



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:14 PM GMT

PDB ID : 4BXH
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
<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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

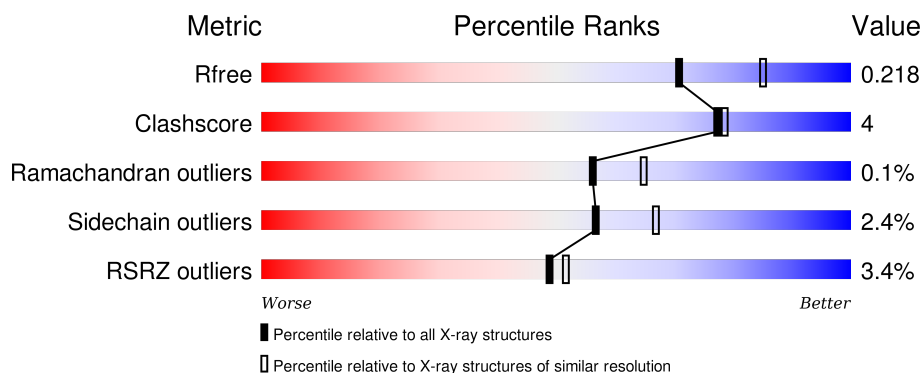
1 Overall quality at a glance ⓘ

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}	91344	1611 (2.26-2.22)
Clashscore	102246	1764 (2.26-2.22)
Ramachandran outliers	100387	1724 (2.26-2.22)
Sidechain outliers	100360	1724 (2.26-2.22)
RSRZ outliers	91569	1616 (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 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	990	<div> <div>4%</div> <div>84%</div> <div>8% • 6%</div> </div>
2	B	990	<div> <div>3%</div> <div>83%</div> <div>9% • 6%</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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	EDO	A	1002	-	-	-	X
3	EDO	B	1002	-	-	-	X
3	EDO	B	1003	-	-	-	X

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	C	N	O	S	0	4	0
			7466	4741	1298	1392	35			

There are 25 discrepancies between the modelled and reference sequences:

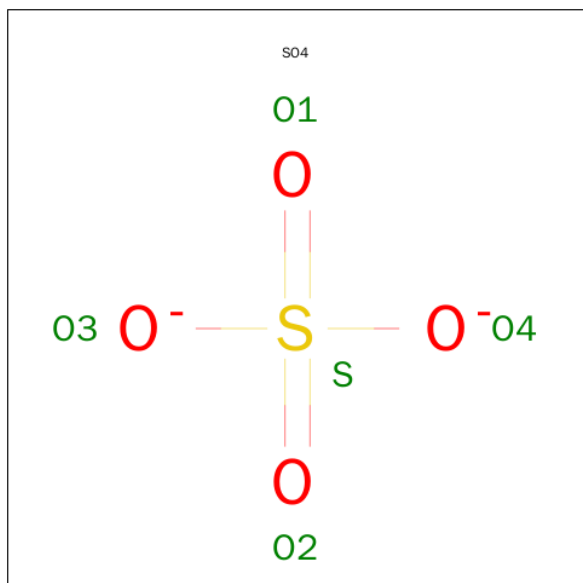
Chain	Residue	Modelled	Actual	Comment	Reference
B	-23	MET	-	EXPRESSION TAG	UNP P30694
B	-22	GLY	-	EXPRESSION TAG	UNP P30694
B	-21	HIS	-	EXPRESSION TAG	UNP P30694
B	-20	HIS	-	EXPRESSION TAG	UNP P30694
B	-19	HIS	-	EXPRESSION TAG	UNP P30694
B	-18	HIS	-	EXPRESSION TAG	UNP P30694
B	-17	HIS	-	EXPRESSION TAG	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 (three-letter code: 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 (three-letter code: 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		

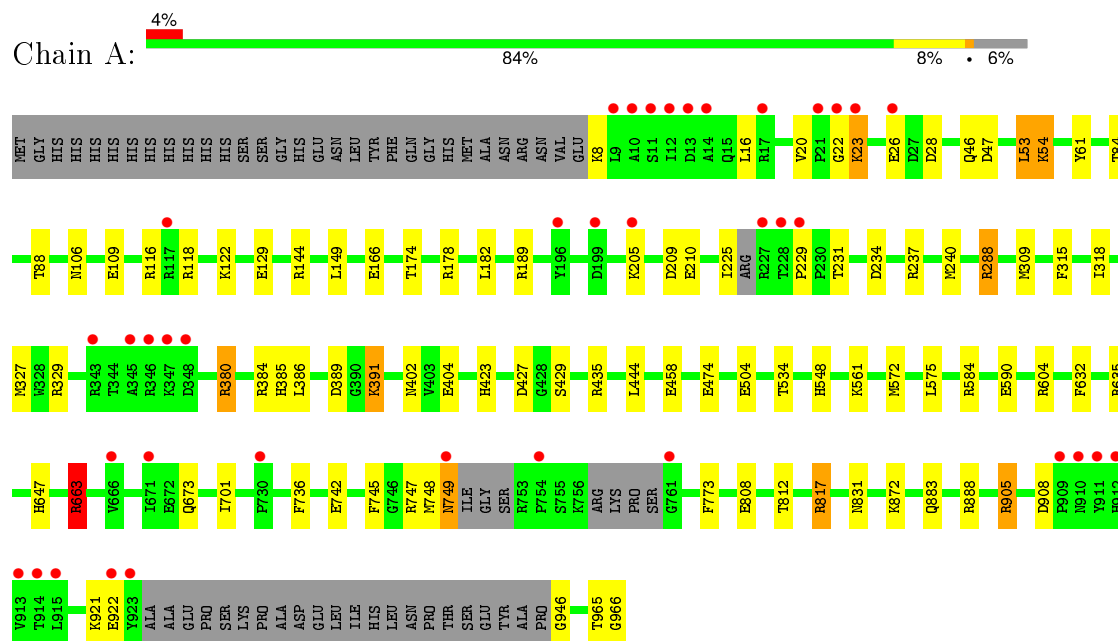
- Molecule 5 is water.

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

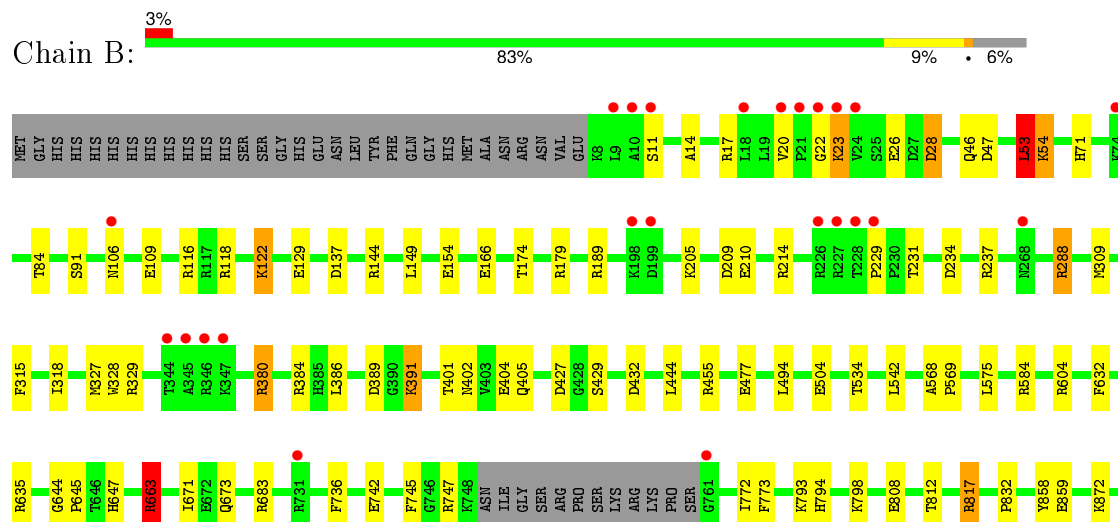
3 Residue-property plots

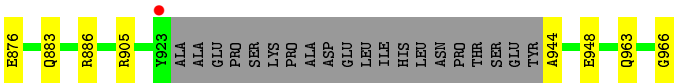
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 2 ₁ 2 ₁ 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 40.69 – 2.24	Depositor EDS
% Data completeness (in resolution range)	99.6 (41.00-2.24) 99.7 (40.69-2.24)	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 (2.10%)	DCC
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 , 39.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 126691 reflections (0.001%)	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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.86	2/7647 (0.0%)	0.99	31/10339 (0.3%)
2	B	0.92	5/7636 (0.1%)	1.03	35/10327 (0.3%)
All	All	0.89	7/15283 (0.0%)	1.01	66/20666 (0.3%)

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 (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	590	GLU	CD-OE2	5.43	1.31	1.25
2	B	328	TRP	CB-CG	5.32	1.59	1.50
2	B	288	ARG	CD-NE	-5.30	1.37	1.46
2	B	109	GLU	CD-OE2	-5.28	1.19	1.25
2	B	477	GLU	CD-OE1	5.27	1.31	1.25
1	A	109	GLU	CD-OE1	-5.01	1.20	1.25
2	B	154	GLU	CG-CD	5.01	1.59	1.51

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	144	ARG	NE-CZ-NH2	-17.14	111.73	120.30
1	A	144	ARG	NE-CZ-NH2	-16.61	111.99	120.30
1	A	663	ARG	NE-CZ-NH1	16.21	128.41	120.30
2	B	288	ARG	NE-CZ-NH2	-16.14	112.23	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	663	ARG	NE-CZ-NH1	16.12	128.36	120.30
1	A	663	ARG	NE-CZ-NH2	-15.67	112.47	120.30
2	B	663	ARG	NE-CZ-NH2	-15.37	112.61	120.30
1	A	144	ARG	NE-CZ-NH1	15.27	127.94	120.30
2	B	288	ARG	NE-CZ-NH1	15.09	127.85	120.30
2	B	144	ARG	NE-CZ-NH1	14.94	127.77	120.30
1	A	288	ARG	NE-CZ-NH2	-12.27	114.17	120.30
1	A	288	ARG	NE-CZ-NH1	12.13	126.36	120.30
2	B	817	ARG	NE-CZ-NH2	-11.56	114.52	120.30
1	A	817	ARG	NE-CZ-NH2	-11.07	114.76	120.30
2	B	380	ARG	NE-CZ-NH1	8.44	124.52	120.30
1	A	380	ARG	NE-CZ-NH1	8.27	124.43	120.30
2	B	380	ARG	NE-CZ-NH2	-8.25	116.17	120.30
2	B	604	ARG	NE-CZ-NH2	-7.90	116.35	120.30
2	B	584	ARG	CG-CD-NE	-7.90	95.22	111.80
2	B	817	ARG	NE-CZ-NH1	7.37	123.98	120.30
1	A	380	ARG	NE-CZ-NH2	-7.30	116.65	120.30
2	B	28	ASP	CB-CG-OD1	7.20	124.78	118.30
1	A	584	ARG	CG-CD-NE	-7.07	96.96	111.80
1	A	604	ARG	NE-CZ-NH2	-6.83	116.88	120.30
2	B	663	ARG	CD-NE-CZ	6.79	133.10	123.60
2	B	144	ARG	CD-NE-CZ	6.45	132.62	123.60
1	A	122	LYS	CD-CE-NZ	6.44	126.50	111.70
2	B	432	ASP	CB-CG-OD1	6.38	124.04	118.30
1	A	329	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	A	427	ASP	CB-CG-OD1	6.18	123.86	118.30
1	A	28	ASP	CB-CG-OD1	6.17	123.86	118.30
2	B	329	ARG	NE-CZ-NH1	6.17	123.38	120.30
1	A	663	ARG	CD-NE-CZ	6.14	132.19	123.60
1	A	604	ARG	NE-CZ-NH1	6.10	123.35	120.30
1	A	817	ARG	CG-CD-NE	-6.07	99.05	111.80
2	B	122	LYS	CD-CE-NZ	6.01	125.52	111.70
2	B	817	ARG	CG-CD-NE	-6.00	99.19	111.80
1	A	817	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	A	144	ARG	CD-NE-CZ	5.92	131.88	123.60
1	A	116	ARG	NE-CZ-NH2	5.91	123.26	120.30
1	A	908	ASP	CB-CG-OD2	-5.81	113.07	118.30
1	A	435	ARG	NE-CZ-NH2	-5.67	117.47	120.30
2	B	179	ARG	NE-CZ-NH1	5.65	123.12	120.30
2	B	427	ASP	CB-CG-OD1	5.63	123.37	118.30
1	A	905	ARG	NE-CZ-NH2	-5.57	117.52	120.30
1	A	118	ARG	NE-CZ-NH2	-5.56	117.52	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	747	ARG	NE-CZ-NH1	5.55	123.08	120.30
2	B	118	ARG	NE-CZ-NH2	-5.54	117.53	120.30
2	B	116	ARG	NE-CZ-NH2	5.52	123.06	120.30
1	A	28	ASP	CB-CG-OD2	-5.45	113.39	118.30
2	B	671	ILE	CG1-CB-CG2	-5.41	99.51	111.40
2	B	389	ASP	CB-CG-OD1	5.37	123.13	118.30
2	B	886	ARG	NE-CZ-NH2	-5.36	117.62	120.30
2	B	886	ARG	NE-CZ-NH1	5.27	122.94	120.30
2	B	683	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	A	189	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	A	572[A]	MET	CG-SD-CE	-5.20	91.88	100.20
1	A	572[B]	MET	CG-SD-CE	-5.20	91.88	100.20
1	A	288	ARG	CD-NE-CZ	5.20	130.87	123.60
2	B	53	LEU	CA-CB-CG	-5.19	103.36	115.30
2	B	189	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	A	53	LEU	CA-CB-CG	-5.15	103.46	115.30
2	B	772	ILE	CB-CA-C	-5.07	101.45	111.60
2	B	455	ARG	NE-CZ-NH1	5.05	122.83	120.30
2	B	604	ARG	NE-CZ-NH1	5.03	122.82	120.30
2	B	137	ASP	CB-CG-OD1	5.02	122.82	118.30

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	53	0
2	B	7466	0	7439	56	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	420	0	0	16	0
5	B	412	0	0	18	0
All	All	15803	0	14904	109	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 (109) 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
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
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
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
2:B:106[B]:ASN:ND2	2:B:673:GLN:OE1	2.38	0.56
1:A:174:THR:HG21	1:A:773:PHE:HE2	1.68	0.56
2:B:71:HIS:CD2	5:B:2025:HOH:O	2.56	0.56
1:A:745:PHE:CD2	1:A:773:PHE:CE1	2.94	0.56
1:A:548:HIS:HE1	5:A:2261:HOH:O	1.89	0.55
1:A:106[B]:ASN:ND2	1:A:673:GLN:HE21	2.04	0.55
1:A:22:GLY:HA2	1:A:23:LYS:HE3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:745:PHE:CD2	2:B:773:PHE:CE1	2.96	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
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
2:B:174:THR:HG21	2:B:773:PHE:CE2	2.44	0.49
1:A:402:ASN:ND2	1:A:404:GLU:HB2	2.27	0.49
1:A:315:PHE:O	1:A:318:ILE:HG22	2.11	0.49
2:B:402:ASN:ND2	2:B:404:GLU:HB2	2.27	0.49
1:A:88:THR:HG21	1:A:946:GLY:HA3	1.95	0.49
1:A:231:THR:HG22	1:A:234:ASP:CG	2.33	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:17:ARG:HG3	5:B:2002:HOH:O	2.13	0.47
1:A:534:THR:HG23	1:A:575:LEU:HG	1.95	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
2:B:402:ASN:ND2	2:B:404:GLU:H	2.13	0.46
1:A:129:GLU:O	1:A:647:HIS:HB3	2.16	0.46
2:B:231:THR:HG22	2:B:234:ASP:CG	2.36	0.46
2:B:129:GLU:O	2:B:647:HIS:HB3	2.16	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: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
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
1:A:380:ARG:HD3	1:A:384:ARG:CZ	2.48	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
1:A:402:ASN:ND2	1:A:404:GLU:H	2.15	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:174:THR:HG21	1:A:773:PHE:CE2	2.51	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:632:PHE:CD1	1:A:663:ARG:HG2	2.54	0.42
1:A:504:GLU:HG3	5:A:2233:HOH:O	2.19	0.42
2:B:568:ALA:HB3	2:B:569:PRO:HD3	2.00	0.42
1:A:309:MET:HB3	1:A:309:MET:HE2	1.84	0.42
2:B:214:ARG:HD2	5:B:2104:HOH:O	2.18	0.42
1:A:748:MET:O	1:A:749:ASN:C	2.56	0.42
1:A:240:MET:HB3	1:A:309:MET:CE	2.49	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:309:MET:HE2	2:B:309:MET:HB3	1.82	0.42
2:B:53:LEU:O	2:B:53:LEU:HG	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
2:B:632:PHE:CD1	2:B:663:ARG:HG2	2.55	0.41
1:A:46:GLN:NE2	1:A:54:LYS:HE2	2.35	0.41
1:A:872:LYS:CE	5:B:2066:HOH:O	2.68	0.41
1:A:831:ASN:OD1	1:A:831:ASN:C	2.59	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
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:182:LEU:HA	1:A:182:LEU:HD12	1.94	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%)	56	65
2	B	925/990 (93%)	901 (97%)	24 (3%)	0	100	100
All	All	1848/1980 (93%)	1799 (97%)	48 (3%)	1 (0%)	56	65

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%)	58	68
2	B	809/866 (93%)	790 (98%)	19 (2%)	58	68
All	All	1620/1732 (94%)	1582 (98%)	38 (2%)	57	68

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	LYS
1	A	23	LYS
1	A	26	GLU
1	A	47	ASP
1	A	53	LEU

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Mol	Chain	Res	Type
1	A	54	LYS
1	A	149	LEU
1	A	205	LYS
1	A	209	ASP
1	A	210	GLU
1	A	225	ILE
1	A	237	ARG
1	A	327	MET
1	A	391	LYS
1	A	429	SER
1	A	444	LEU
1	A	663	ARG
1	A	749	ASN
1	A	922	GLU
2	B	23	LYS
2	B	26	GLU
2	B	47	ASP
2	B	53	LEU
2	B	54	LYS
2	B	91	SER
2	B	122	LYS
2	B	149	LEU
2	B	205	LYS
2	B	209	ASP
2	B	210	GLU
2	B	237	ARG
2	B	327	MET
2	B	391	LYS
2	B	429	SER
2	B	444	LEU
2	B	663	ARG
2	B	798	LYS
2	B	948	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	46	GLN
1	A	385	HIS
1	A	402	ASN
1	A	802	ASN

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Mol	Chain	Res	Type
1	A	963	GLN
2	B	46	GLN
2	B	385	HIS
2	B	402	ASN
2	B	673	GLN
2	B	802	ASN
2	B	963	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](#)

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	0.48	0
3	EDO	A	1003	-	3,3,3	0.56	0	2,2,2	0.12	0
4	SO4	A	1004	-	4,4,4	0.71	0	6,6,6	0.85	0
3	EDO	B	1002	-	3,3,3	0.33	0	2,2,2	1.15	0
3	EDO	B	1003	-	3,3,3	1.17	0	2,2,2	0.43	0
4	SO4	B	1004	-	4,4,4	0.89	0	6,6,6	0.65	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	A	1002	-	-	0/1/1/1	0/0/0/0
3	EDO	A	1003	-	-	0/1/1/1	0/0/0/0
4	SO4	A	1004	-	-	0/0/0/0	0/0/0/0
3	EDO	B	1002	-	-	0/1/1/1	0/0/0/0
3	EDO	B	1003	-	-	0/1/1/1	0/0/0/0
4	SO4	B	1004	-	-	0/0/0/0	0/0/0/0

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
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	38 (4%) 41 43	29, 44, 82, 121	0
2	B	927/990 (93%)	-0.28	25 (2%) 58 60	25, 39, 73, 134	0
All	All	1856/1980 (93%)	-0.23	63 (3%) 49 51	25, 41, 78, 134	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	10	ALA	6.3
2	B	227	ARG	5.8
2	B	23	LYS	5.3
2	B	923	TYR	5.1
1	A	346	ARG	5.1
2	B	228	THR	4.8
1	A	923	TYR	4.8
1	A	9	LEU	4.7
2	B	24	VAL	4.5
2	B	10	ALA	4.4
1	A	910	ASN	4.2
2	B	21	PRO	3.9
2	B	345	ALA	3.8
1	A	228	THR	3.8
2	B	198	LYS	3.7
2	B	346	ARG	3.4
1	A	14	ALA	3.4
2	B	18	LEU	3.4
2	B	229	PRO	3.4
2	B	761	GLY	3.3
2	B	11	SER	3.3
1	A	912	HIS	3.3
2	B	199	ASP	3.2
2	B	9	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	229	PRO	3.1
2	B	22	GLY	3.0
1	A	26	GLU	3.0
1	A	909	PRO	2.9
1	A	348	ASP	2.9
1	A	12	ILE	2.8
1	A	21	PRO	2.8
1	A	730	PRO	2.7
1	A	911	TYR	2.7
2	B	344	THR	2.7
1	A	13	ASP	2.7
1	A	347	LYS	2.7
1	A	345	ALA	2.7
1	A	914	THR	2.6
1	A	343	ARG	2.6
1	A	761	GLY	2.6
1	A	749	ASN	2.5
1	A	22	GLY	2.4
1	A	199	ASP	2.4
1	A	117	ARG	2.4
1	A	913	VAL	2.3
1	A	205	LYS	2.3
2	B	347	LYS	2.3
1	A	11	SER	2.3
1	A	754	PRO	2.3
1	A	915	LEU	2.2
1	A	922	GLU	2.2
1	A	227	ARG	2.2
2	B	74	LYS	2.2
1	A	671	ILE	2.1
1	A	666	VAL	2.1
2	B	268	ASN	2.1
1	A	23	LYS	2.1
1	A	17	ARG	2.1
1	A	196	TYR	2.1
2	B	20	VAL	2.1
2	B	226	ARG	2.1
2	B	731	ARG	2.0
2	B	106[A]	ASN	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 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
3	EDO	A	1002	4/4	0.90	0.34	3.53	44,49,53,55	0
3	EDO	B	1003	4/4	0.83	0.27	3.04	36,40,42,47	0
3	EDO	B	1002	4/4	0.90	0.21	2.29	40,43,43,51	0
3	EDO	A	1003	4/4	0.95	0.23	1.09	43,47,48,55	0
4	SO4	B	1004	5/5	0.99	0.10	-0.27	39,43,48,48	0
4	SO4	A	1004	5/5	0.99	0.10	-1.03	41,50,51,52	0

6.5 Other polymers [i](#)

There are no such residues in this entry.