



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 13, 2024 – 06:22 pm BST

PDB ID : 6QGB
Title : Crystal structure of Ideonella sakaiensis MHETase bound to benzoic acid
Authors : Palm, G.J.; Reisky, L.; Boettcher, D.; Mueller, H.; Michels, E.A.P.; Walczak, C.; Berndt, L.; Weiss, M.S.; Bornscheuer, U.T.; Weber, G.
Deposited on : 2019-01-10
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

<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	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
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

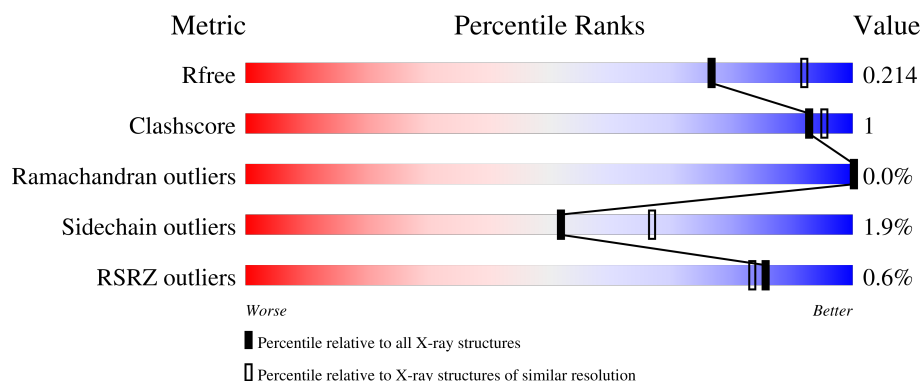
1 Overall quality at a glance

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}	164625	5791 (2.20-2.20)
Clashscore	180529	6634 (2.20-2.20)
Ramachandran outliers	177936	6560 (2.20-2.20)
Sidechain outliers	177891	6561 (2.20-2.20)
RSRZ outliers	164620	5791 (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 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	596	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> % 87% 6% 7% </div> </div>
1	B	596	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> % 90% • 6% </div> </div>
1	C	596	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> % 89% • 6% </div> </div>
1	D	596	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> % 89% • 7% </div> </div>
1	E	596	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> % 89% • 7% </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	596	<div><div><div>%</div><div><div></div><div>89%</div><div></div></div><div><div></div><div></div><div>7%</div></div></div></div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 26826 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 Mono(2-hydroxyethyl) terephthalate hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	557	Total	C	N	O	S	0	0	0
			4116	2580	723	785	28			
1	B	559	Total	C	N	O	S	0	0	0
			4129	2586	725	790	28			
1	C	558	Total	C	N	O	S	0	0	0
			4121	2582	724	787	28			
1	D	557	Total	C	N	O	S	0	0	0
			4117	2580	723	786	28			
1	E	557	Total	C	N	O	S	0	0	0
			4117	2580	723	786	28			
1	F	557	Total	C	N	O	S	0	0	0
			4117	2580	723	786	28			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	8	MET	-	initiating methionine	UNP A0A0K8P8E7
A	9	ASN	-	expression tag	UNP A0A0K8P8E7
A	10	HIS	-	expression tag	UNP A0A0K8P8E7
A	11	LYS	-	expression tag	UNP A0A0K8P8E7
A	12	VAL	-	expression tag	UNP A0A0K8P8E7
A	13	HIS	-	expression tag	UNP A0A0K8P8E7
A	14	HIS	-	expression tag	UNP A0A0K8P8E7
A	15	HIS	-	expression tag	UNP A0A0K8P8E7
A	16	HIS	-	expression tag	UNP A0A0K8P8E7
A	17	HIS	-	expression tag	UNP A0A0K8P8E7
A	18	HIS	-	expression tag	UNP A0A0K8P8E7
A	19	MET	-	expression tag	UNP A0A0K8P8E7
B	8	MET	-	initiating methionine	UNP A0A0K8P8E7
B	9	ASN	-	expression tag	UNP A0A0K8P8E7
B	10	HIS	-	expression tag	UNP A0A0K8P8E7
B	11	LYS	-	expression tag	UNP A0A0K8P8E7
B	12	VAL	-	expression tag	UNP A0A0K8P8E7

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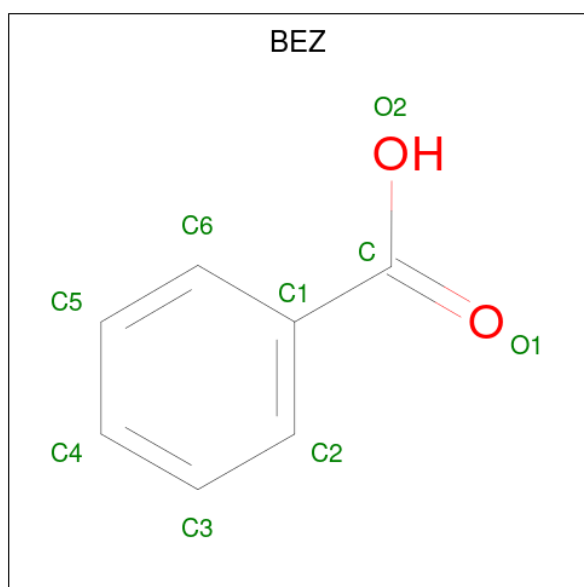
Chain	Residue	Modelled	Actual	Comment	Reference
B	13	HIS	-	expression tag	UNP A0A0K8P8E7
B	14	HIS	-	expression tag	UNP A0A0K8P8E7
B	15	HIS	-	expression tag	UNP A0A0K8P8E7
B	16	HIS	-	expression tag	UNP A0A0K8P8E7
B	17	HIS	-	expression tag	UNP A0A0K8P8E7
B	18	HIS	-	expression tag	UNP A0A0K8P8E7
B	19	MET	-	expression tag	UNP A0A0K8P8E7
C	8	MET	-	initiating methionine	UNP A0A0K8P8E7
C	9	ASN	-	expression tag	UNP A0A0K8P8E7
C	10	HIS	-	expression tag	UNP A0A0K8P8E7
C	11	LYS	-	expression tag	UNP A0A0K8P8E7
C	12	VAL	-	expression tag	UNP A0A0K8P8E7
C	13	HIS	-	expression tag	UNP A0A0K8P8E7
C	14	HIS	-	expression tag	UNP A0A0K8P8E7
C	15	HIS	-	expression tag	UNP A0A0K8P8E7
C	16	HIS	-	expression tag	UNP A0A0K8P8E7
C	17	HIS	-	expression tag	UNP A0A0K8P8E7
C	18	HIS	-	expression tag	UNP A0A0K8P8E7
C	19	MET	-	expression tag	UNP A0A0K8P8E7
D	8	MET	-	initiating methionine	UNP A0A0K8P8E7
D	9	ASN	-	expression tag	UNP A0A0K8P8E7
D	10	HIS	-	expression tag	UNP A0A0K8P8E7
D	11	LYS	-	expression tag	UNP A0A0K8P8E7
D	12	VAL	-	expression tag	UNP A0A0K8P8E7
D	13	HIS	-	expression tag	UNP A0A0K8P8E7
D	14	HIS	-	expression tag	UNP A0A0K8P8E7
D	15	HIS	-	expression tag	UNP A0A0K8P8E7
D	16	HIS	-	expression tag	UNP A0A0K8P8E7
D	17	HIS	-	expression tag	UNP A0A0K8P8E7
D	18	HIS	-	expression tag	UNP A0A0K8P8E7
D	19	MET	-	expression tag	UNP A0A0K8P8E7
E	8	MET	-	initiating methionine	UNP A0A0K8P8E7
E	9	ASN	-	expression tag	UNP A0A0K8P8E7
E	10	HIS	-	expression tag	UNP A0A0K8P8E7
E	11	LYS	-	expression tag	UNP A0A0K8P8E7
E	12	VAL	-	expression tag	UNP A0A0K8P8E7
E	13	HIS	-	expression tag	UNP A0A0K8P8E7
E	14	HIS	-	expression tag	UNP A0A0K8P8E7
E	15	HIS	-	expression tag	UNP A0A0K8P8E7
E	16	HIS	-	expression tag	UNP A0A0K8P8E7
E	17	HIS	-	expression tag	UNP A0A0K8P8E7
E	18	HIS	-	expression tag	UNP A0A0K8P8E7

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Chain	Residue	Modelled	Actual	Comment	Reference
E	19	MET	-	expression tag	UNP A0A0K8P8E7
F	8	MET	-	initiating methionine	UNP A0A0K8P8E7
F	9	ASN	-	expression tag	UNP A0A0K8P8E7
F	10	HIS	-	expression tag	UNP A0A0K8P8E7
F	11	LYS	-	expression tag	UNP A0A0K8P8E7
F	12	VAL	-	expression tag	UNP A0A0K8P8E7
F	13	HIS	-	expression tag	UNP A0A0K8P8E7
F	14	HIS	-	expression tag	UNP A0A0K8P8E7
F	15	HIS	-	expression tag	UNP A0A0K8P8E7
F	16	HIS	-	expression tag	UNP A0A0K8P8E7
F	17	HIS	-	expression tag	UNP A0A0K8P8E7
F	18	HIS	-	expression tag	UNP A0A0K8P8E7
F	19	MET	-	expression tag	UNP A0A0K8P8E7

- Molecule 2 is BENZOIC ACID (three-letter code: BEZ) (formula: $C_7H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			9	7	2		
2	B	1	Total	C	O	0	0
			9	7	2		
2	C	1	Total	C	O	0	0
			8	7	1		
2	D	1	Total	C	O	0	0
			9	7	2		
2	E	1	Total	C	O	0	0
			9	7	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	F	1	Total	C	O	0	0
			9	7	2		

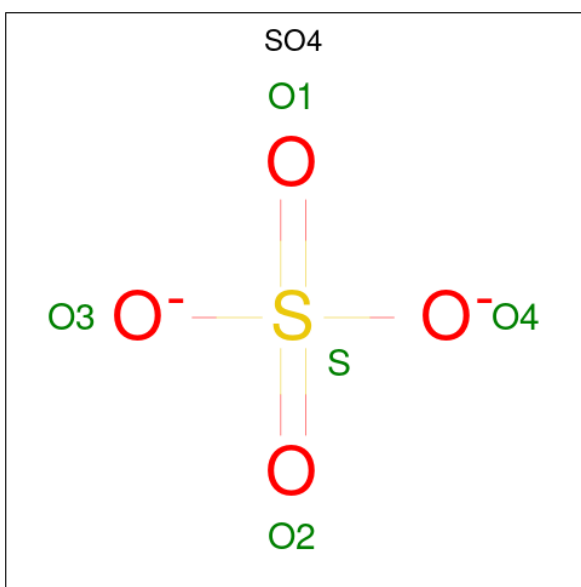
- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		
3	B	1	Total	Ca	0	0
			1	1		
3	C	1	Total	Ca	0	0
			1	1		
3	D	1	Total	Ca	0	0
			1	1		
3	E	1	Total	Ca	0	0
			1	1		
3	F	1	Total	Ca	0	0
			1	1		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

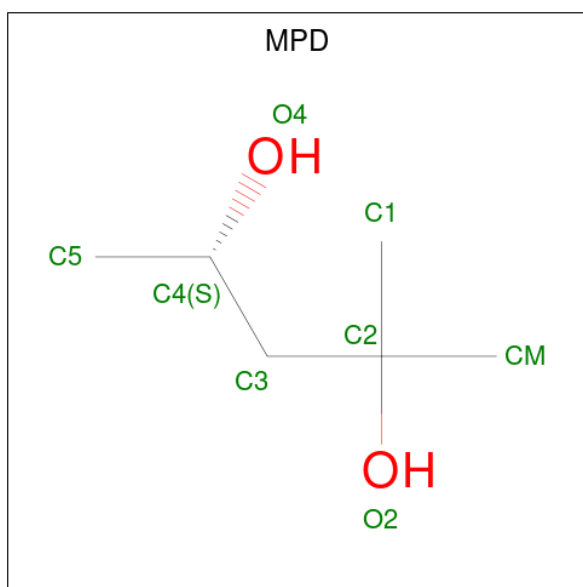
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Cl	0	0
			2	2		
4	B	1	Total	Cl	0	0
			1	1		
4	C	1	Total	Cl	0	0
			1	1		
4	D	1	Total	Cl	0	0
			1	1		
4	E	1	Total	Cl	0	0
			1	1		
4	F	2	Total	Cl	0	0
			2	2		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

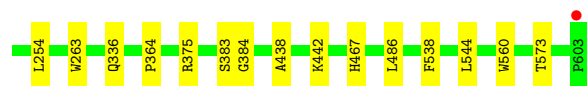
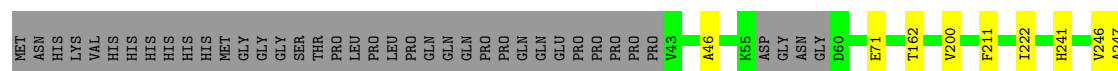
- Molecule 6 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C₆H₁₄O₂).



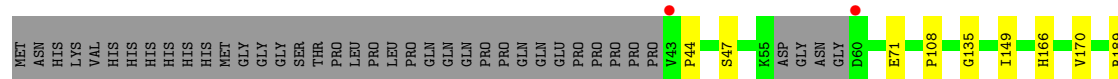
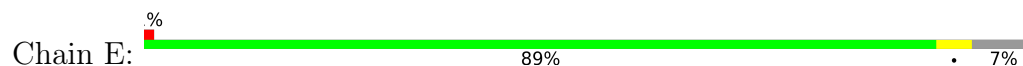
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			8	6	2		

- Molecule 7 is water.

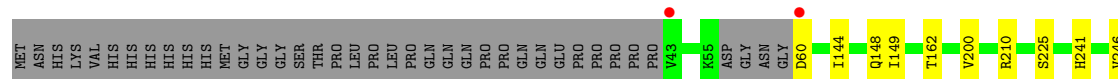
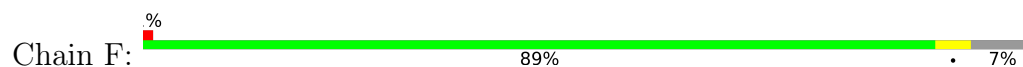
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	291	Total	O	0	0
			291	291		
7	B	379	Total	O	0	0
			379	379		
7	C	312	Total	O	0	0
			312	312		
7	D	327	Total	O	0	0
			327	327		
7	E	351	Total	O	0	0
			351	351		
7	F	324	Total	O	0	0
			324	324		



- Molecule 1: Mono(2-hydroxyethyl) terephthalate hydrolase



- Molecule 1: Mono(2-hydroxyethyl) terephthalate hydrolase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	111.14Å 184.05Å 247.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.09 – 2.20 46.09 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.9 (46.09-2.20) 99.0 (46.09-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.22 (at 2.20Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.185 , 0.213 0.185 , 0.214	Depositor DCC
R_{free} test set	2667 reflections (1.05%)	wwPDB-VP
Wilson B-factor (Å ²)	29.9	Xtriage
Anisotropy	0.169	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 36.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	26826	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.57% 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: SO4, CL, MPD, BEZ, CA

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	0.37	0/4223	0.50	0/5750
1	B	0.38	0/4236	0.53	0/5766
1	C	0.37	0/4228	0.51	0/5755
1	D	0.38	0/4224	0.51	0/5750
1	E	0.38	0/4224	0.52	0/5750
1	F	0.37	0/4224	0.51	0/5750
All	All	0.37	0/25359	0.51	0/34521

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	4116	0	3912	15	0
1	B	4129	0	3919	9	0
1	C	4121	0	3915	11	0
1	D	4117	0	3912	10	0
1	E	4117	0	3912	9	0
1	F	4117	0	3912	12	0
2	A	9	0	5	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	9	0	5	0	0
2	C	8	0	5	0	0
2	D	9	0	5	0	0
2	E	9	0	5	0	0
2	F	9	0	5	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	2	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	2	0	0	0	0
5	A	10	0	0	0	0
5	B	15	0	0	0	0
5	C	5	0	0	0	0
5	D	5	0	0	0	0
5	E	5	0	0	1	0
5	F	10	0	0	0	0
6	B	8	0	14	0	0
7	A	291	0	0	1	0
7	B	379	0	0	0	1
7	C	312	0	0	1	1
7	D	327	0	0	0	2
7	E	351	0	0	1	2
7	F	324	0	0	0	1
All	All	26826	0	23526	67	4

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 1.

The worst 5 of 67 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:F:60:ASP:O	1:F:210:ARG:NH2	2.30	0.65
1:A:246:VAL:HG23	1:A:544:LEU:HD22	1.79	0.63
1:C:246:VAL:HG23	1:C:544:LEU:HD22	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:VAL:HG23	1:B:544:LEU:HD22	1.82	0.60
1:E:246:VAL:HG23	1:E:544:LEU:HD22	1.84	0.59

All (4) 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)
7:C:1091:HOH:O	7:F:1102:HOH:O[2_455]	1.99	0.21
7:D:1045:HOH:O	7:E:1063:HOH:O[2_554]	2.13	0.07
7:D:1115:HOH:O	7:E:1072:HOH:O[2_554]	2.14	0.06
7:B:923:HOH:O	7:B:1202:HOH:O[4_545]	2.16	0.04

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	553/596 (93%)	537 (97%)	16 (3%)	0	100	100
1	B	555/596 (93%)	539 (97%)	15 (3%)	1 (0%)	44	52
1	C	554/596 (93%)	536 (97%)	18 (3%)	0	100	100
1	D	553/596 (93%)	537 (97%)	16 (3%)	0	100	100
1	E	553/596 (93%)	535 (97%)	18 (3%)	0	100	100
1	F	553/596 (93%)	538 (97%)	15 (3%)	0	100	100
All	All	3321/3576 (93%)	3222 (97%)	98 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	60	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	405/439 (92%)	392 (97%)	13 (3%)	34	45
1	B	406/439 (92%)	397 (98%)	9 (2%)	47	61
1	C	405/439 (92%)	399 (98%)	6 (2%)	60	75
1	D	405/439 (92%)	398 (98%)	7 (2%)	56	71
1	E	405/439 (92%)	397 (98%)	8 (2%)	50	65
1	F	405/439 (92%)	401 (99%)	4 (1%)	73	84
All	All	2431/2634 (92%)	2384 (98%)	47 (2%)	52	67

5 of 47 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	71	GLU
1	E	71	GLU
1	D	241	HIS
1	D	375	ARG
1	E	210	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	202	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 31 ligands modelled in this entry, 14 are monoatomic - leaving 17 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	SO4	A	706	-	4,4,4	0.15	0	6,6,6	0.15	0
2	BEZ	F	701	-	9,9,9	0.71	0	11,11,11	0.96	1 (9%)
5	SO4	B	805	-	4,4,4	0.14	0	6,6,6	0.11	0
6	MPD	B	801	-	7,7,7	0.29	0	9,10,10	0.51	0
2	BEZ	D	701	-	9,9,9	0.66	0	11,11,11	1.07	1 (9%)
5	SO4	B	807	-	4,4,4	0.13	0	6,6,6	0.09	0
5	SO4	C	704	-	4,4,4	0.14	0	6,6,6	0.15	0
2	BEZ	C	701	-	8,8,9	0.41	0	9,9,11	0.95	1 (11%)
5	SO4	D	704	-	4,4,4	0.14	0	6,6,6	0.12	0
5	SO4	B	806	-	4,4,4	0.16	0	6,6,6	0.18	0
2	BEZ	E	701	-	9,9,9	0.76	1 (11%)	11,11,11	0.88	0
5	SO4	A	705	-	4,4,4	0.17	0	6,6,6	0.16	0
2	BEZ	B	802	-	9,9,9	0.76	1 (11%)	11,11,11	0.90	0
5	SO4	E	704	-	4,4,4	0.14	0	6,6,6	0.12	0
5	SO4	F	705	-	4,4,4	0.13	0	6,6,6	0.17	0
5	SO4	F	706	-	4,4,4	0.13	0	6,6,6	0.17	0
2	BEZ	A	701	-	9,9,9	0.72	0	11,11,11	0.88	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
2	BEZ	F	701	-	-	0/4/4/4	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	MPD	B	801	-	-	3/5/5/5	-
2	BEZ	D	701	-	-	0/4/4/4	0/1/1/1
2	BEZ	C	701	-	-	0/2/2/4	0/1/1/1
2	BEZ	E	701	-	-	0/4/4/4	0/1/1/1
2	BEZ	B	802	-	-	0/4/4/4	0/1/1/1
2	BEZ	A	701	-	-	0/4/4/4	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	802	BEZ	O2-C	-2.04	1.24	1.30
2	E	701	BEZ	O2-C	-2.01	1.24	1.30

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	701	BEZ	O2-C-C1	2.53	121.41	114.85
2	F	701	BEZ	O2-C-C1	2.07	120.22	114.85
2	C	701	BEZ	C6-C1-C2	2.04	120.66	117.64

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	801	MPD	C2-C3-C4-O4
6	B	801	MPD	CM-C2-C3-C4
6	B	801	MPD	O2-C2-C3-C4

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	701	BEZ	1	0
5	E	704	SO4	1	0
2	A	701	BEZ	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	557/596 (93%)	-0.31	5 (0%) 81 78	24, 32, 52, 73	0
1	B	559/596 (93%)	-0.53	4 (0%) 84 82	21, 28, 41, 84	0
1	C	558/596 (93%)	-0.37	4 (0%) 84 82	24, 31, 47, 97	0
1	D	557/596 (93%)	-0.37	1 (0%) 92 90	23, 30, 46, 62	0
1	E	557/596 (93%)	-0.50	3 (0%) 87 85	22, 28, 39, 69	0
1	F	557/596 (93%)	-0.41	4 (0%) 84 82	23, 30, 43, 69	0
All	All	3345/3576 (93%)	-0.41	21 (0%) 85 83	21, 30, 45, 97	0

The worst 5 of 21 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	43	VAL	5.9
1	E	43	VAL	5.0
1	B	43	VAL	4.7
1	F	43	VAL	4.7
1	A	43	VAL	4.6

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 monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	SO4	B	807	5/5	0.80	0.18	90,90,91,93	0
5	SO4	F	706	5/5	0.80	0.28	106,107,109,111	0
5	SO4	F	705	5/5	0.82	0.17	89,90,92,93	0
5	SO4	D	704	5/5	0.83	0.21	95,96,98,99	0
2	BEZ	C	701	8/9	0.84	0.09	24,25,26,26	0
5	SO4	E	704	5/5	0.85	0.20	118,119,121,123	0
5	SO4	A	706	5/5	0.85	0.15	88,88,90,92	0
5	SO4	B	806	5/5	0.85	0.15	96,97,99,100	0
5	SO4	A	705	5/5	0.86	0.19	81,83,87,88	0
5	SO4	C	704	5/5	0.87	0.18	92,93,96,97	0
5	SO4	B	805	5/5	0.88	0.20	98,98,101,101	0
6	MPD	B	801	8/8	0.91	0.12	31,38,40,43	0
4	CL	F	703	1/1	0.93	0.08	46,46,46,46	0
4	CL	A	704	1/1	0.93	0.12	59,59,59,59	0
4	CL	E	703	1/1	0.93	0.15	73,73,73,73	0
4	CL	B	804	1/1	0.94	0.13	65,65,65,65	0
4	CL	A	703	1/1	0.94	0.11	50,50,50,50	0
4	CL	D	703	1/1	0.95	0.12	53,53,53,53	0
4	CL	F	704	1/1	0.96	0.09	50,50,50,50	0
4	CL	C	703	1/1	0.96	0.12	49,49,49,49	0
2	BEZ	F	701	9/9	0.97	0.07	21,25,30,32	0
2	BEZ	B	802	9/9	0.97	0.06	21,22,23,24	0
2	BEZ	D	701	9/9	0.97	0.07	22,23,25,27	0
2	BEZ	E	701	9/9	0.97	0.06	22,23,24,25	0
2	BEZ	A	701	9/9	0.98	0.06	24,25,28,29	0
3	CA	E	702	1/1	0.99	0.04	23,23,23,23	0
3	CA	A	702	1/1	0.99	0.06	27,27,27,27	0
3	CA	B	803	1/1	0.99	0.03	28,28,28,28	0
3	CA	C	702	1/1	0.99	0.03	33,33,33,33	0
3	CA	F	702	1/1	1.00	0.02	25,25,25,25	0
3	CA	D	702	1/1	1.00	0.01	29,29,29,29	0

6.5 Other polymers [i](#)

There are no such residues in this entry.