



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 06:59 pm GMT

PDB ID : 1O57
Title : CRYSTAL STRUCTURE OF THE PURINE OPERON REPRESSOR OF BACILLUS SUBTILIS
Authors : Sinha, S.C.; Krahn, J.; Shin, B.S.; Tomchick, D.R.; Zalkin, H.; Smith, J.L.
Deposited on : 2003-04-20
Resolution : 2.20 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

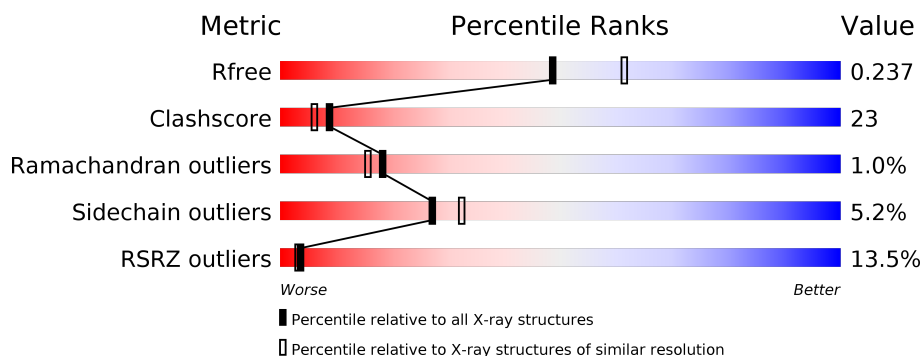
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	100719	4002 (2.20-2.20)
Clashscore	112137	4730 (2.20-2.20)
Ramachandran outliers	110173	4656 (2.20-2.20)
Sidechain outliers	110143	4657 (2.20-2.20)
RSRZ outliers	101464	4033 (2.20-2.20)

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. 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	291	<div> <div>15%</div> <div> <div>57%</div> <div>31%</div> <div>•</div> <div>7%</div> </div> </div>
1	B	291	<div> <div>12%</div> <div> <div>63%</div> <div>26%</div> <div>•</div> <div>8%</div> </div> </div>
1	C	291	<div> <div>9%</div> <div> <div>63%</div> <div>26%</div> <div>•</div> <div>8%</div> </div> </div>
1	D	291	<div> <div>13%</div> <div> <div>60%</div> <div>28%</div> <div>•</div> <div>7%</div> </div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	B	589	-	-	-	X
2	SO4	C	590	-	-	-	X
3	EPE	A	570	-	-	-	X
3	EPE	D	571	-	-	-	X
4	P6G	A	572	-	-	-	X
4	P6G	D	573	-	-	-	X
5	2PE	A	574	-	-	-	X
6	PG4	B	575	-	-	-	X
7	1PE	C	576	-	-	-	X
7	1PE	D	577	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 9132 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 PUR OPERON REPRESSOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	270	Total	C	N	O	S	0	8	0
			2099	1338	347	400	14			
1	B	269	Total	C	N	O	S	0	8	0
			2091	1334	346	397	14			
1	C	269	Total	C	N	O	S	0	9	0
			2097	1340	346	395	16			
1	D	270	Total	C	N	O	S	0	7	0
			2096	1337	346	399	14			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	286	HIS	-	EXPRESSION TAG	UNP P37551
A	287	HIS	-	EXPRESSION TAG	UNP P37551
A	288	HIS	-	EXPRESSION TAG	UNP P37551
A	289	HIS	-	EXPRESSION TAG	UNP P37551
A	290	HIS	-	EXPRESSION TAG	UNP P37551
A	291	HIS	-	EXPRESSION TAG	UNP P37551
B	286	HIS	-	EXPRESSION TAG	UNP P37551
B	287	HIS	-	EXPRESSION TAG	UNP P37551
B	288	HIS	-	EXPRESSION TAG	UNP P37551
B	289	HIS	-	EXPRESSION TAG	UNP P37551
B	290	HIS	-	EXPRESSION TAG	UNP P37551
B	291	HIS	-	EXPRESSION TAG	UNP P37551
C	286	HIS	-	EXPRESSION TAG	UNP P37551
C	287	HIS	-	EXPRESSION TAG	UNP P37551
C	288	HIS	-	EXPRESSION TAG	UNP P37551
C	289	HIS	-	EXPRESSION TAG	UNP P37551
C	290	HIS	-	EXPRESSION TAG	UNP P37551
C	291	HIS	-	EXPRESSION TAG	UNP P37551
D	286	HIS	-	EXPRESSION TAG	UNP P37551
D	287	HIS	-	EXPRESSION TAG	UNP P37551
D	288	HIS	-	EXPRESSION TAG	UNP P37551

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Chain	Residue	Modelled	Actual	Comment	Reference
D	289	HIS	-	EXPRESSION TAG	UNP P37551
D	290	HIS	-	EXPRESSION TAG	UNP P37551
D	291	HIS	-	EXPRESSION TAG	UNP P37551

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



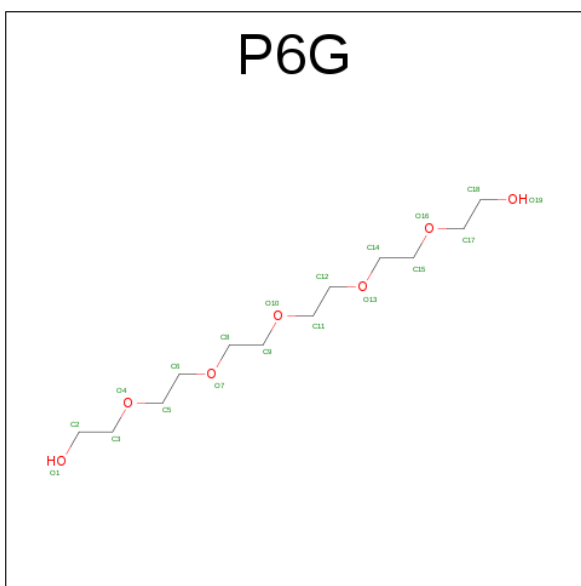
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C₈H₁₈N₂O₄S).



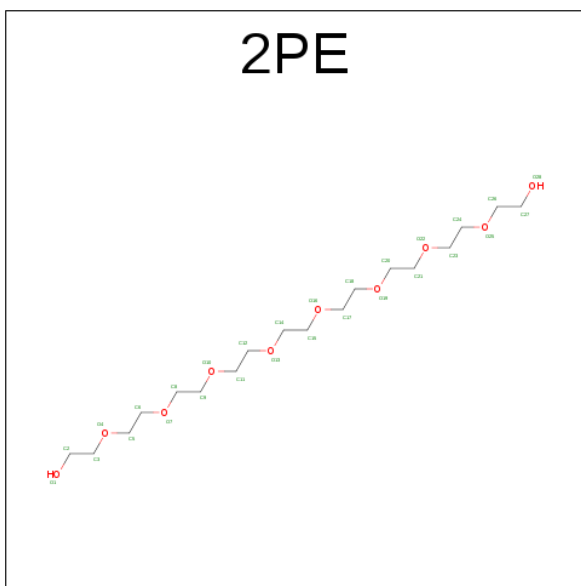
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
3	D	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 4 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula: $C_{12}H_{26}O_7$).



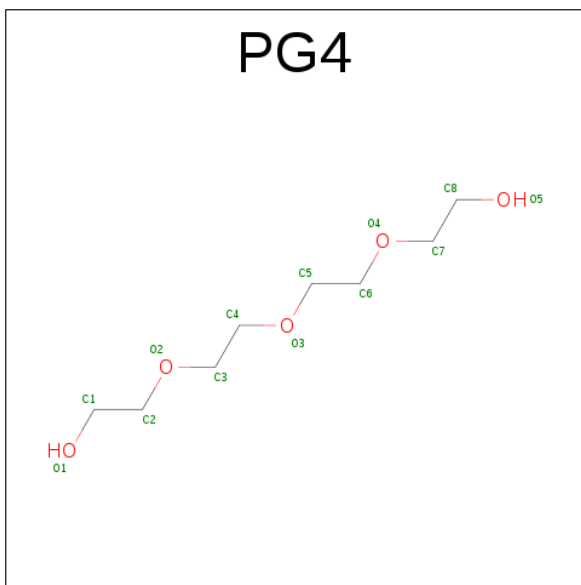
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			19	12	7		
4	D	1	Total	C	O	0	0
			19	12	7		

- Molecule 5 is NONAETHYLENE GLYCOL (three-letter code: 2PE) (formula: $C_{18}H_{38}O_{10}$).



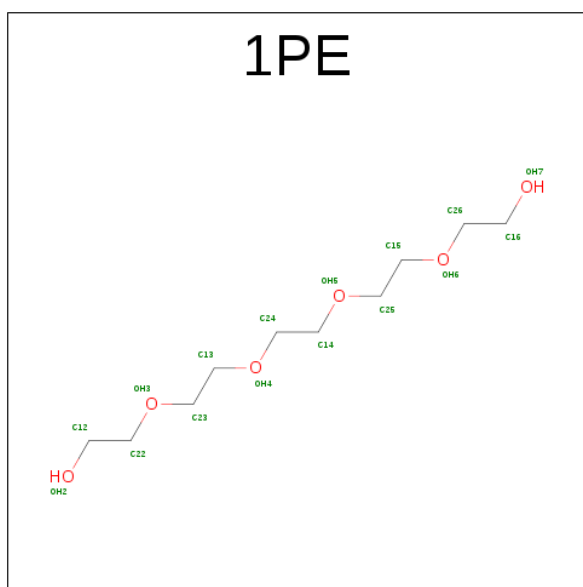
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			28	18	10		

- Molecule 6 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



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

- Molecule 7 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	C	O	0	0
			16	10	6		
7	D	1	Total	C	O	0	0
			16	10	6		

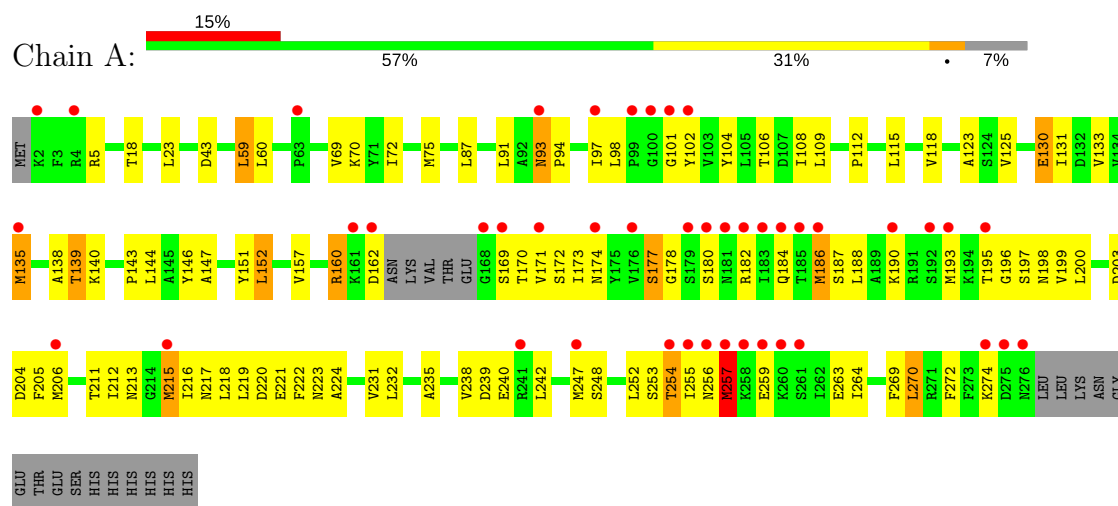
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	121	Total O 121 121	0	0
8	B	138	Total O 138 138	0	0
8	C	177	Total O 177 177	0	0
8	D	132	Total O 132 132	0	0

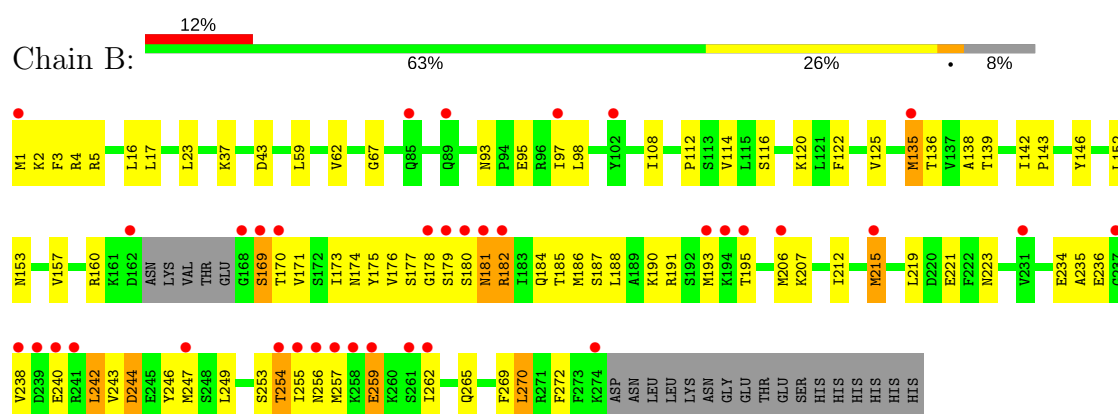
3 Residue-property plots

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.

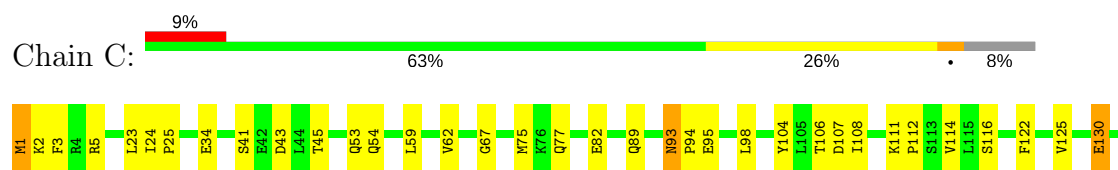
• Molecule 1: PUR OPERON REPRESSOR

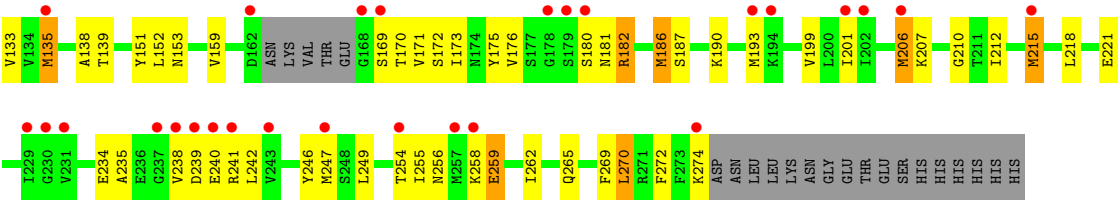


• Molecule 1: PUR OPERON REPRESSOR

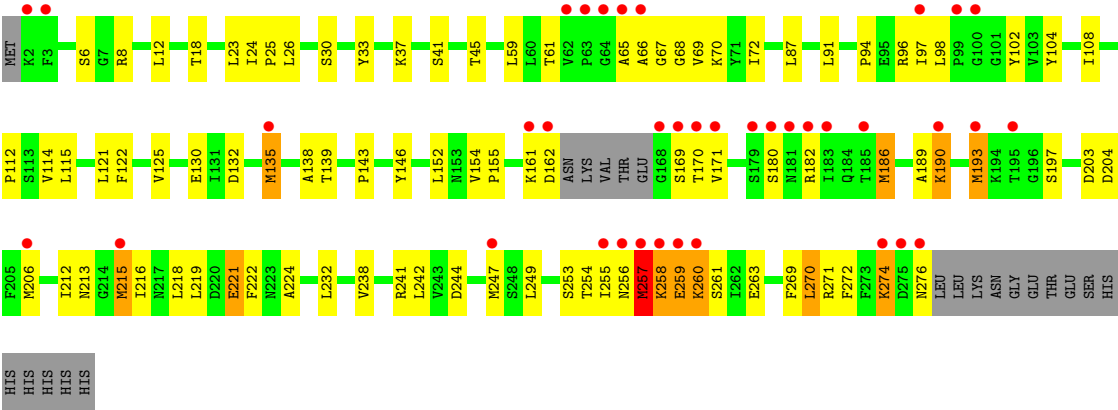


• Molecule 1: PUR OPERON REPRESSOR





• Molecule 1: PUR OPERON REPRESSOR



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	65.08Å 72.16Å 82.97Å 84.75° 84.03° 67.47°	Depositor
Resolution (Å)	20.00 – 2.20 27.68 – 2.17	Depositor EDS
% Data completeness (in resolution range)	94.4 (20.00-2.20) 91.8 (27.68-2.17)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.83 (at 2.18Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.188 , 0.237 0.194 , 0.237	Depositor DCC
R_{free} test set	3335 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	38.1	Xtriage
Anisotropy	0.154	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 63.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9132	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.62% 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: 1PE, PG4, 2PE, SO4, P6G, EPE

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	10/2169 (0.5%)	0.70	0/2924
1	B	0.70	7/2162 (0.3%)	0.71	0/2914
1	C	0.76	10/2173 (0.5%)	0.74	0/2926
1	D	0.69	9/2161 (0.4%)	0.72	0/2913
All	All	0.71	36/8665 (0.4%)	0.72	0/11677

The worst 5 of 36 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	135[A]	MET	CG-SD	7.06	1.99	1.81
1	C	135[B]	MET	CG-SD	7.06	1.99	1.81
1	B	135[A]	MET	CG-SD	6.59	1.98	1.81
1	B	135[B]	MET	CG-SD	6.59	1.98	1.81
1	D	215[A]	MET	CG-SD	6.59	1.98	1.81

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	2099	0	2164	105	0
1	B	2091	0	2161	79	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2097	0	2177	102	0
1	D	2096	0	2162	106	0
2	A	5	0	0	0	0
2	B	15	0	0	0	0
2	C	15	0	0	0	0
2	D	5	0	0	0	0
3	A	15	0	17	3	0
3	D	15	0	17	1	0
4	A	19	0	26	2	0
4	D	19	0	26	2	0
5	A	28	0	38	10	0
6	B	13	0	18	6	0
7	C	16	0	22	5	0
7	D	16	0	22	4	0
8	A	121	0	0	1	0
8	B	138	0	0	7	0
8	C	177	0	0	6	0
8	D	132	0	0	7	0
All	All	9132	0	8850	395	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 23.

The worst 5 of 395 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:97:ILE:HG22	1:A:255:ILE:HD11	1.32	1.12
1:B:182:ARG:HH11	1:B:182:ARG:HG2	1.18	1.04
1:B:182:ARG:HG2	1:B:182:ARG:NH1	1.86	0.88
1:B:178:GLY:C	1:B:180:SER:H	1.78	0.87
1:D:190:LYS:HA	1:D:190:LYS:NZ	1.93	0.83

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	274/291 (94%)	258 (94%)	13 (5%)	3 (1%)	17	13
1	B	273/291 (94%)	262 (96%)	8 (3%)	3 (1%)	17	13
1	C	274/291 (94%)	265 (97%)	7 (3%)	2 (1%)	25	24
1	D	273/291 (94%)	258 (94%)	12 (4%)	3 (1%)	17	13
All	All	1094/1164 (94%)	1043 (95%)	40 (4%)	11 (1%)	18	16

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	254	THR
1	B	179	SER
1	B	254	THR
1	D	254	THR
1	B	169	SER

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	238/250 (95%)	227 (95%)	11 (5%)	31	39
1	B	237/250 (95%)	222 (94%)	15 (6%)	21	23
1	C	238/250 (95%)	225 (94%)	13 (6%)	25	29
1	D	237/250 (95%)	226 (95%)	11 (5%)	31	39
All	All	950/1000 (95%)	900 (95%)	50 (5%)	27	31

5 of 50 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	242	LEU
1	C	23	LEU
1	D	258	LYS

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Mol	Chain	Res	Type
1	B	244	ASP
1	B	270	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	181	ASN
1	B	266	ASN
1	D	213	ASN
1	B	223	ASN
1	C	54	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

16 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	$\# Z > 2$
3	EPE	A	570	-	15,15,15	1.22	1 (6%)	18,20,20	0.76	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	P6G	A	572	-	18,18,18	0.45	0	17,17,17	0.32	0
5	2PE	A	574	-	27,27,27	0.52	0	26,26,26	0.30	0
2	SO4	A	581	-	4,4,4	0.23	0	6,6,6	0.40	0
6	PG4	B	575	-	12,12,12	0.39	0	11,11,11	0.48	0
2	SO4	B	582	-	4,4,4	0.16	0	6,6,6	0.34	0
2	SO4	B	586	-	4,4,4	0.38	0	6,6,6	0.09	0
2	SO4	B	589	-	4,4,4	0.35	0	6,6,6	0.15	0
7	1PE	C	576	-	15,15,15	0.40	0	14,14,14	0.44	0
2	SO4	C	583	-	4,4,4	0.18	0	6,6,6	0.40	0
2	SO4	C	587	-	4,4,4	0.37	0	6,6,6	0.13	0
2	SO4	C	590	-	4,4,4	0.39	0	6,6,6	0.10	0
3	EPE	D	571	-	15,15,15	1.09	0	18,20,20	0.77	0
4	P6G	D	573	-	18,18,18	0.47	0	17,17,17	0.36	0
7	1PE	D	577	-	15,15,15	0.58	0	14,14,14	0.36	0
2	SO4	D	584	-	4,4,4	0.27	0	6,6,6	0.38	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	EPE	A	570	-	-	0/9/19/19	0/1/1/1
4	P6G	A	572	-	-	0/16/16/16	0/0/0/0
5	2PE	A	574	-	-	0/25/25/25	0/0/0/0
2	SO4	A	581	-	-	0/0/0/0	0/0/0/0
6	PG4	B	575	-	-	0/10/10/10	0/0/0/0
2	SO4	B	582	-	-	0/0/0/0	0/0/0/0
2	SO4	B	586	-	-	0/0/0/0	0/0/0/0
2	SO4	B	589	-	-	0/0/0/0	0/0/0/0
7	1PE	C	576	-	-	0/13/13/13	0/0/0/0
2	SO4	C	583	-	-	0/0/0/0	0/0/0/0
2	SO4	C	587	-	-	0/0/0/0	0/0/0/0
2	SO4	C	590	-	-	0/0/0/0	0/0/0/0
3	EPE	D	571	-	-	0/9/19/19	0/1/1/1
4	P6G	D	573	-	-	0/16/16/16	0/0/0/0
7	1PE	D	577	-	-	0/13/13/13	0/0/0/0
2	SO4	D	584	-	-	0/0/0/0	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	570	EPE	C10-S	2.42	1.81	1.77

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	570	EPE	3	0
4	A	572	P6G	2	0
5	A	574	2PE	10	0
6	B	575	PG4	6	0
7	C	576	1PE	5	0
3	D	571	EPE	1	0
4	D	573	P6G	2	0
7	D	577	1PE	4	0

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	270/291 (92%)	0.61	44 (16%) 2 2	23, 46, 108, 163	0
1	B	269/291 (92%)	0.37	36 (13%) 4 3	23, 43, 94, 125	0
1	C	269/291 (92%)	0.27	27 (10%) 8 7	22, 39, 88, 115	0
1	D	270/291 (92%)	0.54	38 (14%) 3 3	24, 46, 97, 154	0
All	All	1078/1164 (92%)	0.45	145 (13%) 3 3	22, 43, 99, 163	0

The worst 5 of 145 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	255	ILE	11.2
1	B	179	SER	10.8
1	A	257	MET	10.3
1	D	257	MET	8.4
1	A	275	ASP	7.6

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 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
2	SO4	B	589	5/5	0.72	0.28	9.14	84,84,92,92	5
2	SO4	C	590	5/5	0.77	0.32	6.07	88,88,91,92	5
6	PG4	B	575	13/13	0.85	0.35	5.26	75,83,94,98	0
4	P6G	A	572	19/19	0.85	0.25	5.08	48,81,91,92	0
7	1PE	D	577	16/16	0.78	0.35	4.85	80,94,103,107	0
5	2PE	A	574	28/28	0.80	0.30	4.67	79,91,100,102	0
3	EPE	A	570	15/15	0.74	0.50	4.00	93,106,109,110	15
3	EPE	D	571	15/15	0.76	0.53	3.80	100,104,112,115	15
7	1PE	C	576	16/16	0.79	0.28	3.30	82,93,96,98	0
4	P6G	D	573	19/19	0.83	0.24	2.11	53,77,97,98	0
2	SO4	C	583	5/5	0.99	0.14	-0.77	42,44,54,69	0
2	SO4	B	582	5/5	0.99	0.10	-1.03	50,51,64,66	0
2	SO4	A	581	5/5	0.98	0.11	-1.06	56,56,67,68	0
2	SO4	C	587	5/5	0.97	0.10	-1.29	55,55,59,63	5
2	SO4	D	584	5/5	0.97	0.10	-1.32	52,53,57,64	0
2	SO4	B	586	5/5	0.95	0.11	-	56,62,65,67	5

6.5 Other polymers [i](#)

There are no such residues in this entry.