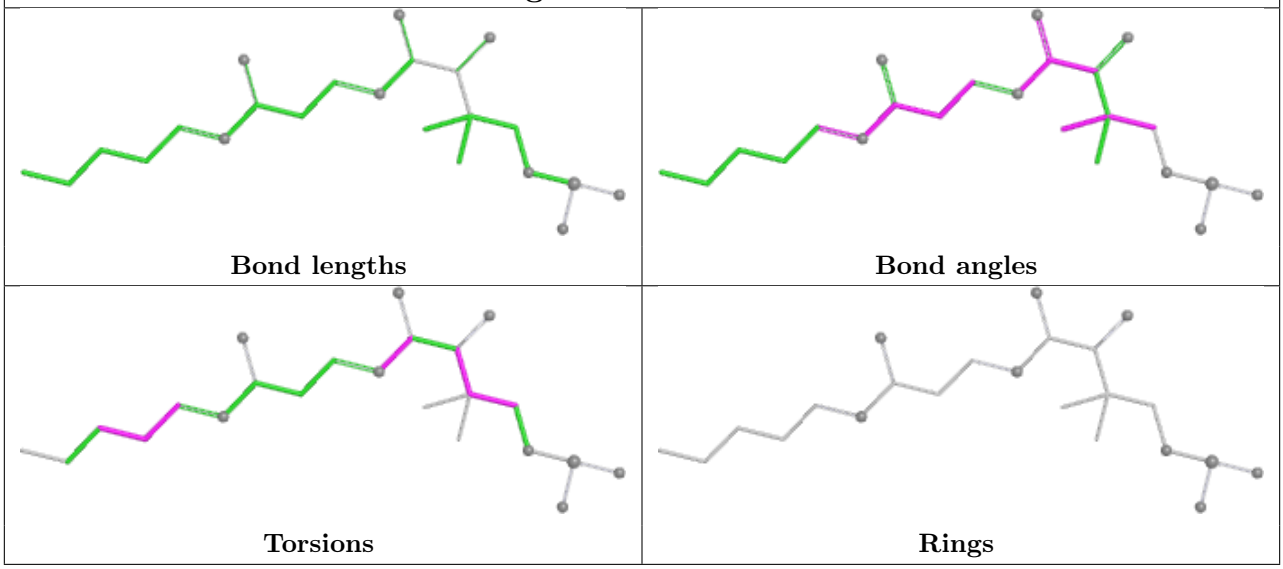
There are no ring outliers.

8 monomers are involved in 17 short contacts:

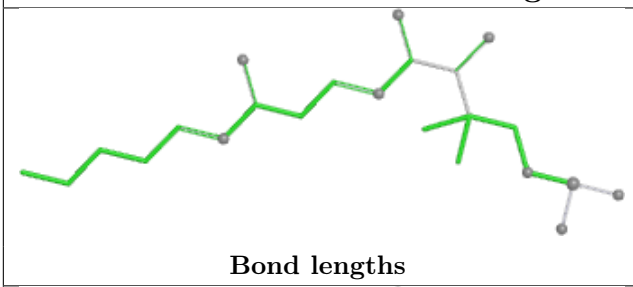
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	605	MES	2	0
4	A	612	GOL	4	0
5	B	608	2GH	5	0
2	B	601	SO4	1	0
4	B	609	GOL	1	0
5	A	610	2GH	3	0
3	A	603	MES	1	0
4	A	605	GOL	2	0

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 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.

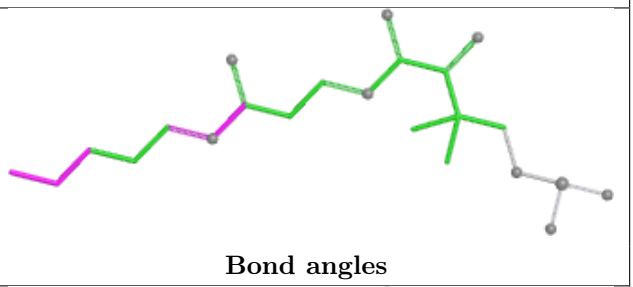
Ligand 2GH B 608



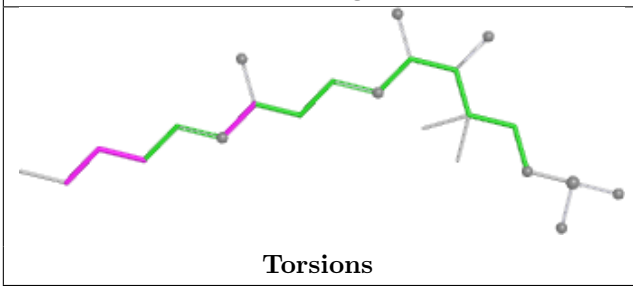
Ligand 2GH A 610



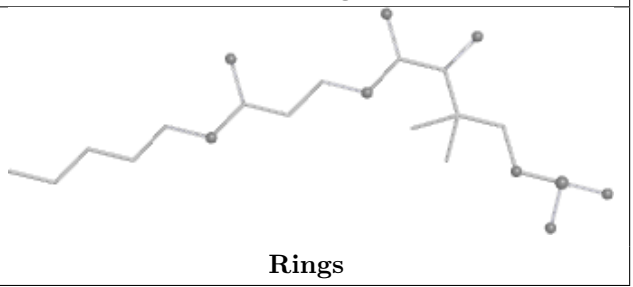
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	533/555 (96%)	-0.03	23 (4%)	40	39	24, 41, 76, 115	0
1	B	532/555 (95%)	-0.03	13 (2%)	59	58	26, 41, 72, 111	0
All	All	1065/1110 (95%)	-0.03	36 (3%)	48	47	24, 41, 74, 115	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	162	GLY	5.3
1	A	301	VAL	4.8
1	B	310	THR	4.3
1	B	162	GLY	3.9
1	B	209	GLY	3.6
1	B	544	LYS	3.6
1	A	209	GLY	3.6
1	B	161	ASN	3.6
1	A	310	THR	3.5
1	A	307	TYR	3.2
1	B	442	LEU	3.2
1	A	11	GLN	3.2
1	A	34	GLY	3.2
1	A	74	LEU	3.1
1	A	402	GLN	3.1
1	A	380	GLN	3.1
1	A	90	THR	3.0
1	B	444	PHE	2.9
1	A	543	GLU	2.8
1	A	161	ASN	2.7
1	A	75	ASN	2.7
1	A	299	LYS	2.6
1	B	159	HIS	2.6
1	A	45	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	309	VAL	2.5
1	B	448	PRO	2.3
1	A	12	ALA	2.3
1	B	443	SER	2.3
1	A	302	SER	2.3
1	A	73	LEU	2.2
1	B	543	GLU	2.2
1	A	397	LEU	2.1
1	B	445	ARG	2.1
1	B	87	LYS	2.1
1	A	322	ILE	2.1
1	A	311	ASP	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	B	607	5/5	0.65	0.16	106,111,119,127	0
3	MES	B	605	12/12	0.72	0.20	71,82,131,152	0
2	SO4	A	609	5/5	0.75	0.15	58,63,79,81	0
4	GOL	A	612	6/6	0.79	0.19	60,63,70,71	2
4	GOL	B	609	6/6	0.80	0.18	56,65,79,80	2
2	SO4	A	607	5/5	0.82	0.10	97,109,121,122	0
2	SO4	A	608	5/5	0.85	0.11	70,72,76,90	0
4	GOL	A	605	6/6	0.85	0.21	56,59,67,67	2
2	SO4	A	611	5/5	0.87	0.11	78,85,89,95	0
2	SO4	A	604	5/5	0.87	0.11	64,67,74,80	0
2	SO4	B	604	5/5	0.91	0.09	57,64,75,83	0

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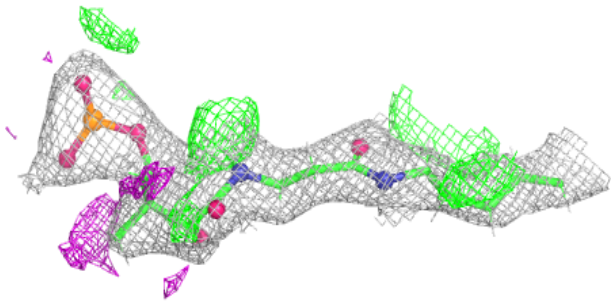
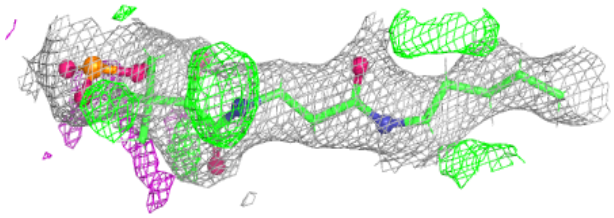
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	A	602	5/5	0.91	0.07	67,75,78,81	0
4	GOL	B	606	6/6	0.91	0.19	46,59,77,78	2
2	SO4	B	601	5/5	0.91	0.07	67,70,75,78	0
5	2GH	B	608	23/24	0.92	0.12	37,47,58,64	1
2	SO4	A	606	5/5	0.93	0.11	110,113,123,126	0
2	SO4	A	601	5/5	0.94	0.06	78,79,83,88	0
2	SO4	B	602	5/5	0.94	0.07	62,63,77,77	0
5	2GH	A	610	23/24	0.96	0.09	33,40,60,64	1
3	MES	A	603	12/12	0.96	0.09	34,39,42,44	0
3	MES	B	603	12/12	0.98	0.05	30,33,34,37	0

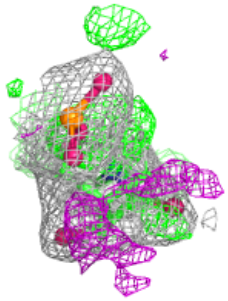
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 2GH B 608:

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

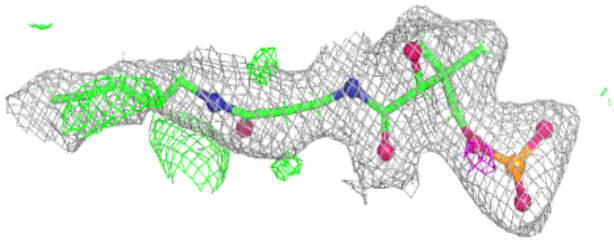


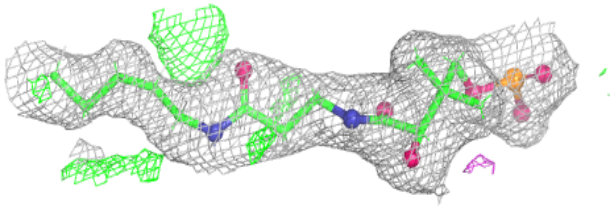


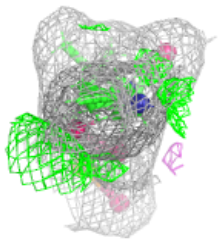


Electron density around 2GH A 610:

$2mF_o$-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.