



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 09:02 PM BST

PDB ID : 4MG4
Title : Crystal structure of a putative phosphonmutase from Burkholderia cenocepacia J2315
Authors : Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on : 2013-08-28
Resolution : 1.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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 : 2.13.1
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) : 2.13.1

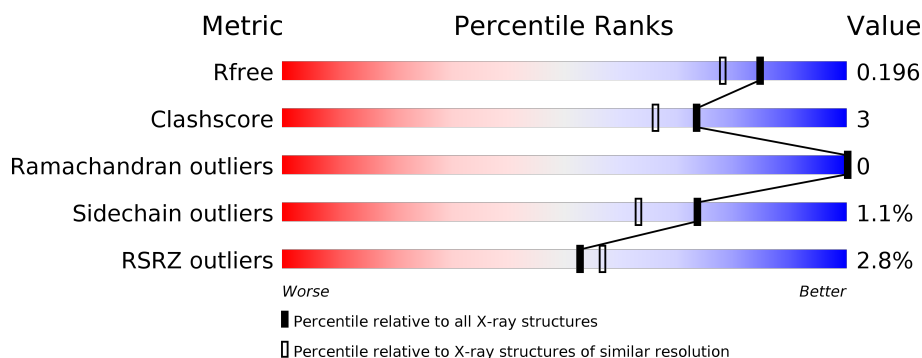
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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 $\leq 5\%$. 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	261	<div> <div>2%</div> <div> <div></div> <div>87%</div> <div>7%</div> <div>• •</div> </div> </div>
1	B	261	<div> <div>2%</div> <div> <div></div> <div>93%</div> <div>• •</div> </div> </div>
1	C	261	<div> <div>3%</div> <div> <div></div> <div>87%</div> <div>10%</div> <div>•</div> </div> </div>
1	D	261	<div> <div>3%</div> <div> <div></div> <div>87%</div> <div>7%</div> <div>6%</div> </div> </div>
1	E	261	<div> <div>2%</div> <div> <div></div> <div>91%</div> <div>5%</div> <div>•</div> </div> </div>
1	F	261	<div> <div>3%</div> <div> <div></div> <div>92%</div> <div>• • •</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	261	<div><div><div></div><div></div><div></div></div><div><div>3%</div><div>91%</div><div>5% . .</div></div></div>
1	H	261	<div><div><div></div><div></div><div></div></div><div><div>3%</div><div>90%</div><div>. 7%</div></div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16446 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 Phosphonomutase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	250	Total	C	N	O	S	0	2	0
			1852	1160	332	352	8			
1	B	251	Total	C	N	O	S	0	2	0
			1826	1144	325	348	9			
1	C	253	Total	C	N	O	S	0	3	0
			1855	1161	330	355	9			
1	D	246	Total	C	N	O	S	0	2	0
			1792	1128	318	338	8			
1	E	253	Total	C	N	O	S	0	2	0
			1850	1158	324	359	9			
1	F	250	Total	C	N	O	S	0	1	0
			1809	1137	318	347	7			
1	G	252	Total	C	N	O	S	0	2	0
			1859	1163	333	354	9			
1	H	243	Total	C	N	O	S	0	3	0
			1765	1110	317	331	7			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	EXPRESSION TAG	UNP B4EL08
A	-6	ALA	-	EXPRESSION TAG	UNP B4EL08
A	-5	HIS	-	EXPRESSION TAG	UNP B4EL08
A	-4	HIS	-	EXPRESSION TAG	UNP B4EL08
A	-3	HIS	-	EXPRESSION TAG	UNP B4EL08
A	-2	HIS	-	EXPRESSION TAG	UNP B4EL08
A	-1	HIS	-	EXPRESSION TAG	UNP B4EL08
A	0	HIS	-	EXPRESSION TAG	UNP B4EL08
B	-7	MET	-	EXPRESSION TAG	UNP B4EL08
B	-6	ALA	-	EXPRESSION TAG	UNP B4EL08
B	-5	HIS	-	EXPRESSION TAG	UNP B4EL08
B	-4	HIS	-	EXPRESSION TAG	UNP B4EL08
B	-3	HIS	-	EXPRESSION TAG	UNP B4EL08

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	HIS	-	EXPRESSION TAG	UNP B4EL08
B	-1	HIS	-	EXPRESSION TAG	UNP B4EL08
B	0	HIS	-	EXPRESSION TAG	UNP B4EL08
C	-7	MET	-	EXPRESSION TAG	UNP B4EL08
C	-6	ALA	-	EXPRESSION TAG	UNP B4EL08
C	-5	HIS	-	EXPRESSION TAG	UNP B4EL08
C	-4	HIS	-	EXPRESSION TAG	UNP B4EL08
C	-3	HIS	-	EXPRESSION TAG	UNP B4EL08
C	-2	HIS	-	EXPRESSION TAG	UNP B4EL08
C	-1	HIS	-	EXPRESSION TAG	UNP B4EL08
C	0	HIS	-	EXPRESSION TAG	UNP B4EL08
D	-7	MET	-	EXPRESSION TAG	UNP B4EL08
D	-6	ALA	-	EXPRESSION TAG	UNP B4EL08
D	-5	HIS	-	EXPRESSION TAG	UNP B4EL08
D	-4	HIS	-	EXPRESSION TAG	UNP B4EL08
D	-3	HIS	-	EXPRESSION TAG	UNP B4EL08
D	-2	HIS	-	EXPRESSION TAG	UNP B4EL08
D	-1	HIS	-	EXPRESSION TAG	UNP B4EL08
D	0	HIS	-	EXPRESSION TAG	UNP B4EL08
E	-7	MET	-	EXPRESSION TAG	UNP B4EL08
E	-6	ALA	-	EXPRESSION TAG	UNP B4EL08
E	-5	HIS	-	EXPRESSION TAG	UNP B4EL08
E	-4	HIS	-	EXPRESSION TAG	UNP B4EL08
E	-3	HIS	-	EXPRESSION TAG	UNP B4EL08
E	-2	HIS	-	EXPRESSION TAG	UNP B4EL08
E	-1	HIS	-	EXPRESSION TAG	UNP B4EL08
E	0	HIS	-	EXPRESSION TAG	UNP B4EL08
F	-7	MET	-	EXPRESSION TAG	UNP B4EL08
F	-6	ALA	-	EXPRESSION TAG	UNP B4EL08
F	-5	HIS	-	EXPRESSION TAG	UNP B4EL08
F	-4	HIS	-	EXPRESSION TAG	UNP B4EL08
F	-3	HIS	-	EXPRESSION TAG	UNP B4EL08
F	-2	HIS	-	EXPRESSION TAG	UNP B4EL08
F	-1	HIS	-	EXPRESSION TAG	UNP B4EL08
F	0	HIS	-	EXPRESSION TAG	UNP B4EL08
G	-7	MET	-	EXPRESSION TAG	UNP B4EL08
G	-6	ALA	-	EXPRESSION TAG	UNP B4EL08
G	-5	HIS	-	EXPRESSION TAG	UNP B4EL08
G	-4	HIS	-	EXPRESSION TAG	UNP B4EL08
G	-3	HIS	-	EXPRESSION TAG	UNP B4EL08
G	-2	HIS	-	EXPRESSION TAG	UNP B4EL08
G	-1	HIS	-	EXPRESSION TAG	UNP B4EL08

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Chain	Residue	Modelled	Actual	Comment	Reference
G	0	HIS	-	EXPRESSION TAG	UNP B4EL08
H	-7	MET	-	EXPRESSION TAG	UNP B4EL08
H	-6	ALA	-	EXPRESSION TAG	UNP B4EL08
H	-5	HIS	-	EXPRESSION TAG	UNP B4EL08
H	-4	HIS	-	EXPRESSION TAG	UNP B4EL08
H	-3	HIS	-	EXPRESSION TAG	UNP B4EL08
H	-2	HIS	-	EXPRESSION TAG	UNP B4EL08
H	-1	HIS	-	EXPRESSION TAG	UNP B4EL08
H	0	HIS	-	EXPRESSION TAG	UNP B4EL08

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	3	Total Cl 3 3	0	0
2	D	3	Total Cl 3 3	0	0
2	E	4	Total Cl 4 4	0	0
2	H	3	Total Cl 3 3	0	0
2	B	3	Total Cl 3 3	0	0
2	C	3	Total Cl 3 3	0	0
2	A	3	Total Cl 3 3	0	0
2	F	3	Total Cl 3 3	0	0

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

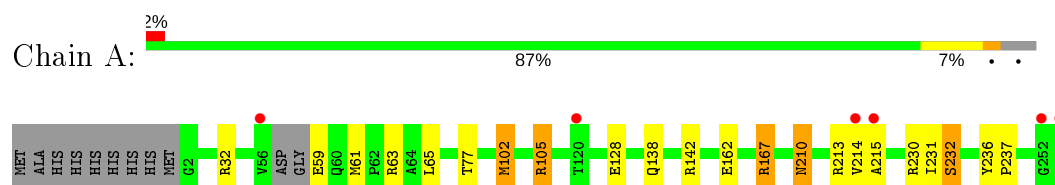
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	243	Total	O	0	0
			243	243		
4	B	281	Total	O	0	0
			281	281		
4	C	265	Total	O	0	0
			265	265		
4	D	214	Total	O	0	0
			214	214		
4	E	190	Total	O	0	0
			190	190		
4	F	210	Total	O	0	0
			210	210		
4	G	244	Total	O	0	0
			244	244		
4	H	150	Total	O	0	0
			150	150		

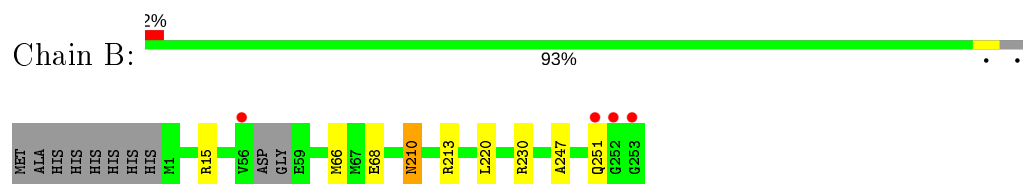
3 Residue-property plots [i](#)

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.

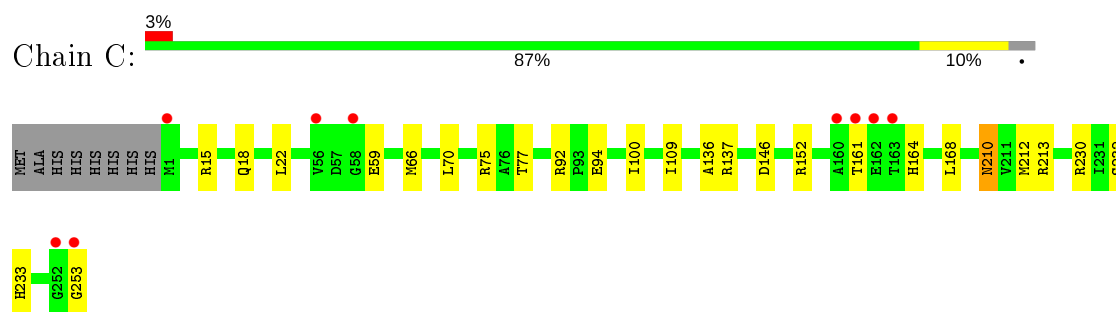
- Molecule 1: Phosphonomutase



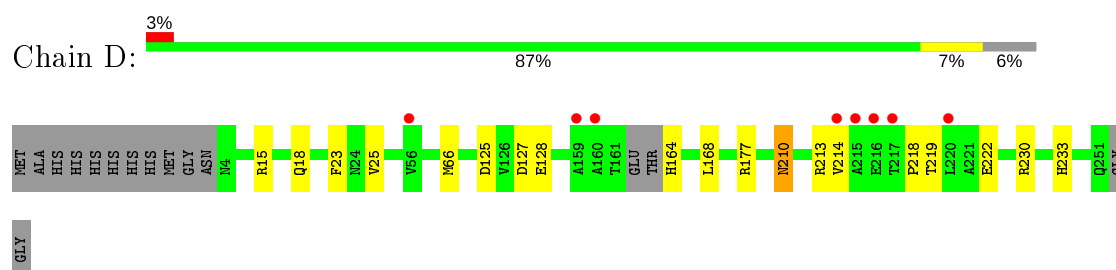
- Molecule 1: Phosphonomutase



- Molecule 1: Phosphonomutase



- Molecule 1: Phosphonomutase

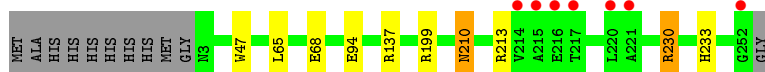


- Molecule 1: Phosphonomutase





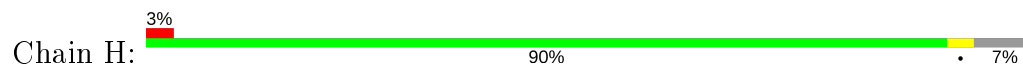
● Molecule 1: Phosphonomutase



● Molecule 1: Phosphonomutase



● Molecule 1: Phosphonomutase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	218.60Å 91.18Å 110.01Å 90.00° 91.53° 90.00°	Depositor
Resolution (Å)	46.29 – 1.70 46.25 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.8 (46.29-1.70) 99.8 (46.25-1.70)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.17 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.158 , 0.189 0.168 , 0.196	Depositor DCC
R_{free} test set	11843 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	17.2	Xtriage
Anisotropy	0.075	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 50.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.014 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	16446	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.05% 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: EDO, CL

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	0.82	2/1883 (0.1%)	1.00	6/2560 (0.2%)
1	B	0.76	0/1857	0.88	2/2531 (0.1%)
1	C	0.76	0/1887	0.87	2/2570 (0.1%)
1	D	0.72	0/1824	0.84	3/2489 (0.1%)
1	E	0.72	0/1883	0.85	3/2565 (0.1%)
1	F	0.67	0/1842	0.80	2/2517 (0.1%)
1	G	0.79	0/1891	0.90	4/2573 (0.2%)
1	H	0.66	0/1797	0.80	0/2453
All	All	0.74	2/14864 (0.0%)	0.87	22/20258 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	232	SER	CB-OG	-9.22	1.30	1.42
1	A	232	SER	CA-CB	5.47	1.61	1.52

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	102[A]	MET	CG-SD-CE	12.78	120.65	100.20
1	A	102[B]	MET	CG-SD-CE	12.78	120.65	100.20
1	G	63	ARG	NE-CZ-NH2	7.56	124.08	120.30
1	B	15[A]	ARG	NE-CZ-NH2	-7.36	116.62	120.30
1	B	15[B]	ARG	NE-CZ-NH2	-7.36	116.62	120.30
1	A	105	ARG	NE-CZ-NH1	6.69	123.65	120.30
1	F	230	ARG	NE-CZ-NH2	-6.57	117.02	120.30
1	A	105	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	E	27	ASP	CB-CG-OD1	6.27	123.95	118.30
1	G	137	ARG	NE-CZ-NH2	-6.03	117.28	120.30
1	A	167[A]	ARG	NE-CZ-NH1	5.94	123.27	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	167[B]	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	D	66[A]	MET	CG-SD-CE	5.84	109.54	100.20
1	D	66[B]	MET	CG-SD-CE	5.84	109.54	100.20
1	G	175	ARG	NE-CZ-NH1	5.83	123.21	120.30
1	F	230	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	C	137	ARG	NE-CZ-NH1	5.59	123.10	120.30
1	C	152	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	D	127	ASP	CB-CG-OD1	5.12	122.91	118.30
1	G	105	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	E	66[A]	MET	CG-SD-CE	5.02	108.23	100.20
1	E	66[B]	MET	CG-SD-CE	5.02	108.23	100.20

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	1852	0	1830	21	1
1	B	1826	0	1774	9	0
1	C	1855	0	1809	21	1
1	D	1792	0	1742	17	0
1	E	1850	0	1792	14	0
1	F	1809	0	1751	6	0
1	G	1859	0	1830	13	0
1	H	1765	0	1705	5	0
2	A	3	0	0	1	0
2	B	3	0	0	0	0
2	C	3	0	0	0	0
2	D	3	0	0	0	0
2	E	4	0	0	0	0
2	F	3	0	0	0	0
2	G	3	0	0	1	0
2	H	3	0	0	0	0
3	D	4	0	6	0	0
3	E	4	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	4	0	6	1	0
3	H	4	0	6	0	0
4	A	243	0	0	3	0
4	B	281	0	0	3	0
4	C	265	0	0	5	0
4	D	214	0	0	4	1
4	E	190	0	0	3	1
4	F	210	0	0	1	0
4	G	244	0	0	1	0
4	H	150	0	0	0	0
All	All	16446	0	14257	96	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 (96) 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:102[A]:MET:HE2	1:A:105:ARG:HD2	1.14	1.07
1:A:102[A]:MET:CE	1:A:105:ARG:HD2	1.94	0.98
1:G:102[B]:MET:HE2	1:G:105:ARG:HD2	1.49	0.93
1:A:102[A]:MET:HE2	1:A:105:ARG:CD	2.02	0.90
1:G:102[B]:MET:HE2	1:G:105:ARG:HH11	1.37	0.88
1:D:213:ARG:HD3	1:D:233[A]:HIS:CD2	2.11	0.85
1:B:68:GLU:OE2	1:D:177:ARG:NH1	2.13	0.82
1:C:66[B]:MET:O	1:C:66[B]:MET:HE2	1.81	0.81
1:H:219:THR:HG23	1:H:222:GLU:H	1.48	0.77
1:G:102[B]:MET:CE	1:G:105:ARG:HH11	1.99	0.76
1:F:213:ARG:HD3	1:F:233[A]:HIS:CD2	2.21	0.75
1:D:219:THR:HG21	4:D:555:HOH:O	1.86	0.75
1:A:102[A]:MET:CE	1:A:105:ARG:CD	2.63	0.74
1:E:213:ARG:HD3	1:E:233[A]:HIS:CD2	2.23	0.73
1:C:233:HIS:HE1	1:E:253:GLY:OXT	1.75	0.68
1:E:213:ARG:HD3	1:E:233[A]:HIS:NE2	2.09	0.68
1:H:213:ARG:HD3	1:H:233[A]:HIS:CD2	2.30	0.66
1:F:199:ARG:NH1	4:F:608:HOH:O	2.17	0.64
1:C:233:HIS:CE1	1:E:253:GLY:OXT	2.50	0.64
1:C:75:ARG:NH1	4:C:612:HOH:O	2.30	0.64
1:H:164:HIS:HA	1:H:168:LEU:HD12	1.80	0.62
1:C:15:ARG:CZ	1:C:18:GLN:HE21	2.11	0.62
1:C:66[B]:MET:O	1:C:66[B]:MET:CE	2.48	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:59:GLU:OE1	4:C:557:HOH:O	2.16	0.60
1:A:102[A]:MET:CE	1:A:105:ARG:HH11	2.13	0.60
1:D:213:ARG:HD3	1:D:233[A]:HIS:NE2	2.16	0.60
1:D:125:ASP:HB2	1:D:128:GLU:OE1	2.03	0.59
1:G:22:LEU:HD12	4:G:486:HOH:O	2.02	0.58
1:D:219:THR:HG23	1:D:222:GLU:H	1.68	0.58
1:C:66[B]:MET:SD	1:C:66[B]:MET:C	2.82	0.58
1:C:161:THR:HA	1:C:164:HIS:CD2	2.39	0.57
1:E:68:GLU:OE2	4:E:436:HOH:O	2.17	0.57
1:C:164:HIS:HA	1:C:168:LEU:HD12	1.86	0.56
1:C:66[B]:MET:O	1:C:66[B]:MET:SD	2.63	0.56
1:A:102[A]:MET:HE2	1:A:105:ARG:HH11	1.72	0.55
1:G:102[B]:MET:CE	1:G:105:ARG:HD2	2.32	0.54
1:D:23:PHE:CE1	1:G:253:GLY:O	2.60	0.54
1:A:138:GLN:HG2	1:A:142:ARG:NH1	2.23	0.53
1:G:102[B]:MET:HE2	1:G:105:ARG:CD	2.33	0.53
1:D:23:PHE:HE1	1:G:253:GLY:O	1.92	0.53
1:B:66[B]:MET:SD	1:B:66[B]:MET:C	2.89	0.52
1:A:167[B]:ARG:HD3	4:A:634:HOH:O	2.10	0.51
1:B:220:LEU:HD22	4:B:648:HOH:O	2.10	0.51
1:G:193:ARG:NH2	1:G:215:ALA:HB3	2.24	0.51
1:A:63:ARG:CZ	1:A:102[B]:MET:SD	2.99	0.51
1:A:128:GLU:HG2	4:A:447:HOH:O	2.11	0.50
1:D:25:VAL:O	4:D:568:HOH:O	2.19	0.50
1:C:92:ARG:CZ	1:C:94:GLU:OE1	2.59	0.50
1:A:210:ASN:HA	1:A:230:ARG:O	2.12	0.49
1:C:253:GLY:OXT	1:E:23:PHE:CE1	2.65	0.49
1:A:63:ARG:NH1	1:A:102[B]:MET:SD	2.86	0.49
1:B:220:LEU:CD2	4:B:648:HOH:O	2.61	0.48
1:G:210:ASN:HA	1:G:230:ARG:O	2.14	0.47
1:A:59:GLU:OE1	4:A:639:HOH:O	2.20	0.47
1:C:210:ASN:HA	1:C:230:ARG:O	2.15	0.47
1:G:155:VAL:HG12	1:G:168:LEU:HG	1.96	0.47
1:B:66[B]:MET:SD	1:B:66[B]:MET:O	2.73	0.47
1:A:61:MET:HE2	1:A:65:LEU:HG	1.97	0.47
1:B:68:GLU:OE2	1:D:177:ARG:CZ	2.63	0.47
1:B:247:ALA:O	1:B:251:GLN:HG2	2.16	0.46
1:C:213:ARG:HD3	1:E:253:GLY:O	2.15	0.46
1:E:114:GLU:OE2	1:E:154:ASP:OD2	2.33	0.46
1:B:210:ASN:HA	1:B:230:ARG:O	2.15	0.46
1:H:210:ASN:HA	1:H:230:ARG:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:TYR:HE2	1:H:248:LEU:HD22	1.80	0.46
1:D:164:HIS:HA	1:D:168:LEU:HD12	1.98	0.46
1:D:15:ARG:CZ	1:D:18:GLN:HE21	2.29	0.46
1:G:66[B]:MET:C	1:G:66[B]:MET:SD	2.95	0.45
1:E:210:ASN:HA	1:E:230:ARG:O	2.17	0.45
1:C:253:GLY:OXT	1:E:23:PHE:HE1	2.00	0.45
1:C:232:SER:HB3	4:C:475:HOH:O	2.17	0.45
1:D:210:ASN:HA	1:D:230:ARG:O	2.16	0.45
1:A:32:ARG:HD3	1:A:32:ARG:O	2.17	0.45
1:A:61:MET:CE	1:A:65:LEU:HG	2.46	0.44
1:A:213:ARG:HG3	1:A:231:ILE:CG2	2.48	0.44
1:E:94:GLU:CD	1:E:94:GLU:H	2.21	0.44
1:D:218:PRO:HD2	4:D:472:HOH:O	2.18	0.44
1:C:212:MET:CE	4:C:661:HOH:O	2.65	0.44
1:D:214:VAL:O	1:D:233[B]:HIS:HE1	2.00	0.44
1:G:45:GLY:HA3	2:G:301:CL:CL	2.54	0.44
1:A:232:SER:HB3	2:A:302:CL:CL	2.54	0.43
1:A:214:VAL:HG13	1:A:215:ALA:N	2.34	0.43
1:C:66[B]:MET:HE1	1:C:70:LEU:HB2	2.00	0.43
1:C:22:LEU:HD12	4:C:475:HOH:O	2.18	0.42
1:F:210:ASN:HA	1:F:230:ARG:O	2.18	0.42
1:F:47:TRP:CD1	3:F:301:EDO:H22	2.54	0.41
1:D:233[A]:HIS:HB2	4:D:425:HOH:O	2.20	0.41
1:E:25:VAL:O	4:E:447:HOH:O	2.21	0.41
1:F:94:GLU:H	1:F:94:GLU:CD	2.23	0.41
1:E:66[A]:MET:CE	4:E:558:HOH:O	2.68	0.41
1:C:100:ILE:HG13	1:C:136:ALA:CB	2.51	0.41
1:E:214:VAL:O	1:E:233[B]:HIS:HE1	2.04	0.41
1:A:236:TYR:HB3	1:A:237:PRO:HD3	2.03	0.40
1:D:219:THR:HG22	1:D:222:GLU:CG	2.51	0.40
1:B:213:ARG:HG3	4:B:565:HOH:O	2.20	0.40
1:F:65:LEU:O	1:F:68:GLU:HG2	2.22	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:162:GLU:OE1	1:C:146:ASP:OD2[4_758]	1.96	0.24
4:D:477:HOH:O	4:E:437:HOH:O[2_769]	1.98	0.22

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	248/261 (95%)	248 (100%)	0	0	100	100
1	B	249/261 (95%)	247 (99%)	2 (1%)	0	100	100
1	C	254/261 (97%)	250 (98%)	4 (2%)	0	100	100
1	D	244/261 (94%)	241 (99%)	3 (1%)	0	100	100
1	E	253/261 (97%)	251 (99%)	2 (1%)	0	100	100
1	F	249/261 (95%)	246 (99%)	3 (1%)	0	100	100
1	G	252/261 (97%)	250 (99%)	2 (1%)	0	100	100
1	H	242/261 (93%)	235 (97%)	7 (3%)	0	100	100
All	All	1991/2088 (95%)	1968 (99%)	23 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	178/189 (94%)	176 (99%)	2 (1%)	73	63
1	B	171/189 (90%)	170 (99%)	1 (1%)	86	80
1	C	175/189 (93%)	172 (98%)	3 (2%)	60	46
1	D	168/189 (89%)	167 (99%)	1 (1%)	86	80
1	E	175/189 (93%)	170 (97%)	5 (3%)	42	23
1	F	170/189 (90%)	168 (99%)	2 (1%)	71	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	178/189 (94%)	177 (99%)	1 (1%)	86	80
1	H	162/189 (86%)	161 (99%)	1 (1%)	86	80
All	All	1377/1512 (91%)	1361 (99%)	16 (1%)	73	59

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	THR
1	A	210	ASN
1	B	210	ASN
1	C	77	THR
1	C	109	ILE
1	C	210	ASN
1	D	210	ASN
1	E	66[A]	MET
1	E	66[B]	MET
1	E	109	ILE
1	E	137	ARG
1	E	210	ASN
1	F	137	ARG
1	F	210	ASN
1	G	210	ASN
1	H	210	ASN

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

Mol	Chain	Res	Type
1	C	18	GLN
1	C	233	HIS
1	D	18	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 monosaccharides in this entry.

5.6 Ligand geometry

Of 29 ligands modelled in this entry, 25 are monoatomic - leaving 4 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	$\# Z > 2$
3	EDO	H	301	-	3,3,3	0.65	0	2,2,2	0.13	0
3	EDO	E	301	-	3,3,3	0.52	0	2,2,2	0.46	0
3	EDO	D	301	-	3,3,3	0.53	0	2,2,2	0.44	0
3	EDO	F	301	-	3,3,3	0.45	0	2,2,2	0.44	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	EDO	H	301	-	-	0/1/1/1	-
3	EDO	E	301	-	-	0/1/1/1	-
3	EDO	D	301	-	-	0/1/1/1	-
3	EDO	F	301	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	301	EDO	1	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 ⓘ

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, 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	250/261 (95%)	-0.21	6 (2%) 59 63	9, 16, 37, 49	0
1	B	251/261 (96%)	-0.24	4 (1%) 72 76	9, 15, 35, 56	0
1	C	253/261 (96%)	-0.15	9 (3%) 42 47	9, 16, 37, 58	0
1	D	246/261 (94%)	-0.17	8 (3%) 46 51	11, 20, 39, 60	0
1	E	253/261 (96%)	-0.17	4 (1%) 72 76	12, 22, 39, 50	0
1	F	250/261 (95%)	-0.19	7 (2%) 53 57	13, 21, 37, 53	0
1	G	252/261 (96%)	-0.14	8 (3%) 47 52	8, 15, 35, 46	0
1	H	243/261 (93%)	-0.03	9 (3%) 41 46	14, 26, 43, 59	0
All	All	1998/2088 (95%)	-0.17	55 (2%) 53 57	8, 19, 39, 60	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	253	GLY	6.0
1	B	253	GLY	5.2
1	D	215	ALA	4.8
1	A	253	GLY	4.5
1	F	214	VAL	4.5
1	A	56	VAL	4.4
1	C	56	VAL	4.4
1	G	253	GLY	4.3
1	A	252	GLY	4.3
1	C	160	ALA	4.1
1	H	215	ALA	4.1
1	E	215	ALA	4.0
1	G	58	GLY	3.9
1	F	217	THR	3.7
1	D	160	ALA	3.7
1	E	56	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
1	G	56	VAL	3.7
1	D	214	VAL	3.6
1	H	159	ALA	3.4
1	C	163	THR	3.4
1	C	252	GLY	3.3
1	H	217	THR	3.3
1	E	58	GLY	3.2
1	F	215	ALA	3.1
1	A	120	THR	3.0
1	D	217	THR	3.0
1	G	252	GLY	3.0
1	G	214	VAL	3.0
1	H	164	HIS	3.0
1	H	216	GLU	3.0
1	F	220	LEU	2.9
1	E	216	GLU	2.9
1	F	216	GLU	2.9
1	B	252	GLY	2.8
1	A	214	VAL	2.8
1	C	58	GLY	2.8
1	C	162	GLU	2.6
1	D	56	VAL	2.6
1	H	220	LEU	2.6
1	F	252	GLY	2.5
1	C	1	MET	2.5
1	F	221	ALA	2.5
1	B	251	GLN	2.4
1	C	161	THR	2.4
1	B	56	VAL	2.3
1	D	220	LEU	2.3
1	A	215	ALA	2.2
1	G	215	ALA	2.2
1	G	57	ASP	2.1
1	D	216	GLU	2.1
1	H	252	GLY	2.1
1	G	217	THR	2.1
1	D	159	ALA	2.1
1	H	218	PRO	2.0
1	H	214	VAL	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, 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(\AA^2)	Q<0.9
3	EDO	F	301	4/4	0.87	0.11	32,33,34,37	0
3	EDO	D	301	4/4	0.88	0.17	24,29,32,34	0
3	EDO	E	301	4/4	0.92	0.18	25,32,35,41	0
2	CL	H	304	1/1	0.92	0.07	40,40,40,40	0
2	CL	C	303	1/1	0.95	0.08	29,29,29,29	0
2	CL	H	303	1/1	0.96	0.06	30,30,30,30	0
3	EDO	H	301	4/4	0.96	0.07	19,22,22,24	0
2	CL	D	304	1/1	0.98	0.06	30,30,30,30	0
2	CL	B	302	1/1	0.98	0.04	21,21,21,21	0
2	CL	A	301	1/1	0.98	0.04	19,19,19,19	0
2	CL	E	305	1/1	0.98	0.06	35,35,35,35	0
2	CL	F	303	1/1	0.98	0.05	24,24,24,24	0
2	CL	G	303	1/1	0.98	0.06	16,16,16,16	0
2	CL	C	302	1/1	0.98	0.04	21,21,21,21	0
2	CL	E	302	1/1	0.98	0.08	17,17,17,17	0
2	CL	A	303	1/1	0.98	0.05	23,23,23,23	0
2	CL	E	304	1/1	0.98	0.06	22,22,22,22	0
2	CL	B	301	1/1	0.99	0.04	18,18,18,18	0
2	CL	B	303	1/1	0.99	0.06	24,24,24,24	0
2	CL	E	303	1/1	0.99	0.04	21,21,21,21	0
2	CL	G	302	1/1	0.99	0.05	20,20,20,20	0
2	CL	H	302	1/1	0.99	0.04	21,21,21,21	0
2	CL	D	302	1/1	0.99	0.06	16,16,16,16	0
2	CL	F	304	1/1	0.99	0.06	23,23,23,23	0
2	CL	D	303	1/1	0.99	0.06	19,19,19,19	0
2	CL	F	302	1/1	0.99	0.07	18,18,18,18	0
2	CL	A	302	1/1	0.99	0.04	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	CL	G	301	1/1	0.99	0.05	15,15,15,15	0
2	CL	C	301	1/1	1.00	0.04	15,15,15,15	0

6.5 Other polymers [i](#)

There are no such residues in this entry.