wwPDB X-ray Structure Validation Summary Report (i)

May 14, 2020 – 03:12 pm BST

PDB ID	:	4A2L
Title	:	Structure of the periplasmic domain of the heparin and heparan sulphate sensing hybrid two component system BT4663 in apo and ligand bound forms
Authors	:	Lowe, E.C.; Basle, A.; Czjzek, M.; Firbank, S.J.; Bolam, D.N.
Deposited on	:	2011-09-27
Resolution	:	2.60 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 following versions of software and data (see references (1)) were used in the production of this report:

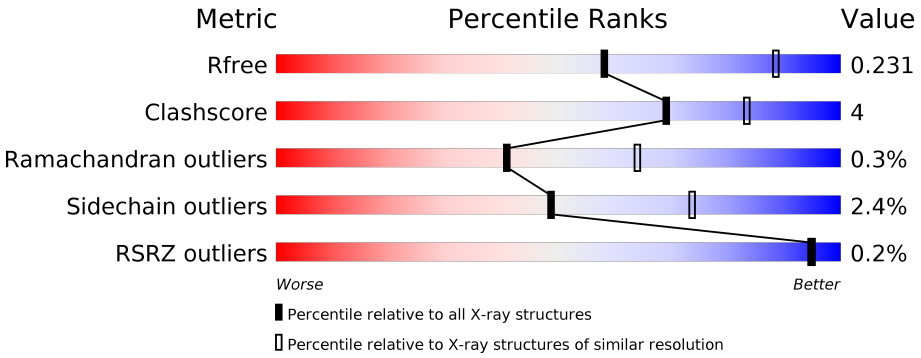
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 on 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	795	84% 9% • 6%
1	B	795	83% 10% 6%
1	C	795	84% 10% • 6%
1	D	795	85% 9% 6%
1	E	795	84% 9% • 6%
1	F	795	85% 9% 6%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 35839 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 TWO-COMPONENT SYSTEM SENSOR HISTIDINE KINASE/RESPONSE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	747	Total	C	N	O	S	0	0	0
			5869	3734	980	1143	12			
1	B	744	Total	C	N	O	S	0	0	0
			5873	3739	977	1145	12			
1	C	749	Total	C	N	O	S	0	0	0
			5910	3757	988	1153	12			
1	D	745	Total	C	N	O	S	0	0	0
			5880	3739	977	1152	12			
1	E	744	Total	C	N	O	S	0	0	0
			5893	3748	980	1153	12			
1	F	749	Total	C	N	O	S	0	0	0
			5889	3745	983	1149	12			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	788	LEU	-	expression tag	UNP Q89YR8
A	789	GLU	-	expression tag	UNP Q89YR8
A	790	HIS	-	expression tag	UNP Q89YR8
A	791	HIS	-	expression tag	UNP Q89YR8
A	792	HIS	-	expression tag	UNP Q89YR8
A	793	HIS	-	expression tag	UNP Q89YR8
A	794	HIS	-	expression tag	UNP Q89YR8
A	795	HIS	-	expression tag	UNP Q89YR8
B	788	LEU	-	expression tag	UNP Q89YR8
B	789	GLU	-	expression tag	UNP Q89YR8
B	790	HIS	-	expression tag	UNP Q89YR8
B	791	HIS	-	expression tag	UNP Q89YR8
B	792	HIS	-	expression tag	UNP Q89YR8
B	793	HIS	-	expression tag	UNP Q89YR8
B	794	HIS	-	expression tag	UNP Q89YR8
B	795	HIS	-	expression tag	UNP Q89YR8

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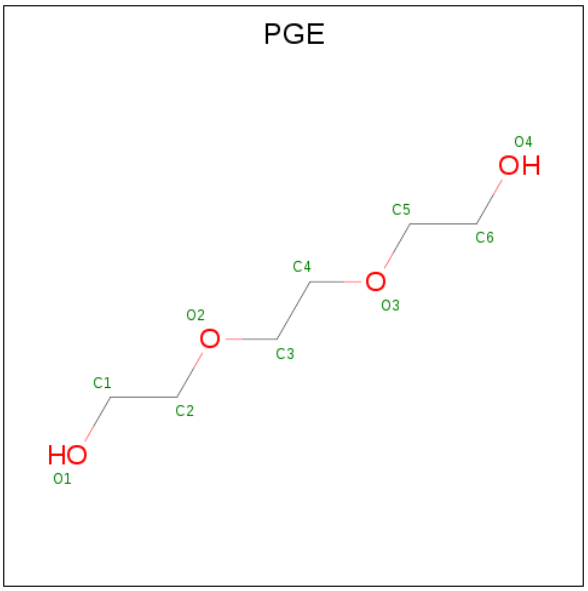
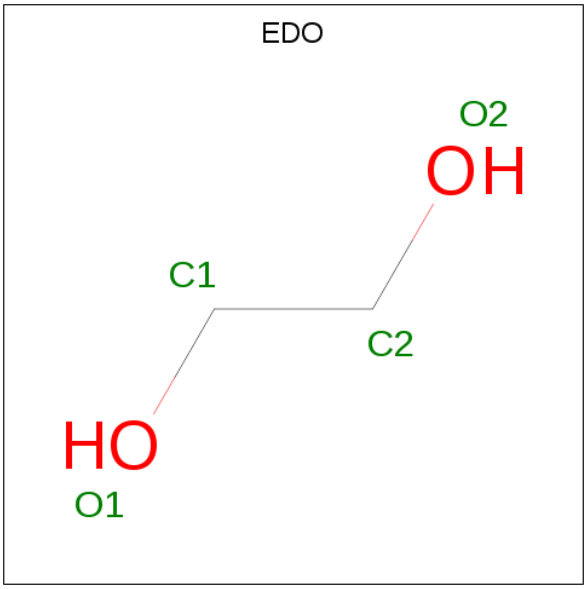
Chain	Residue	Modelled	Actual	Comment	Reference
C	788	LEU	-	expression tag	UNP Q89YR8
C	789	GLU	-	expression tag	UNP Q89YR8
C	790	HIS	-	expression tag	UNP Q89YR8
C	791	HIS	-	expression tag	UNP Q89YR8
C	792	HIS	-	expression tag	UNP Q89YR8
C	793	HIS	-	expression tag	UNP Q89YR8
C	794	HIS	-	expression tag	UNP Q89YR8
C	795	HIS	-	expression tag	UNP Q89YR8
D	788	LEU	-	expression tag	UNP Q89YR8
D	789	GLU	-	expression tag	UNP Q89YR8
D	790	HIS	-	expression tag	UNP Q89YR8
D	791	HIS	-	expression tag	UNP Q89YR8
D	792	HIS	-	expression tag	UNP Q89YR8
D	793	HIS	-	expression tag	UNP Q89YR8
D	794	HIS	-	expression tag	UNP Q89YR8
D	795	HIS	-	expression tag	UNP Q89YR8
E	788	LEU	-	expression tag	UNP Q89YR8
E	789	GLU	-	expression tag	UNP Q89YR8
E	790	HIS	-	expression tag	UNP Q89YR8
E	791	HIS	-	expression tag	UNP Q89YR8
E	792	HIS	-	expression tag	UNP Q89YR8
E	793	HIS	-	expression tag	UNP Q89YR8
E	794	HIS	-	expression tag	UNP Q89YR8
E	795	HIS	-	expression tag	UNP Q89YR8
F	788	LEU	-	expression tag	UNP Q89YR8
F	789	GLU	-	expression tag	UNP Q89YR8
F	790	HIS	-	expression tag	UNP Q89YR8
F	791	HIS	-	expression tag	UNP Q89YR8
F	792	HIS	-	expression tag	UNP Q89YR8
F	793	HIS	-	expression tag	UNP Q89YR8
F	794	HIS	-	expression tag	UNP Q89YR8
F	795	HIS	-	expression tag	UNP Q89YR8

- Molecule 2 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



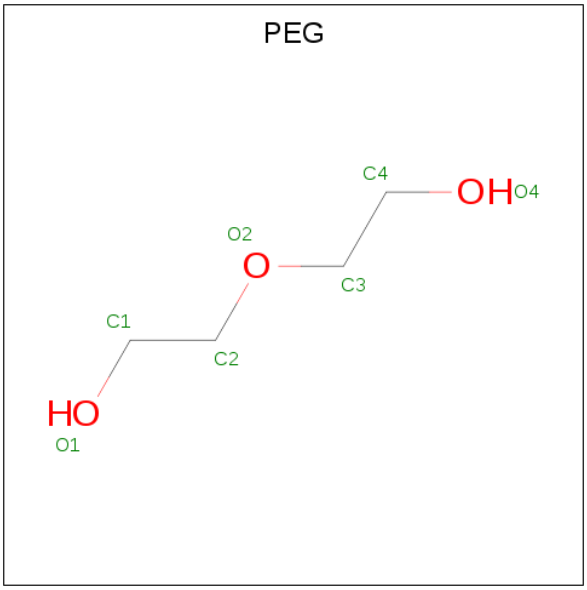
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 10 6 4	0	0
2	A	1	Total C O 10 6 4	0	0
2	B	1	Total C O 10 6 4	0	0
2	E	1	Total C O 7 4 3	0	0
2	F	1	Total C O 10 6 4	0	0

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 7 4 3	0	0
4	B	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 7 4 3	0	0
4	C	1	Total C O 7 4 3	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 7 4 3	0	0

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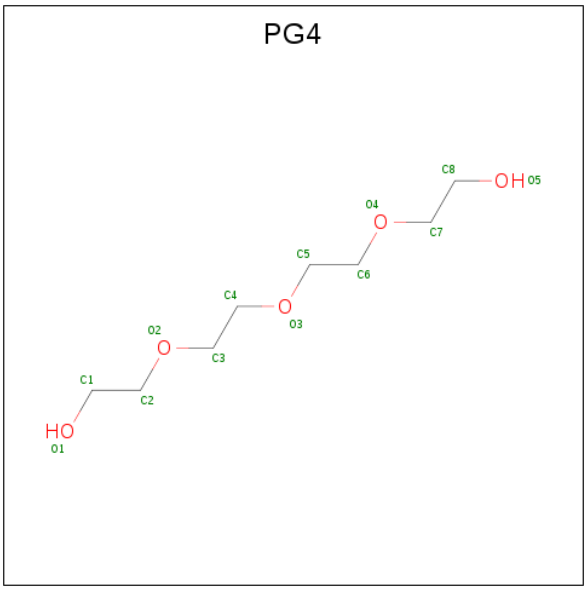
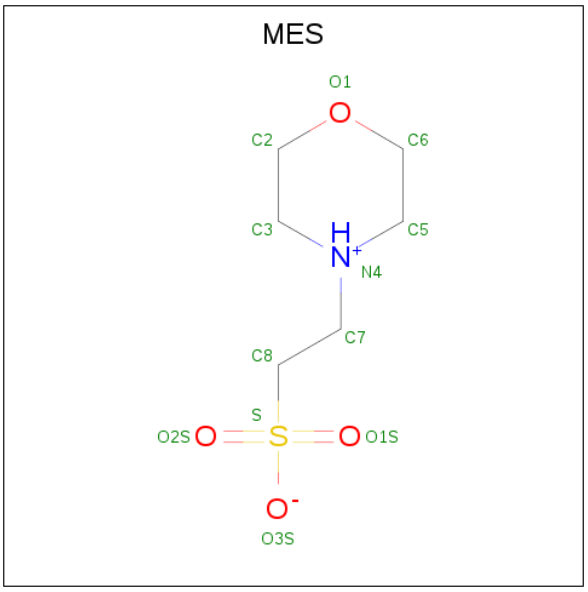
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	E	1	Total C O 7 4 3	0	0
4	F	1	Total C O 7 4 3	0	0

- Molecule 5 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



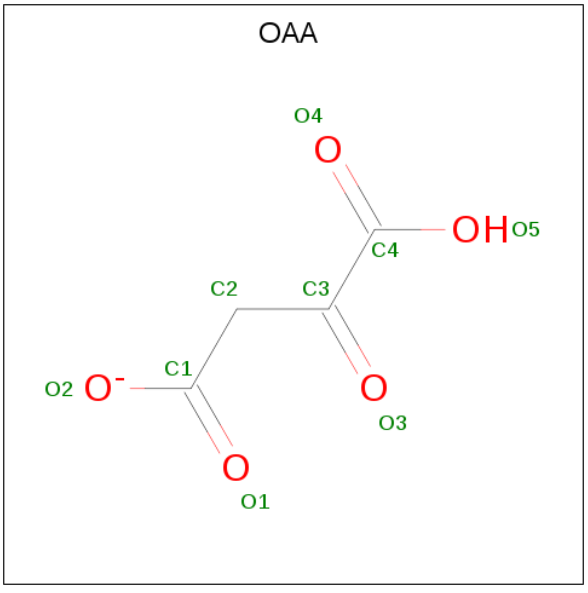
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 13 8 5	0	0

- Molecule 6 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
6	D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
6	E	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 7 is OXALOACETATE ION (three-letter code: OAA) (formula: $C_4H_3O_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	C	1	Total	C	O		0	0
			9	4	5			

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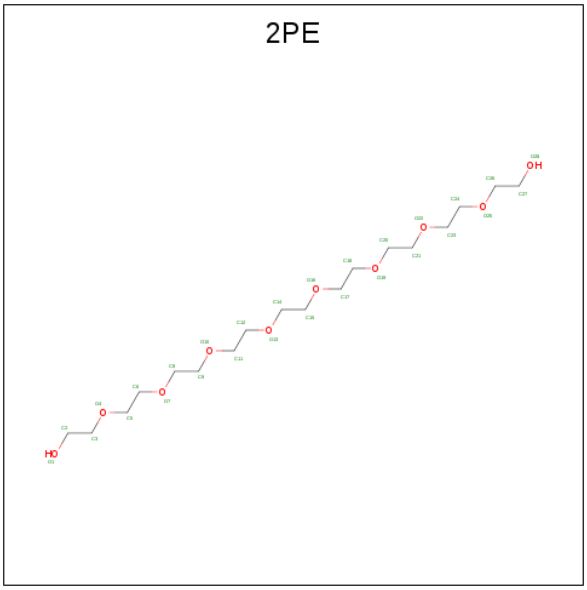
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	C	1	Total C O 9 4 5	0	0
7	E	1	Total C O 9 4 5	0	0

- Molecule 8 is NONAETHYLENE GLYCOL (three-letter code: 2PE) (formula: $C_{18}H_{38}O_{10}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	D	1	Total C O 19 12 7	0	0

- Molecule 9 is water.

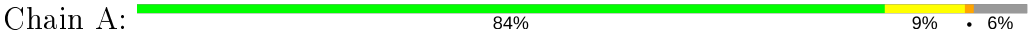
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	68	Total O 68 68	0	0
9	B	36	Total O 36 36	0	0
9	C	75	Total O 75 75	0	0
9	D	37	Total O 37 37	0	0
9	E	36	Total O 36 36	0	0
9	F	49	Total O 49 49	0	0

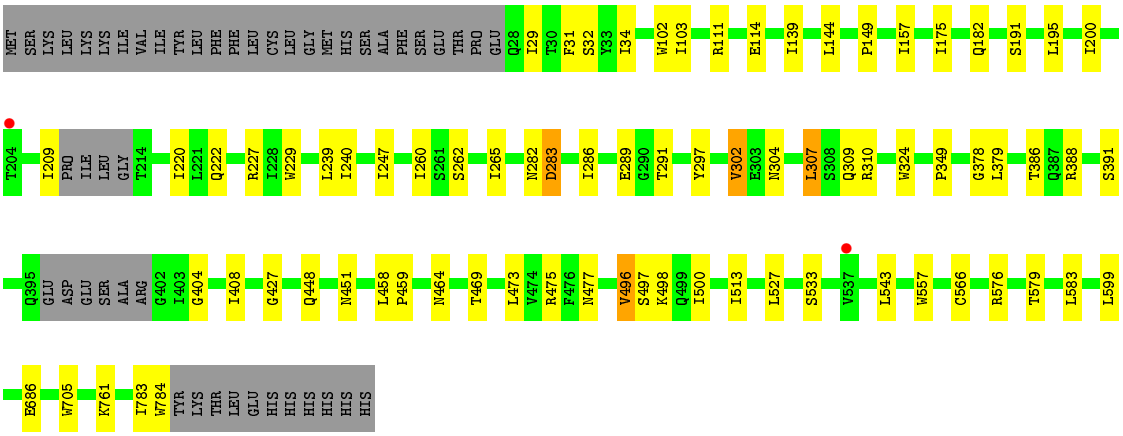
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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: TWO-COMPONENT SYSTEM SENSOR HISTIDINE KINASE/RESPONSE

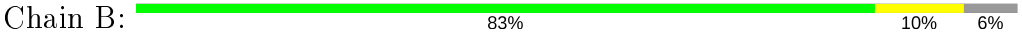
Chain A:

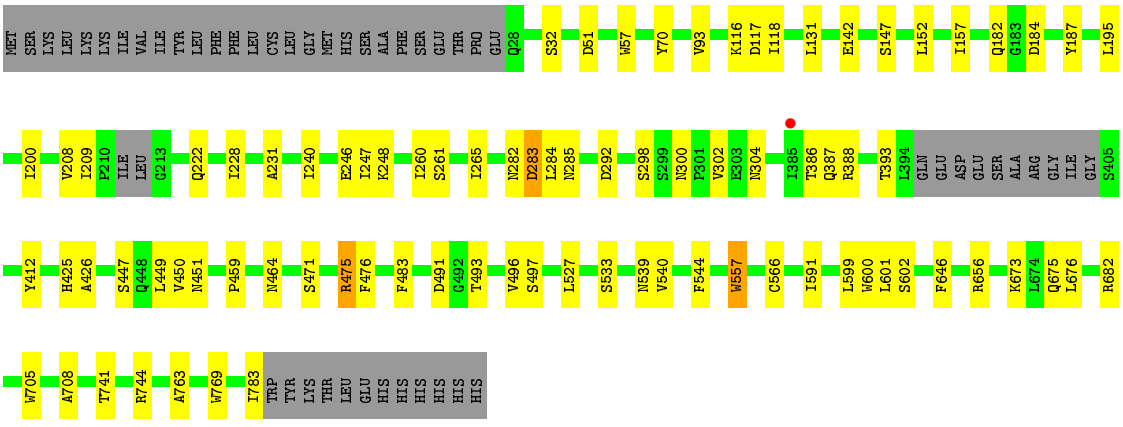




• Molecule 1: TWO-COMPONENT SYSTEM SENSOR HISTIDINE KINASE/RESPONSE

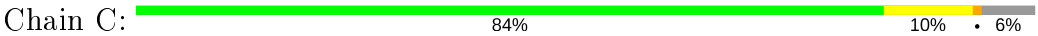
Chain B:

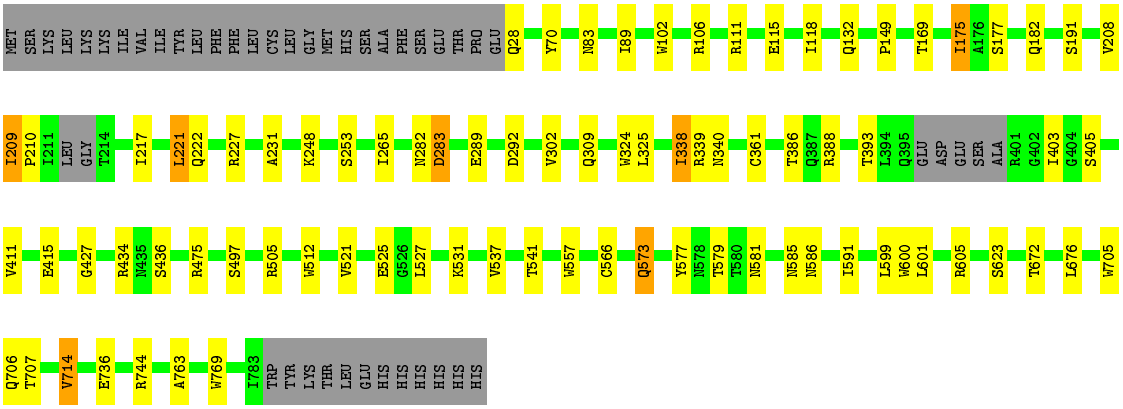




• Molecule 1: TWO-COMPONENT SYSTEM SENSOR HISTIDINE KINASE/RESPONSE

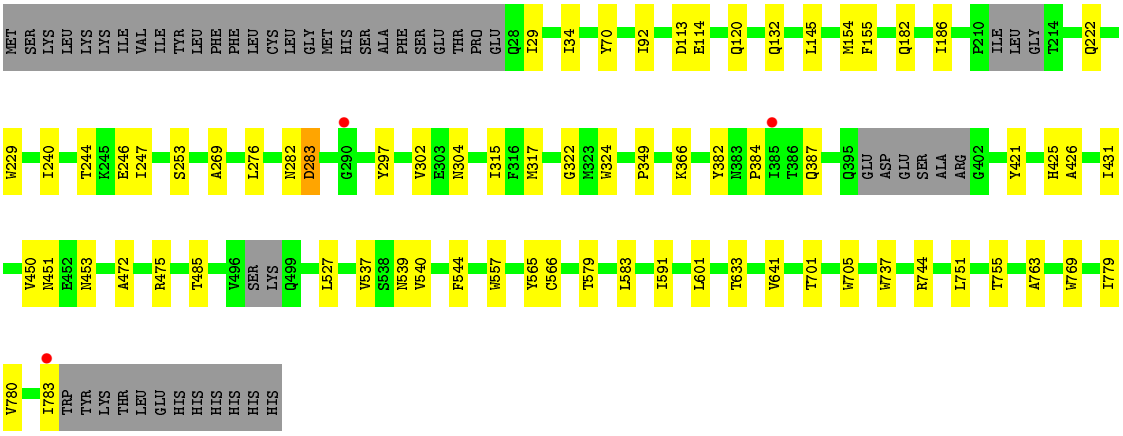
Chain C:





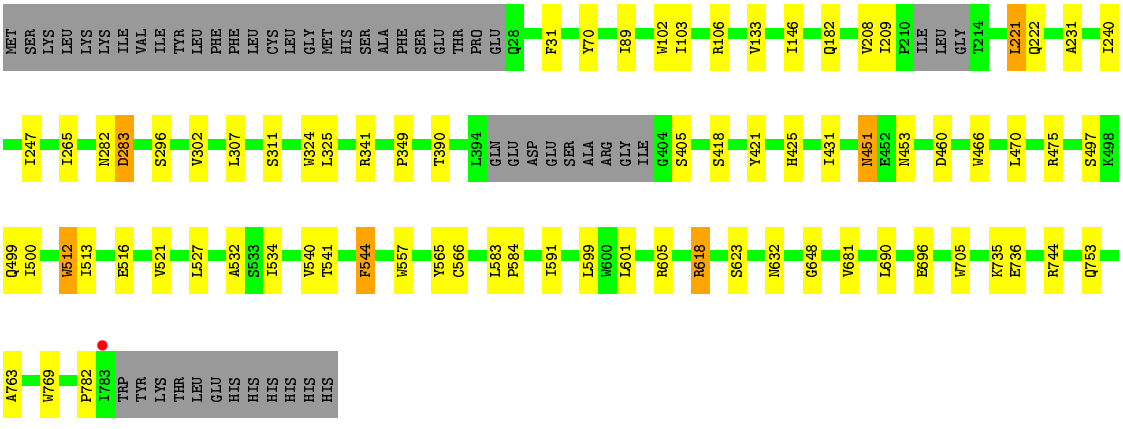
• Molecule 1: TWO-COMPONENT SYSTEM SENSOR HISTIDINE KINASE/RESPONSE

Chain D:



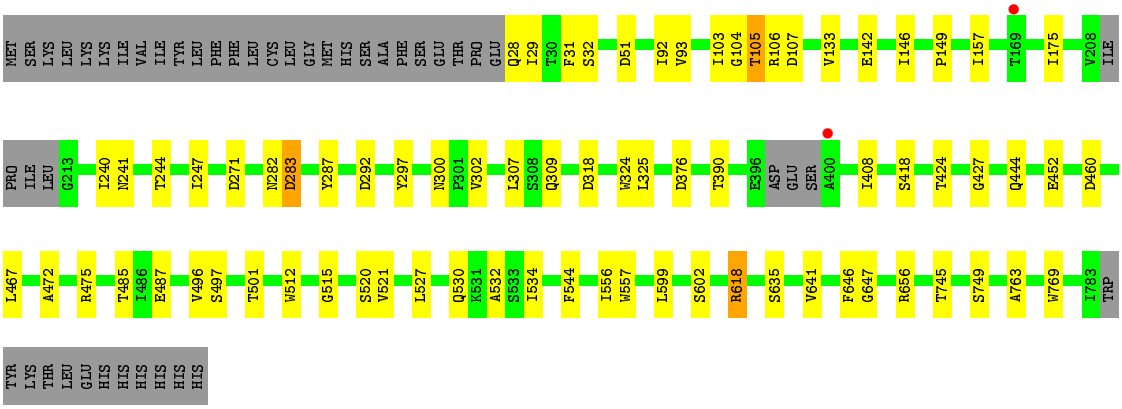
• Molecule 1: TWO-COMPONENT SYSTEM SENSOR HISTIDINE KINASE/RESPONSE

Chain E:



• Molecule 1: TWO-COMPONENT SYSTEM SENSOR HISTIDINE KINASE/RESPONSE

Chain F:


MET SER LYS LEU LYS LYS ILE VAL ILE TYR LEU PHE PHE LEU CYS LEU GLY MET HIS SER ALA PHE SER GLU THR PRO GLU Q28 I29 T30 F31 S32 D51 I92 V93 I103 G104 T105 R106 D107 V133 E142 I146 P149 I157 T169 I175 V208 ILE
PRO ILE LEU G213 I240 N241 T244 I247 D271 N282 D283 Y287 D292 Y297 N300 P301 V302 L307 S308 Q309 D318 W324 L325 D376 T390 E396 ASP GLU SER A400 I408 S418 T424 G427 Q444 E452 D460
L467 A472 R475 T485 I486 E487 V496 S497 T501 W512 G515 S520 V521 L527 Q530 K531 A532 S533 I534 F544 I556 W557 L599 S602 R618 S635 V641 F646 G647 R656 T745 S749 A763 W769 I783 TRP
TYR LYS THR LEU GLU HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α, β, γ	342.47Å 342.47Å 97.85Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	296.59 – 2.60 62.97 – 2.60	Depositor EDS
% Data completeness (in resolution range)	95.0 (296.59-2.60) 90.3 (62.97-2.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.12 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.186 , 0.231 0.188 , 0.231	Depositor DCC
R_{free} test set	9134 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	46.1	Xtriage
Anisotropy	0.302	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 37.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.029 for -h,-k,l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	35839	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% 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: PGE, OAA, EDO, PG4, 2PE, MES, PEG

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	0.59	2/6006 (0.0%)	0.69	0/8175
1	B	0.59	2/6009 (0.0%)	0.70	1/8172 (0.0%)
1	C	0.59	1/6046 (0.0%)	0.70	1/8222 (0.0%)
1	D	0.58	2/6015 (0.0%)	0.68	0/8183
1	E	0.58	3/6029 (0.0%)	0.68	1/8196 (0.0%)
1	F	0.59	0/6024	0.69	1/8194 (0.0%)
All	All	0.59	10/36129 (0.0%)	0.69	4/49142 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	784	TRP	CD2-CE2	6.03	1.48	1.41
1	E	512	TRP	CD2-CE2	5.64	1.48	1.41
1	D	705	TRP	CD2-CE2	5.52	1.48	1.41
1	E	466	TRP	CD2-CE2	5.49	1.48	1.41
1	D	737	TRP	CD2-CE2	5.25	1.47	1.41

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	475	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	E	618	ARG	NE-CZ-NH2	-5.34	117.63	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	618	ARG	NE-CZ-NH1	5.25	122.93	120.30
1	C	434	ARG	NE-CZ-NH2	-5.12	117.74	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	404	GLY	Peptide

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	5869	0	5549	38	0
1	B	5873	0	5582	50	0
1	C	5910	0	5615	48	0
1	D	5880	0	5556	37	0
1	E	5893	0	5609	51	0
1	F	5889	0	5568	41	0
2	A	20	0	28	0	0
2	B	10	0	14	0	0
2	E	7	0	9	0	0
2	F	10	0	14	0	0
3	A	4	0	6	0	0
3	B	8	0	12	0	0
3	C	4	0	6	0	0
3	D	4	0	6	0	0
4	A	7	0	10	0	0
4	B	4	0	5	0	0
4	C	18	0	25	1	0
4	D	19	0	25	1	0
4	E	7	0	10	0	0
4	F	7	0	10	0	0
5	B	13	0	18	0	0
6	B	12	0	12	0	0
6	D	12	0	12	0	0
6	E	12	0	12	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	C	18	0	4	0	0
7	E	9	0	2	0	0
8	D	19	0	25	0	0
9	A	68	0	0	0	0
9	B	36	0	0	1	0
9	C	75	0	0	0	0
9	D	37	0	0	0	0
9	E	36	0	0	1	0
9	F	49	0	0	0	0
All	All	35839	0	33744	259	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 259 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:755:THR:HG22	1:D:779:ILE:HG23	1.45	0.96
1:B:208:VAL:HG12	1:B:209:ILE:HD13	1.59	0.82
1:E:425:HIS:O	1:E:453:ASN:ND2	2.14	0.80
1:C:393:THR:C	1:C:403:ILE:HG22	2.06	0.77
1:F:105:THR:HG22	1:F:107:ASP:H	1.48	0.75

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	741/795 (93%)	713 (96%)	25 (3%)	3 (0%)	34 57
1	B	738/795 (93%)	709 (96%)	27 (4%)	2 (0%)	41 64

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	743/795 (94%)	721 (97%)	19 (3%)	3 (0%)	34 57
1	D	737/795 (93%)	720 (98%)	16 (2%)	1 (0%)	51 75
1	E	738/795 (93%)	716 (97%)	20 (3%)	2 (0%)	41 64
1	F	743/795 (94%)	710 (96%)	30 (4%)	3 (0%)	34 57
All	All	4440/4770 (93%)	4289 (97%)	137 (3%)	14 (0%)	41 64

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	497	SER
1	B	283	ASP
1	E	497	SER
1	A	283	ASP
1	C	283	ASP

5.3.2 Protein sidechains

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	632/712 (89%)	615 (97%)	17 (3%)	44 71
1	B	635/712 (89%)	619 (98%)	16 (2%)	47 73
1	C	640/712 (90%)	621 (97%)	19 (3%)	41 67
1	D	634/712 (89%)	622 (98%)	12 (2%)	57 79
1	E	641/712 (90%)	630 (98%)	11 (2%)	60 81
1	F	631/712 (89%)	616 (98%)	15 (2%)	49 74
All	All	3813/4272 (89%)	3723 (98%)	90 (2%)	49 74

5 of 90 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	309	GLN
1	C	714	VAL

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Mol	Chain	Res	Type
1	F	487	GLU
1	C	338	ILE
1	C	525	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	120	GLN
1	E	304	ASN
1	F	241	ASN
1	C	722	GLN
1	F	222	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 carbohydrates in this entry.

5.6 Ligand geometry

29 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	$\#\|Z\| > 2$
7	OAA	C	1789	-	2,8,8	9.82	2 (100%)	2,10,10	5.56	1 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	EDO	B	1788	-	3,3,3	0.54	0	2,2,2	0.23	0
4	PEG	E	1784	-	6,6,6	0.51	0	5,5,5	0.31	0
2	PGE	B	1786	-	9,9,9	0.55	0	8,8,8	0.37	0
2	PGE	F	1784	-	9,9,9	0.64	0	8,8,8	0.44	0
3	EDO	B	1787	-	3,3,3	0.53	0	2,2,2	0.32	0
6	MES	D	1790	-	12,12,12	1.97	1 (8%)	14,16,16	7.06	10 (71%)
4	PEG	D	1786	-	3,3,6	0.49	0	2,2,5	0.20	0
3	EDO	C	1786	-	3,3,3	0.52	0	2,2,2	0.27	0
7	OAA	E	1786	-	2,8,8	9.93	2 (100%)	2,10,10	2.57	1 (50%)
3	EDO	A	1787	-	3,3,3	0.55	0	2,2,2	0.21	0
7	OAA	C	1788	-	2,8,8	9.51	2 (100%)	2,10,10	4.30	1 (50%)
4	PEG	B	1784	-	3,3,6	0.61	0	2,2,5	0.08	0
4	PEG	C	1784	-	3,3,6	0.40	0	2,2,5	0.34	0
4	PEG	D	1784	-	3,3,6	0.60	0	2,2,5	0.12	0
4	PEG	C	1785	-	6,6,6	0.54	0	5,5,5	0.30	0
2	PGE	A	1786	-	9,9,9	0.64	0	8,8,8	0.41	0
4	PEG	C	1787	-	6,6,6	0.63	0	5,5,5	0.59	0
5	PG4	B	1785	-	12,12,12	0.58	0	11,11,11	0.34	0
8	2PE	D	1788	-	18,18,27	0.57	0	17,17,26	0.42	0
6	MES	B	1789	-	12,12,12	2.25	2 (16%)	14,16,16	6.29	10 (71%)
4	PEG	A	1788	-	6,6,6	0.57	0	5,5,5	0.46	0
2	PGE	A	1785	-	9,9,9	0.53	0	8,8,8	0.53	0
3	EDO	D	1787	-	3,3,3	0.49	0	2,2,2	0.33	0
4	PEG	D	1789	-	3,3,6	0.56	0	2,2,5	0.27	0
4	PEG	D	1785	-	6,6,6	0.44	0	5,5,5	0.41	0
4	PEG	F	1785	-	6,6,6	0.51	0	5,5,5	0.19	0
6	MES	E	1787	-	12,12,12	2.36	1 (8%)	14,16,16	7.28	10 (71%)
2	PGE	E	1785	-	6,6,9	0.59	0	5,5,8	0.35	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
7	OAA	C	1789	-	-	1/2/8/8	-
3	EDO	B	1788	-	-	0/1/1/1	-
4	PEG	E	1784	-	-	1/4/4/4	-
2	PGE	B	1786	-	-	6/7/7/7	-
2	PGE	F	1784	-	-	5/7/7/7	-
3	EDO	B	1787	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	MES	D	1790	-	-	3/6/14/14	0/1/1/1
4	PEG	D	1786	-	-	1/1/1/4	-
3	EDO	C	1786	-	-	1/1/1/1	-
7	OAA	E	1786	-	-	2/2/8/8	-
3	EDO	A	1787	-	-	0/1/1/1	-
7	OAA	C	1788	-	-	1/2/8/8	-
4	PEG	B	1784	-	-	1/1/1/4	-
4	PEG	C	1784	-	-	1/1/1/4	-
4	PEG	D	1784	-	-	0/1/1/4	-
4	PEG	C	1785	-	-	2/4/4/4	-
2	PGE	A	1786	-	-	3/7/7/7	-
4	PEG	C	1787	-	-	3/4/4/4	-
5	PG4	B	1785	-	-	4/10/10/10	-
8	2PE	D	1788	-	-	8/16/16/25	-
6	MES	B	1789	-	-	3/6/14/14	0/1/1/1
4	PEG	A	1788	-	-	3/4/4/4	-
2	PGE	A	1785	-	-	3/7/7/7	-
3	EDO	D	1787	-	-	1/1/1/1	-
4	PEG	D	1789	-	-	1/1/1/4	-
4	PEG	D	1785	-	-	3/4/4/4	-
4	PEG	F	1785	-	-	3/4/4/4	-
6	MES	E	1787	-	-	4/6/14/14	0/1/1/1
2	PGE	E	1785	-	-	2/4/4/7	-

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	E	1786	OAA	O3-C3	13.85	1.44	1.22
7	C	1789	OAA	O3-C3	13.69	1.44	1.22
7	C	1788	OAA	O3-C3	13.23	1.43	1.22
6	E	1787	MES	C8-S	-7.71	1.66	1.77
6	B	1789	MES	C8-S	-6.94	1.67	1.77

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	E	1787	MES	O2S-S-C8	17.28	127.72	106.92
6	D	1790	MES	O1S-S-C8	-17.21	86.19	106.92
6	E	1787	MES	O1S-S-C8	-13.88	90.20	106.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	1789	MES	O2S-S-C8	12.72	122.23	106.92
6	B	1789	MES	O1S-S-C8	-11.66	92.87	106.92

There are no chirality outliers.

5 of 67 torsion outliers are listed below:

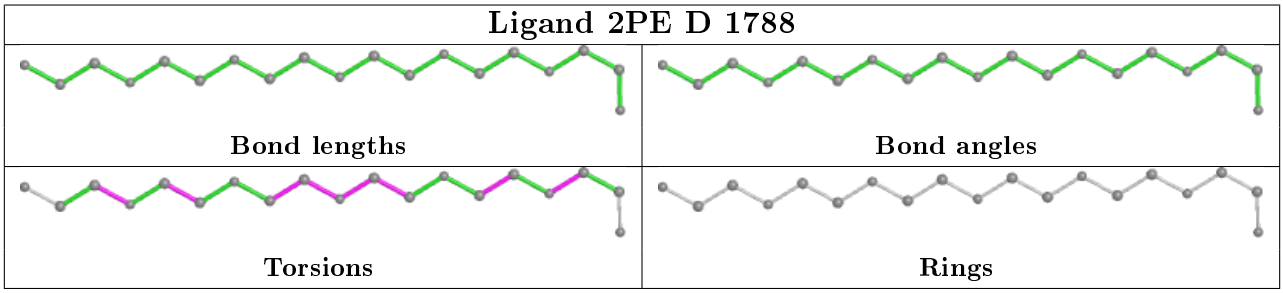
Mol	Chain	Res	Type	Atoms
6	D	1790	MES	N4-C7-C8-S
6	D	1790	MES	C7-C8-S-O3S
7	E	1786	OAA	C1-C2-C3-C4
6	B	1789	MES	C8-C7-N4-C3
6	E	1787	MES	C8-C7-N4-C3

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1787	PEG	1	0
4	D	1785	PEG	1	0
6	E	1787	MES	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.



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	747/795 (93%)	-0.48	2 (0%)	94	93	22, 41, 76, 95	0
1	B	744/795 (93%)	-0.49	1 (0%)	95	95	25, 42, 69, 97	0
1	C	749/795 (94%)	-0.53	0	100	100	23, 39, 67, 93	0
1	D	745/795 (93%)	-0.44	3 (0%)	92	91	26, 42, 70, 101	0
1	E	744/795 (93%)	-0.45	1 (0%)	95	95	26, 43, 66, 89	0
1	F	749/795 (94%)	-0.47	2 (0%)	94	93	23, 40, 71, 87	0
All	All	4478/4770 (93%)	-0.48	9 (0%)	95	95	22, 41, 70, 101	0

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	783	ILE	3.5
1	B	385	ILE	2.8
1	A	537	VAL	2.5
1	A	204	THR	2.4
1	F	400	ALA	2.4

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands (i)

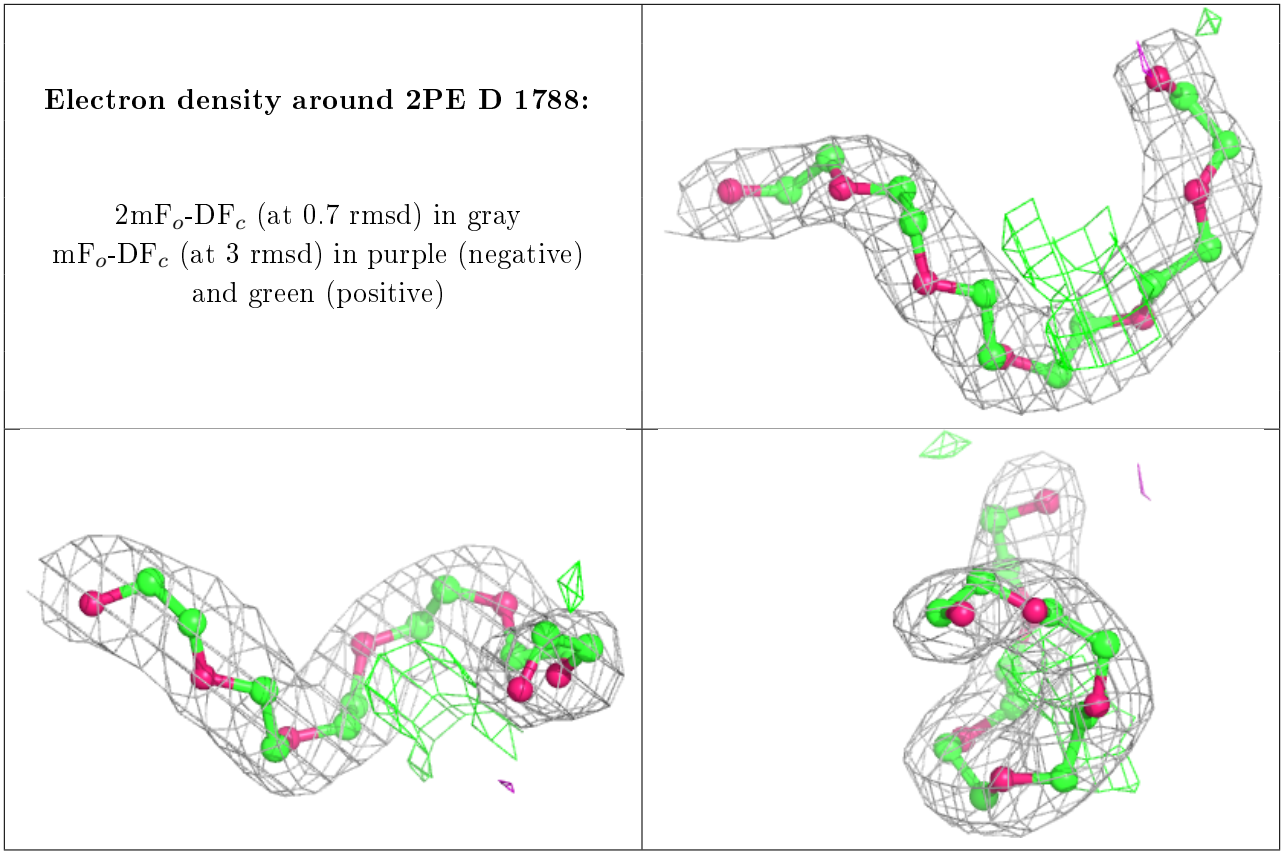
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	PEG	D	1786	4/7	0.72	0.27	58,61,63,64	0
3	EDO	B	1788	4/4	0.76	0.14	65,69,70,70	0
4	PEG	F	1785	7/7	0.76	0.30	61,67,72,72	0
7	OAA	C	1789	9/9	0.80	0.23	69,71,72,73	0
3	EDO	A	1787	4/4	0.81	0.19	47,48,51,51	0
2	PGE	E	1785	7/10	0.81	0.22	60,62,68,69	0
4	PEG	D	1785	7/7	0.82	0.33	69,70,79,80	0
7	OAA	E	1786	9/9	0.87	0.24	74,75,78,79	0
4	PEG	C	1787	7/7	0.87	0.30	54,56,58,60	0
4	PEG	A	1788	7/7	0.87	0.17	52,54,55,57	0
4	PEG	C	1785	7/7	0.88	0.20	67,73,77,78	0
5	PG4	B	1785	13/13	0.88	0.19	47,49,51,52	0
7	OAA	C	1788	9/9	0.90	0.22	63,67,71,77	0
4	PEG	E	1784	7/7	0.90	0.24	60,62,65,66	0
3	EDO	C	1786	4/4	0.91	0.14	60,60,60,61	0
4	PEG	D	1784	4/7	0.91	0.23	49,52,55,59	0
2	PGE	A	1785	10/10	0.91	0.20	50,52,55,57	0
4	PEG	D	1789	4/7	0.92	0.13	50,51,54,54	0
3	EDO	B	1787	4/4	0.92	0.19	56,58,58,62	0
2	PGE	A	1786	10/10	0.92	0.18	49,55,58,59	0
6	MES	E	1787	12/12	0.92	0.20	60,63,75,84	0
3	EDO	D	1787	4/4	0.92	0.12	54,56,57,60	0
6	MES	B	1789	12/12	0.93	0.18	71,75,95,99	0
4	PEG	B	1784	4/7	0.93	0.19	49,49,50,50	0
6	MES	D	1790	12/12	0.93	0.17	66,70,74,78	0
8	2PE	D	1788	19/28	0.94	0.16	44,48,57,60	0
2	PGE	F	1784	10/10	0.94	0.14	43,47,49,52	0
4	PEG	C	1784	4/7	0.95	0.10	51,51,52,53	0
2	PGE	B	1786	10/10	0.96	0.13	43,49,51,53	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 2PE D 1788:

$2mF_o$-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.