



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:30 PM UTC

PDB ID : 4BXH / pdb_00004bxh
Title : Resolving the activation site of positive regulators in plant phosphoenolpyruvate carboxylase
Authors : Schlieper, D.; Foerster, K.; Paulus, J.K.; Groth, G.
Deposited on : 2013-07-11
Resolution : 2.24 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 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

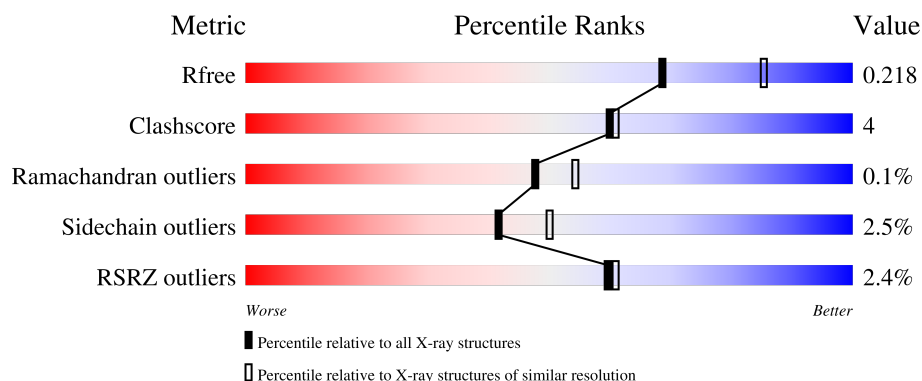
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

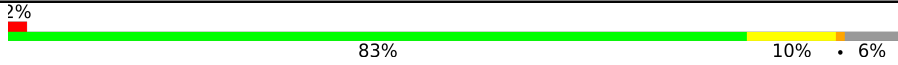
The reported resolution of this entry is 2.24 Å.

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}	180053	3416 (2.26-2.22)
Clashscore	190562	3556 (2.26-2.22)
Ramachandran outliers	187476	3500 (2.26-2.22)
Sidechain outliers	187428	3501 (2.26-2.22)
RSRZ outliers	180081	3415 (2.26-2.22)

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	990	 2% 83% 10% • 6%
2	B	990	 2% 82% 11% • 6%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15803 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 C4 PHOSPHOENOLPYRUVATE CARBOXYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	929	7479	4747	1300	1396	36	0	4	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-23	MET	-	expression tag	UNP P30694
A	-22	GLY	-	expression tag	UNP P30694
A	-21	HIS	-	expression tag	UNP P30694
A	-20	HIS	-	expression tag	UNP P30694
A	-19	HIS	-	expression tag	UNP P30694
A	-18	HIS	-	expression tag	UNP P30694
A	-17	HIS	-	expression tag	UNP P30694
A	-16	HIS	-	expression tag	UNP P30694
A	-15	HIS	-	expression tag	UNP P30694
A	-14	HIS	-	expression tag	UNP P30694
A	-13	HIS	-	expression tag	UNP P30694
A	-12	HIS	-	expression tag	UNP P30694
A	-11	SER	-	expression tag	UNP P30694
A	-10	SER	-	expression tag	UNP P30694
A	-9	GLY	-	expression tag	UNP P30694
A	-8	HIS	-	expression tag	UNP P30694
A	-7	GLU	-	expression tag	UNP P30694
A	-6	ASN	-	expression tag	UNP P30694
A	-5	LEU	-	expression tag	UNP P30694
A	-4	TYR	-	expression tag	UNP P30694
A	-3	PHE	-	expression tag	UNP P30694
A	-2	GLN	-	expression tag	UNP P30694
A	-1	GLY	-	expression tag	UNP P30694
A	0	HIS	-	expression tag	UNP P30694

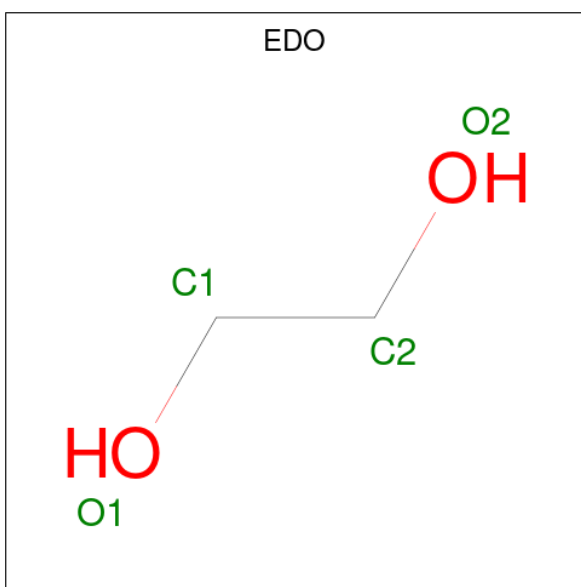
- Molecule 2 is a protein called C4 PHOSPHOENOLPYRUVATE CARBOXYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	927	Total 7466	C 4741	N 1298	O 1392	S 35	0	4	0

There are 25 discrepancies between the modelled and reference sequences:

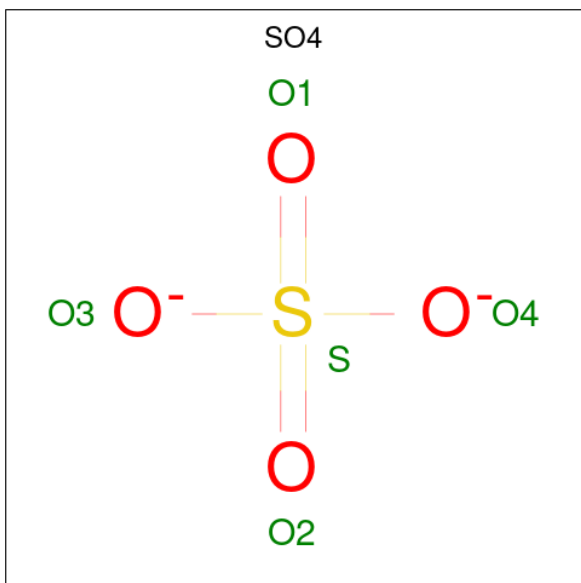
Chain	Residue	Modelled	Actual	Comment	Reference
B	-23	MET	-	expression tag	UNP P30694
B	-22	GLY	-	expression tag	UNP P30694
B	-21	HIS	-	expression tag	UNP P30694
B	-20	HIS	-	expression tag	UNP P30694
B	-19	HIS	-	expression tag	UNP P30694
B	-18	HIS	-	expression tag	UNP P30694
B	-17	HIS	-	expression tag	UNP P30694
B	-16	HIS	-	expression tag	UNP P30694
B	-15	HIS	-	expression tag	UNP P30694
B	-14	HIS	-	expression tag	UNP P30694
B	-13	HIS	-	expression tag	UNP P30694
B	-12	HIS	-	expression tag	UNP P30694
B	-11	SER	-	expression tag	UNP P30694
B	-10	SER	-	expression tag	UNP P30694
B	-9	GLY	-	expression tag	UNP P30694
B	-8	HIS	-	expression tag	UNP P30694
B	-7	GLU	-	expression tag	UNP P30694
B	-6	ASN	-	expression tag	UNP P30694
B	-5	LEU	-	expression tag	UNP P30694
B	-4	TYR	-	expression tag	UNP P30694
B	-3	PHE	-	expression tag	UNP P30694
B	-2	GLN	-	expression tag	UNP P30694
B	-1	GLY	-	expression tag	UNP P30694
B	0	HIS	-	expression tag	UNP P30694
B	748	LYS	MET	conflict	UNP P30694

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

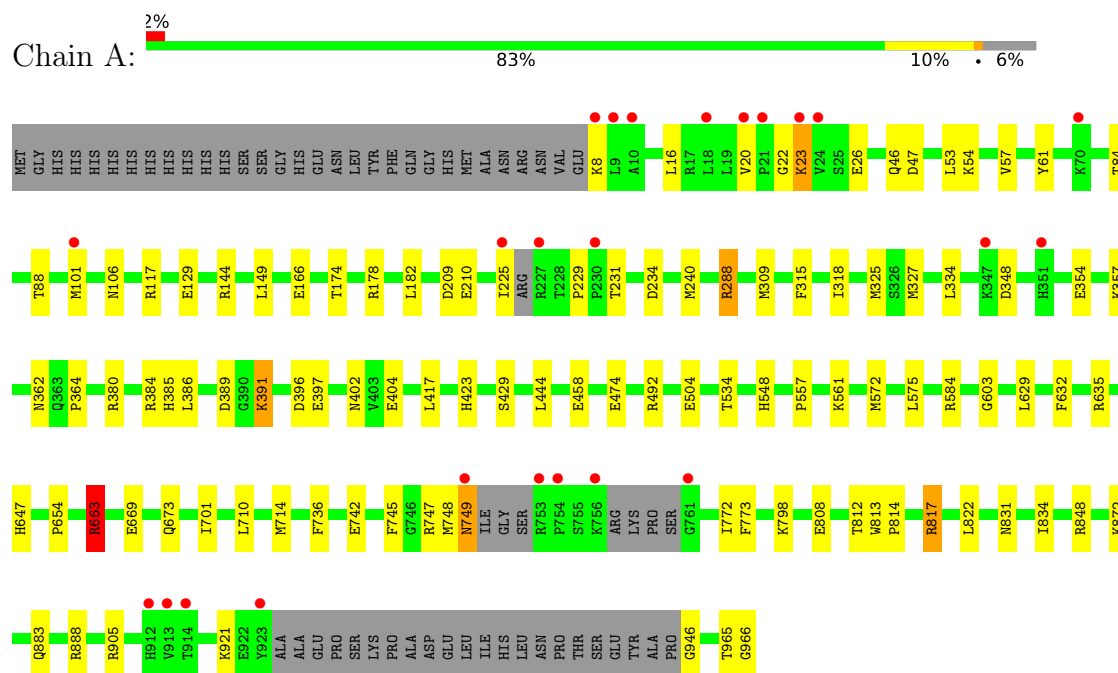
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	420	Total	O	0	0
			420	420		
5	B	412	Total	O	0	0
			412	412		

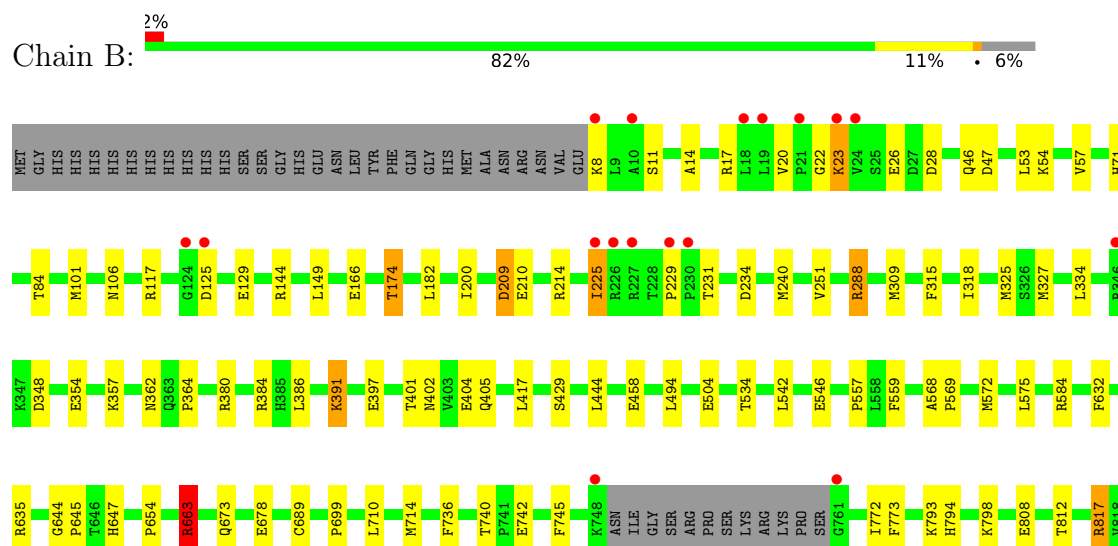
3 Residue-property plots [i](#)

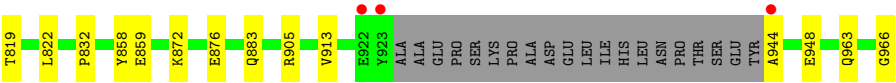
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: C4 PHOSPHOENOLPYRUVATE CARBOXYLASE



• Molecule 2: C4 PHOSPHOENOLPYRUVATE CARBOXYLASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	162.92Å 122.86Å 131.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.00 – 2.24 41.00 – 2.24	Depositor EDS
% Data completeness (in resolution range)	99.6 (41.00-2.24) 99.6 (41.00-2.24)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.11 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.177 , 0.210 0.183 , 0.218	Depositor DCC
R_{free} test set	2600 reflections (2.05%)	wwPDB-VP
Wilson B-factor (Å ²)	40.4	Xtriage
Anisotropy	0.024	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 33.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	15803	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.65% 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, EDO

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	1.13	7/7647 (0.1%)	1.07	17/10339 (0.2%)
2	B	1.22	10/7636 (0.1%)	1.13	23/10327 (0.2%)
All	All	1.18	17/15283 (0.1%)	1.10	40/20666 (0.2%)

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

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	834	ILE	C-O	7.47	1.32	1.24
2	B	699	PRO	CA-C	6.97	1.55	1.51
2	B	288	ARG	CD-NE	-6.29	1.37	1.46
2	B	174	THR	C-O	-6.15	1.16	1.24
2	B	740	THR	C-O	-5.89	1.18	1.24
2	B	546	GLU	C-O	-5.76	1.17	1.24
2	B	663	ARG	CD-NE	-5.43	1.38	1.46
1	A	629	LEU	C-O	-5.41	1.17	1.24
1	A	492	ARG	CA-C	-5.39	1.47	1.52
2	B	125	ASP	CA-C	5.39	1.59	1.52
1	A	584	ARG	C-O	-5.30	1.18	1.24
1	A	288	ARG	CD-NE	-5.29	1.38	1.46
1	A	848	ARG	C-O	-5.28	1.19	1.24
2	B	458	GLU	C-O	-5.28	1.18	1.24
1	A	669	GLU	CA-C	5.16	1.59	1.52
2	B	209	ASP	N-CA	-5.07	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	689	CYS	C-O	-5.04	1.18	1.24

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	144	ARG	NE-CZ-NH2	-8.30	111.73	119.20
2	B	772	ILE	CB-CA-C	-8.07	101.45	112.02
1	A	144	ARG	NE-CZ-NH2	-8.01	111.99	119.20
2	B	288	ARG	NE-CZ-NH2	-7.75	112.23	119.20
2	B	584	ARG	CG-CD-NE	-7.63	95.22	112.00
1	A	772	ILE	CB-CA-C	-7.59	102.25	111.97
1	A	663	ARG	NE-CZ-NH2	-7.48	112.47	119.20
2	B	354	GLU	CA-C-N	-7.36	111.26	123.33
2	B	354	GLU	C-N-CA	-7.36	111.26	123.33
2	B	663	ARG	NE-CZ-NH2	-7.32	112.61	119.20
1	A	354	GLU	CA-C-N	-7.25	111.48	123.37
1	A	354	GLU	C-N-CA	-7.25	111.48	123.37
1	A	654	PRO	O-C-N	7.24	124.64	121.31
1	A	663	ARG	NE-CZ-NH1	6.91	128.41	121.50
2	B	663	ARG	NE-CZ-NH1	6.86	128.36	121.50
1	A	584	ARG	CG-CD-NE	-6.83	96.96	112.00
2	B	654	PRO	O-C-N	6.63	124.36	121.31
1	A	144	ARG	NE-CZ-NH1	6.43	127.94	121.50
2	B	288	ARG	NE-CZ-NH1	6.35	127.85	121.50
2	B	144	ARG	NE-CZ-NH1	6.27	127.77	121.50
2	B	663	ARG	CD-NE-CZ	6.21	133.10	124.40
1	A	817	ARG	CG-CD-NE	-5.89	99.05	112.00
2	B	144	ARG	CD-NE-CZ	5.88	132.62	124.40
2	B	817	ARG	CG-CD-NE	-5.82	99.19	112.00
2	B	354	GLU	N-CA-C	5.79	120.63	112.93
1	A	348	ASP	N-CA-C	5.71	118.09	109.41
2	B	348	ASP	N-CA-C	5.68	118.04	109.41
1	A	288	ARG	NE-CZ-NH2	-5.59	114.17	119.20
1	A	603	GLY	N-CA-C	-5.58	105.72	112.48
1	A	663	ARG	CD-NE-CZ	5.57	132.19	124.40
1	A	354	GLU	N-CA-C	5.49	120.23	112.93
2	B	225	ILE	CB-CA-C	5.47	119.30	111.81
2	B	174	THR	N-CA-C	5.40	121.42	114.56
1	A	144	ARG	CD-NE-CZ	5.34	131.88	124.40
2	B	678	GLU	N-CA-C	5.31	117.82	111.71
2	B	819	THR	N-CA-C	-5.27	105.62	111.36
2	B	251	VAL	CA-C-N	-5.22	113.65	119.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	251	VAL	C-N-CA	-5.22	113.65	119.19
2	B	817	ARG	NE-CZ-NH2	-5.20	114.52	119.20
1	A	396	ASP	N-CA-C	5.19	117.61	111.33

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	921	LYS	Peptide

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	7479	0	7441	62	0
2	B	7466	0	7439	66	0
3	A	8	0	12	0	0
3	B	8	0	12	0	0
4	A	5	0	0	1	0
4	B	5	0	0	0	0
5	A	420	0	0	16	0
5	B	412	0	0	18	0
All	All	15803	0	14904	128	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.

All (128) 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:20:VAL:HG21	1:A:883:GLN:HG3	1.43	0.99
2:B:20:VAL:HG21	2:B:883:GLN:HG3	1.41	0.97
2:B:231:THR:HG21	5:B:2108:HOH:O	1.67	0.94
2:B:673:GLN:HG3	2:B:963:GLN:HE22	1.39	0.88
1:A:229:PRO:HA	5:A:2107:HOH:O	1.78	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:MET:HB3	1:A:309:MET:HE1	1.62	0.80
1:A:386:LEU:HD23	1:A:391:LYS:HA	1.61	0.79
5:A:2040:HOH:O	2:B:28:ASP:HB2	1.82	0.79
2:B:386:LEU:HD23	2:B:391:LYS:HA	1.62	0.79
2:B:240:MET:HB3	2:B:309:MET:HE1	1.68	0.76
2:B:557:PRO:HG3	2:B:572[A]:MET:HE1	1.69	0.74
1:A:288:ARG:HD2	5:A:2189:HOH:O	1.89	0.72
2:B:673:GLN:CG	2:B:963:GLN:HE22	2.01	0.72
2:B:859:GLU:OE1	5:B:2391:HOH:O	2.08	0.71
1:A:557:PRO:HG3	1:A:572[A]:MET:HE1	1.73	0.69
2:B:229:PRO:HA	5:B:2107:HOH:O	1.92	0.69
1:A:808:GLU:HB3	5:A:2387:HOH:O	1.92	0.68
2:B:288:ARG:HD2	5:B:2256:HOH:O	1.95	0.66
1:A:84:THR:O	1:A:905:ARG:NH2	2.27	0.66
2:B:174:THR:HG21	2:B:773:PHE:HE2	1.60	0.65
1:A:106[B]:ASN:HD21	1:A:673:GLN:HE21	1.44	0.63
2:B:84:THR:O	2:B:905:ARG:NH2	2.32	0.62
2:B:166:GLU:OE1	2:B:663:ARG:HD2	1.99	0.62
2:B:635:ARG:NH1	5:B:2321:HOH:O	2.28	0.62
1:A:166:GLU:OE1	1:A:663:ARG:HD2	2.00	0.61
1:A:458:GLU:HG2	5:A:2193:HOH:O	2.01	0.59
1:A:817:ARG:HD2	5:A:2388:HOH:O	2.00	0.59
2:B:71:HIS:HD2	5:B:2025:HOH:O	1.85	0.57
1:A:174:THR:HG21	1:A:773:PHE:HE2	1.68	0.56
2:B:106[B]:ASN:ND2	2:B:673:GLN:OE1	2.38	0.56
1:A:745:PHE:CD2	1:A:773:PHE:CE1	2.94	0.56
2:B:71:HIS:CD2	5:B:2025:HOH:O	2.56	0.56
2:B:710:LEU:HG	2:B:714:MET:HE2	1.88	0.55
1:A:548:HIS:HE1	5:A:2261:HOH:O	1.89	0.55
2:B:240:MET:CB	2:B:309:MET:HE1	2.37	0.55
1:A:106[B]:ASN:ND2	1:A:673:GLN:HE21	2.04	0.55
1:A:325:MET:HE1	1:A:417:LEU:HD11	1.89	0.54
1:A:231:THR:HG22	1:A:234:ASP:CG	2.33	0.54
1:A:22:GLY:HA2	1:A:23:LYS:HE3	1.89	0.54
2:B:745:PHE:CD2	2:B:773:PHE:CE1	2.96	0.53
1:A:240:MET:CB	1:A:309:MET:HE1	2.33	0.53
2:B:325:MET:HE1	2:B:417:LEU:HD11	1.90	0.53
1:A:808:GLU:O	1:A:812:THR:HB	2.08	0.53
2:B:673:GLN:HG3	2:B:963:GLN:NE2	2.18	0.52
1:A:178:ARG:NH2	4:A:1004:SO4:O3	2.40	0.52
2:B:288:ARG:HD3	5:B:2148:HOH:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:710:LEU:HG	1:A:714:MET:HE2	1.93	0.51
2:B:231:THR:HG22	2:B:234:ASP:CG	2.36	0.51
2:B:22:GLY:HA2	2:B:23:LYS:HE3	1.93	0.50
1:A:423:HIS:HB3	5:A:2182:HOH:O	2.11	0.50
2:B:315:PHE:O	2:B:318:ILE:HG22	2.11	0.50
2:B:944:ALA:N	5:B:2410:HOH:O	2.44	0.50
5:A:2040:HOH:O	2:B:28:ASP:CB	2.51	0.50
1:A:315:PHE:O	1:A:318:ILE:HG22	2.11	0.49
1:A:402:ASN:ND2	1:A:404:GLU:HB2	2.27	0.49
2:B:174:THR:HG21	2:B:773:PHE:CE2	2.44	0.49
1:A:88:THR:HG21	1:A:946:GLY:HA3	1.95	0.49
2:B:402:ASN:ND2	2:B:404:GLU:HB2	2.27	0.49
2:B:534:THR:HG23	2:B:575:LEU:HG	1.96	0.48
2:B:808:GLU:O	2:B:812:THR:HB	2.12	0.48
2:B:736:PHE:CZ	2:B:742:GLU:HG3	2.49	0.48
1:A:736:PHE:CZ	1:A:742:GLU:HG3	2.49	0.48
2:B:57:VAL:CG1	2:B:101:MET:HE1	2.43	0.48
1:A:534:THR:HG23	1:A:575:LEU:HG	1.95	0.47
2:B:17:ARG:HG3	5:B:2002:HOH:O	2.13	0.47
1:A:748:MET:O	1:A:749:ASN:C	2.56	0.47
2:B:876:GLU:O	5:B:2400:HOH:O	2.20	0.47
1:A:16:LEU:HD23	1:A:61:TYR:OH	2.14	0.47
2:B:794:HIS:HB3	5:B:2370:HOH:O	2.14	0.46
1:A:129:GLU:O	1:A:647:HIS:HB3	2.16	0.46
2:B:402:ASN:ND2	2:B:404:GLU:H	2.13	0.46
1:A:57:VAL:CG1	1:A:101:MET:HE1	2.46	0.46
2:B:129:GLU:O	2:B:647:HIS:HB3	2.16	0.45
1:A:831:ASN:OD1	1:A:831:ASN:C	2.59	0.45
1:A:16:LEU:CD2	1:A:61:TYR:OH	2.65	0.45
1:A:22:GLY:CA	1:A:23:LYS:HE3	2.47	0.45
1:A:561:LYS:NZ	5:A:2270:HOH:O	2.50	0.45
2:B:362:ASN:C	2:B:364:PRO:HD3	2.42	0.45
2:B:635:ARG:NH2	2:B:966:GLY:O	2.50	0.45
2:B:817:ARG:HD2	5:B:2378:HOH:O	2.16	0.44
1:A:231:THR:CG2	1:A:234:ASP:H	2.30	0.44
1:A:380:ARG:HD3	1:A:384:ARG:CZ	2.48	0.44
5:A:2055:HOH:O	2:B:872:LYS:HE2	2.18	0.44
2:B:793:LYS:CE	5:B:2371:HOH:O	2.66	0.44
2:B:174:THR:CG2	2:B:773:PHE:CE2	3.01	0.44
2:B:17:ARG:CG	5:B:2002:HOH:O	2.66	0.43
2:B:773:PHE:CD1	2:B:773:PHE:C	2.96	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:402:ASN:ND2	1:A:404:GLU:H	2.15	0.43
2:B:822:LEU:C	2:B:822:LEU:HD23	2.43	0.43
1:A:20:VAL:HG21	1:A:883:GLN:CG	2.31	0.43
1:A:231:THR:HG23	1:A:234:ASP:H	1.83	0.43
1:A:46:GLN:HE21	1:A:54:LYS:HE2	1.84	0.43
1:A:166:GLU:CD	1:A:663:ARG:HD2	2.43	0.43
2:B:334:LEU:C	2:B:334:LEU:HD23	2.44	0.43
1:A:174:THR:HG21	1:A:773:PHE:CE2	2.51	0.43
1:A:822:LEU:C	1:A:822:LEU:HD23	2.44	0.43
5:A:2055:HOH:O	2:B:872:LYS:CE	2.67	0.43
2:B:46:GLN:NE2	2:B:54:LYS:HE2	2.34	0.43
2:B:380:ARG:HD3	2:B:384:ARG:CZ	2.48	0.43
1:A:504:GLU:HG3	5:A:2233:HOH:O	2.19	0.42
1:A:632:PHE:CD1	1:A:663:ARG:HG2	2.54	0.42
2:B:568:ALA:HB3	2:B:569:PRO:HD3	2.00	0.42
2:B:559:PHE:CE2	2:B:572[A]:MET:HE3	2.54	0.42
2:B:214:ARG:HD2	5:B:2104:HOH:O	2.18	0.42
1:A:334:LEU:HD23	1:A:334:LEU:C	2.44	0.42
1:A:635:ARG:NH2	1:A:966:GLY:O	2.52	0.42
1:A:385:HIS:HD2	1:A:389:ASP:OD2	2.02	0.42
1:A:701:ILE:HD11	1:A:812:THR:O	2.20	0.42
2:B:22:GLY:CA	2:B:23:LYS:HE3	2.49	0.42
1:A:474:GLU:HB3	5:A:2206:HOH:O	2.20	0.41
1:A:362:ASN:C	1:A:364:PRO:HD3	2.44	0.41
1:A:46:GLN:NE2	1:A:54:LYS:HE2	2.35	0.41
2:B:632:PHE:CD1	2:B:663:ARG:HG2	2.55	0.41
1:A:813:TRP:O	1:A:814:PRO:C	2.62	0.41
2:B:166:GLU:CD	2:B:663:ARG:HD2	2.46	0.41
1:A:872:LYS:CE	5:B:2066:HOH:O	2.68	0.41
2:B:504:GLU:HG3	5:B:2252:HOH:O	2.21	0.41
2:B:644:GLY:N	2:B:645:PRO:CD	2.83	0.41
2:B:832:PRO:HG3	2:B:858:TYR:CE1	2.56	0.41
1:A:182:LEU:HD12	1:A:182:LEU:HA	1.94	0.40
2:B:231:THR:CG2	2:B:234:ASP:H	2.34	0.40
2:B:401:THR:N	2:B:405:GLN:OE1	2.46	0.40
1:A:888:ARG:NH1	5:A:2412:HOH:O	2.54	0.40
2:B:494:LEU:HD11	2:B:542:LEU:HD21	2.04	0.40
1:A:288:ARG:HD3	5:A:2139:HOH:O	2.21	0.40
1:A:745:PHE:HD2	1:A:773:PHE:CE1	2.39	0.40
1:A:965:THR:OG1	1:A:966:GLY:N	2.54	0.40
2:B:11:SER:O	2:B:14:ALA:HB3	2.21	0.40

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	923/990 (93%)	898 (97%)	24 (3%)	1 (0%)	48	54
2	B	925/990 (93%)	901 (97%)	24 (3%)	0	100	100
All	All	1848/1980 (93%)	1799 (97%)	48 (3%)	1 (0%)	48	54

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	747	ARG

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	811/866 (94%)	792 (98%)	19 (2%)	44	53
2	B	809/866 (93%)	787 (97%)	22 (3%)	39	47
All	All	1620/1732 (94%)	1579 (98%)	41 (2%)	42	50

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	LYS
1	A	23	LYS

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Mol	Chain	Res	Type
1	A	26	GLU
1	A	47	ASP
1	A	53	LEU
1	A	117	ARG
1	A	149	LEU
1	A	209	ASP
1	A	210	GLU
1	A	225	ILE
1	A	327	MET
1	A	357	LYS
1	A	391	LYS
1	A	397	GLU
1	A	429	SER
1	A	444	LEU
1	A	663	ARG
1	A	749	ASN
1	A	798	LYS
2	B	8	LYS
2	B	23	LYS
2	B	26	GLU
2	B	47	ASP
2	B	53	LEU
2	B	117	ARG
2	B	149	LEU
2	B	182	LEU
2	B	200	ILE
2	B	209	ASP
2	B	210	GLU
2	B	225	ILE
2	B	327	MET
2	B	357	LYS
2	B	391	LYS
2	B	397	GLU
2	B	429	SER
2	B	444	LEU
2	B	663	ARG
2	B	798	LYS
2	B	913	VAL
2	B	948	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	46	GLN
1	A	150	ASN
1	A	279	GLN
1	A	385	HIS
1	A	402	ASN
1	A	589	GLN
1	A	610	GLN
1	A	794	HIS
1	A	802	ASN
1	A	899	GLN
1	A	963	GLN
2	B	15	GLN
2	B	46	GLN
2	B	150	ASN
2	B	183	GLN
2	B	279	GLN
2	B	385	HIS
2	B	402	ASN
2	B	589	GLN
2	B	610	GLN
2	B	673	GLN
2	B	794	HIS
2	B	802	ASN
2	B	883	GLN
2	B	899	GLN
2	B	912	HIS
2	B	963	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 oligosaccharides in this entry.

5.6 Ligand geometry

6 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	EDO	A	1002	-	3,3,3	0.87	0	2,2,2	0.46	0
3	EDO	B	1003	-	3,3,3	1.19	0	2,2,2	0.42	0
3	EDO	B	1002	-	3,3,3	0.29	0	2,2,2	1.07	0
3	EDO	A	1003	-	3,3,3	0.55	0	2,2,2	0.12	0
4	SO4	A	1004	-	4,4,4	0.62	0	6,6,6	1.10	0
4	SO4	B	1004	-	4,4,4	0.69	0	6,6,6	1.08	1 (16%)

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	B	1002	-	-	1/1/1/1	-
3	EDO	A	1002	-	-	1/1/1/1	-
3	EDO	A	1003	-	-	1/1/1/1	-
3	EDO	B	1003	-	-	1/1/1/1	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1004	SO4	O4-S-O1	-2.12	98.50	109.56

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1002	EDO	O1-C1-C2-O2
3	B	1003	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	A	1002	EDO	O1-C1-C2-O2
3	A	1003	EDO	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1004	SO4	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	929/990 (93%)	-0.19	24 (2%) 57 58	21, 44, 82, 121	4 (0%)
2	B	927/990 (93%)	-0.34	20 (2%) 62 64	17, 39, 73, 134	4 (0%)
All	All	1856/1980 (93%)	-0.27	44 (2%) 59 61	17, 41, 78, 134	8 (0%)

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	923	TYR	5.2
1	A	923	TYR	4.4
1	A	754	PRO	4.3
2	B	19	LEU	4.3
1	A	24	VAL	4.2
2	B	761	GLY	4.1
1	A	225	ILE	4.1
2	B	24	VAL	3.9
1	A	749	ASN	3.8
2	B	18	LEU	3.4
2	B	10	ALA	3.4
2	B	226	ARG	3.4
1	A	227	ARG	3.3
1	A	756	LYS	3.2
2	B	8	LYS	3.2
2	B	922	GLU	3.2
2	B	944	ALA	3.2
1	A	753	ARG	3.1
1	A	18	LEU	3.0
2	B	23	LYS	3.0
2	B	230	PRO	3.0
1	A	761	GLY	2.9
1	A	10	ALA	2.9
1	A	101	MET	2.9

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Mol	Chain	Res	Type	RSRZ
2	B	225	ILE	2.7
1	A	351[A]	HIS	2.7
1	A	23	LYS	2.6
2	B	346	ARG	2.6
1	A	230	PRO	2.6
1	A	9	LEU	2.5
2	B	227	ARG	2.5
1	A	347	LYS	2.4
1	A	8	LYS	2.4
1	A	913	VAL	2.3
1	A	912	HIS	2.3
1	A	914	THR	2.2
1	A	20	VAL	2.1
2	B	748	LYS	2.1
2	B	229	PRO	2.1
1	A	70	LYS	2.1
2	B	124	GLY	2.1
2	B	21	PRO	2.1
2	B	125	ASP	2.0
1	A	21	PRO	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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
3	EDO	A	1002	4/4	0.88	0.14	44,49,53,55	0
3	EDO	B	1003	4/4	0.90	0.15	36,40,42,47	0
3	EDO	B	1002	4/4	0.91	0.13	40,43,43,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	EDO	A	1003	4/4	0.95	0.12	43,47,48,55	0
4	SO4	A	1004	5/5	0.98	0.08	41,50,51,52	0
4	SO4	B	1004	5/5	0.98	0.07	39,43,48,48	0

6.5 Other polymers [i](#)

There are no such residues in this entry.