



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 04:37 PM UTC

PDB ID : 1U2X / pdb_00001u2x
Title : Crystal Structure of a Hypothetical ADP-dependent Phosphofructokinase from *Pyrococcus horikoshii* OT3
Authors : Wong, A.H.Y.; Jia, Z.; Skarina, T.; Walker, J.R.; Arrowsmith, C.; Joachimiak, A.; Edwards, A.; Savchenko, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on : 2004-07-20
Resolution : 2.00 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

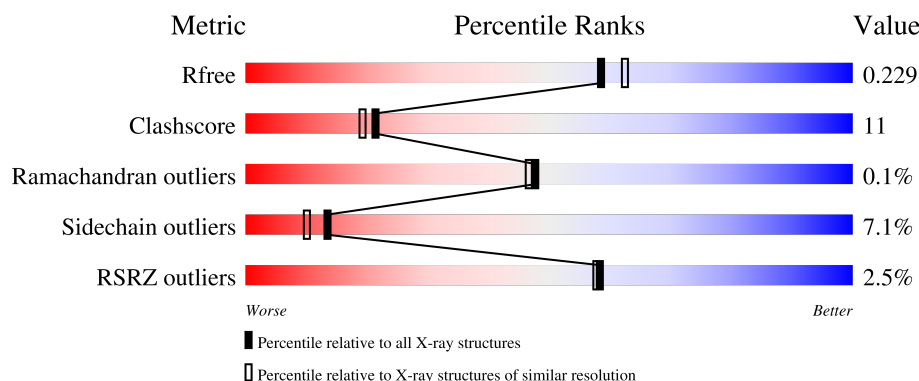
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	474	4% 73% 16% 5% 5%
1	B	474	73% 18% • 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8143 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 ADP-specific phosphofructokinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	450	Total	C	N	O	Se	0	0	0
			3658	2354	625	674	5			
1	B	450	Total	C	N	O	Se	0	0	0
			3658	2354	625	674	5			

There are 58 discrepancies between the modelled and reference sequences:

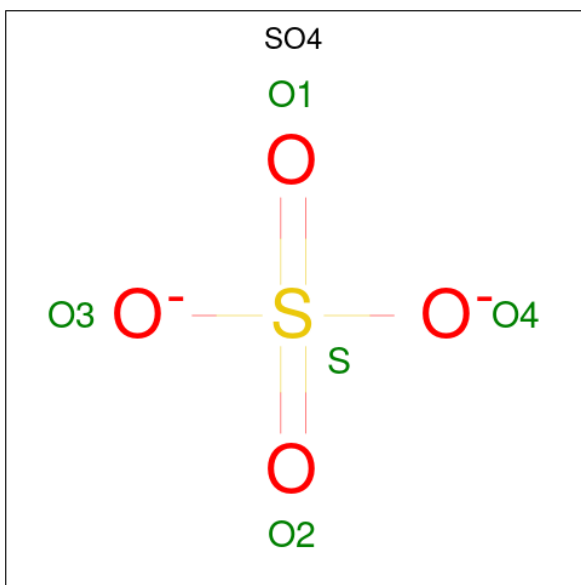
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	expression tag	UNP O59355
A	2	GLY	-	expression tag	UNP O59355
A	3	SER	-	expression tag	UNP O59355
A	4	SER	-	expression tag	UNP O59355
A	5	HIS	-	expression tag	UNP O59355
A	6	HIS	-	expression tag	UNP O59355
A	7	HIS	-	expression tag	UNP O59355
A	8	HIS	-	expression tag	UNP O59355
A	9	HIS	-	expression tag	UNP O59355
A	10	HIS	-	expression tag	UNP O59355
A	11	SER	-	expression tag	UNP O59355
A	12	SER	-	expression tag	UNP O59355
A	13	GLY	-	expression tag	UNP O59355
A	14	ARG	-	expression tag	UNP O59355
A	15	GLU	-	expression tag	UNP O59355
A	16	ASN	-	expression tag	UNP O59355
A	17	LEU	-	expression tag	UNP O59355
A	18	TYR	-	expression tag	UNP O59355
A	19	PHE	-	expression tag	UNP O59355
A	20	GLN	-	expression tag	UNP O59355
A	21	GLY	-	expression tag	UNP O59355
A	22	HIS	-	expression tag	UNP O59355
A	23	MSE	MET	modified residue	UNP O59355
A	101	MSE	MET	modified residue	UNP O59355
A	343	MSE	MET	modified residue	UNP O59355

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Chain	Residue	Modelled	Actual	Comment	Reference
A	363	MSE	MET	modified residue	UNP O59355
A	431	MSE	MET	modified residue	UNP O59355
A	473	GLY	-	cloning artifact	UNP O59355
A	474	SER	-	cloning artifact	UNP O59355
B	1	MSE	-	expression tag	UNP O59355
B	2	GLY	-	expression tag	UNP O59355
B	3	SER	-	expression tag	UNP O59355
B	4	SER	-	expression tag	UNP O59355
B	5	HIS	-	expression tag	UNP O59355
B	6	HIS	-	expression tag	UNP O59355
B	7	HIS	-	expression tag	UNP O59355
B	8	HIS	-	expression tag	UNP O59355
B	9	HIS	-	expression tag	UNP O59355
B	10	HIS	-	expression tag	UNP O59355
B	11	SER	-	expression tag	UNP O59355
B	12	SER	-	expression tag	UNP O59355
B	13	GLY	-	expression tag	UNP O59355
B	14	ARG	-	expression tag	UNP O59355
B	15	GLU	-	expression tag	UNP O59355
B	16	ASN	-	expression tag	UNP O59355
B	17	LEU	-	expression tag	UNP O59355
B	18	TYR	-	expression tag	UNP O59355
B	19	PHE	-	expression tag	UNP O59355
B	20	GLN	-	expression tag	UNP O59355
B	21	GLY	-	expression tag	UNP O59355
B	22	HIS	-	expression tag	UNP O59355
B	23	MSE	MET	modified residue	UNP O59355
B	101	MSE	MET	modified residue	UNP O59355
B	343	MSE	MET	modified residue	UNP O59355
B	363	MSE	MET	modified residue	UNP O59355
B	431	MSE	MET	modified residue	UNP O59355
B	473	GLY	-	cloning artifact	UNP O59355
B	474	SER	-	cloning artifact	UNP O59355

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

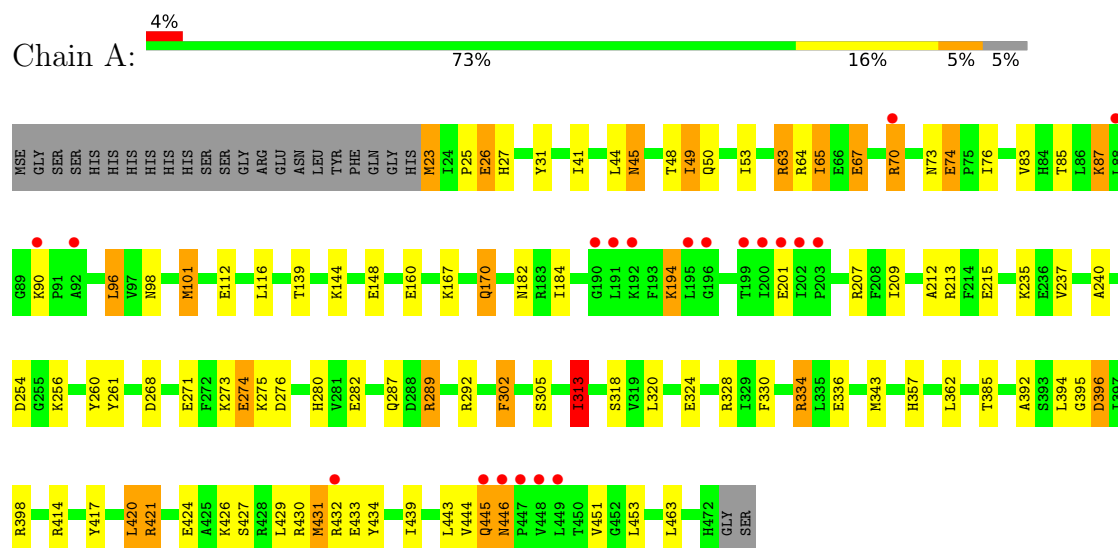
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	400	Total	O	0	0
			400	400		
3	B	412	Total	O	0	0
			412	412		

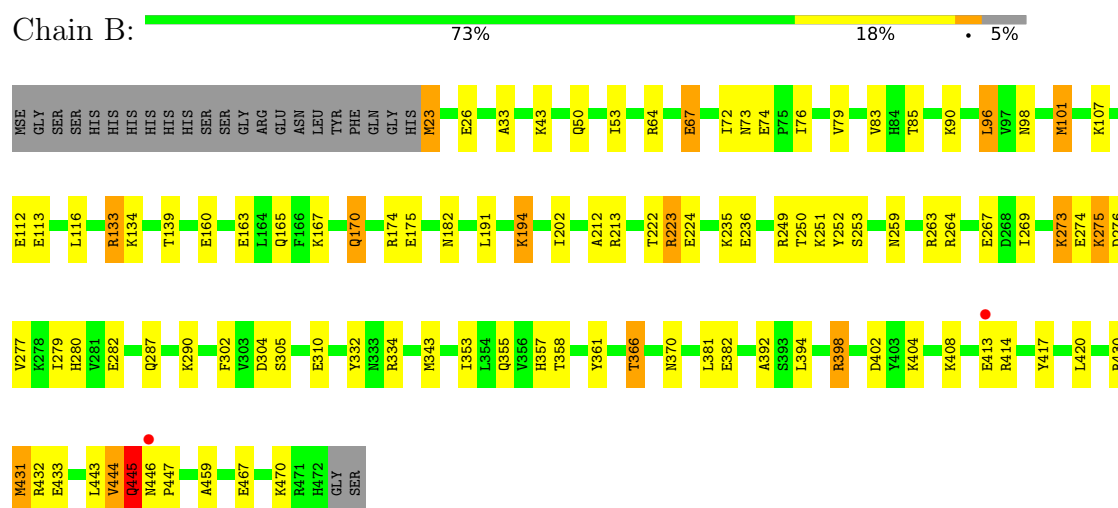
3 Residue-property plots

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: ADP-specific phosphofructokinase



• Molecule 1: ADP-specific phosphofructokinase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	68.06Å 99.93Å 82.58Å 90.00° 110.38° 90.00°	Depositor
Resolution (Å)	39.84 – 2.00 39.84 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.7 (39.84-2.00) 99.0 (39.84-2.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.64 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.174 , 0.226 0.180 , 0.229	Depositor DCC
R_{free} test set	3508 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	25.2	Xtriage
Anisotropy	0.308	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 45.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8143	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 36.16 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.2145e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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	1.48	15/3724 (0.4%)	1.22	4/5016 (0.1%)
1	B	1.51	19/3724 (0.5%)	1.25	9/5016 (0.2%)
All	All	1.49	34/7448 (0.5%)	1.23	13/10032 (0.1%)

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	101	MSE	SE-CE	-9.90	1.65	1.95
1	B	277	VAL	CA-CB	-9.66	1.42	1.54
1	B	101	MSE	SE-CE	-8.91	1.68	1.95
1	B	304	ASP	CA-C	7.92	1.59	1.52
1	A	23	MSE	SE-CE	7.13	2.16	1.95
1	A	343	MSE	SE-CE	-7.04	1.74	1.95
1	A	439	ILE	CA-CB	-6.90	1.49	1.55
1	A	271	GLU	C-O	6.25	1.31	1.24
1	B	459	ALA	C-O	-6.23	1.17	1.24
1	B	417	TYR	C-O	-6.16	1.17	1.24
1	B	249	ARG	CA-C	-6.13	1.45	1.52
1	A	320	LEU	C-O	-6.10	1.16	1.24
1	B	343	MSE	CG-SE	6.09	2.13	1.95
1	A	287	GLN	C-O	-6.07	1.16	1.24
1	B	23	MSE	SE-CE	5.98	2.13	1.95
1	B	116	LEU	C-O	-5.77	1.17	1.23
1	A	74	GLU	N-CA	5.67	1.50	1.45
1	B	222	THR	CA-CB	-5.58	1.45	1.53
1	A	330	PHE	CA-C	5.57	1.60	1.52
1	B	382	GLU	C-O	-5.54	1.17	1.24
1	B	370	ASN	C-O	-5.41	1.17	1.24
1	A	237	VAL	N-CA	5.37	1.52	1.46
1	B	113	GLU	C-O	5.36	1.30	1.23
1	B	381	LEU	C-O	5.29	1.30	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	259	ASN	C-O	-5.22	1.18	1.24
1	B	275	LYS	CA-C	-5.20	1.44	1.52
1	B	252	TYR	CA-C	5.10	1.58	1.52
1	A	268	ASP	CG-OD2	5.09	1.35	1.25
1	A	292	ARG	NE-CZ	5.06	1.38	1.33
1	A	261	TYR	CD2-CE2	5.02	1.53	1.38
1	B	279	ILE	CA-CB	-5.02	1.47	1.54
1	A	434	TYR	N-CA	5.02	1.52	1.46
1	A	274	GLU	C-O	5.02	1.30	1.24
1	B	269	ILE	N-CA	-5.01	1.40	1.46

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	313	ILE	CB-CA-C	-8.00	101.34	112.14
1	B	250	THR	CB-CA-C	-7.42	99.12	110.92
1	B	366	THR	OG1-CB-CG2	-6.81	95.67	109.30
1	A	215	GLU	N-CA-C	5.79	117.59	111.28
1	B	332	TYR	N-CA-C	5.71	121.15	113.72
1	B	334	ARG	NE-CZ-NH1	-5.69	115.81	121.50
1	B	445	GLN	N-CA-C	5.33	117.17	111.36
1	A	289	ARG	CG-CD-NE	-5.27	100.41	112.00
1	B	404	LYS	N-CA-C	-5.19	106.21	112.54
1	B	253	SER	N-CA-C	5.15	119.86	111.37
1	B	33	ALA	CA-C-N	5.12	130.91	121.70
1	B	33	ALA	C-N-CA	5.12	130.91	121.70
1	A	336	GLU	N-CA-C	5.05	116.79	111.28

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	3658	0	3730	84	0
1	B	3658	0	3730	80	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	5	0	0	0	0
2	B	10	0	0	0	0
3	A	400	0	0	27	1
3	B	412	0	0	39	0
All	All	8143	0	7460	161	1

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 11.

All (161) 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:23:MSE:CE	1:A:23:MSE:SE	2.16	1.42
1:A:302:PHE:CD2	3:A:1375:HOH:O	2.05	1.06
1:A:275:LYS:HE3	3:A:1395:HOH:O	1.63	0.96
1:A:446:ASN:O	1:B:445:GLN:NE2	2.01	0.93
1:B:302:PHE:CE2	3:B:1398:HOH:O	2.22	0.93
1:B:50:GLN:HE22	1:B:194:LYS:H	0.95	0.92
1:A:50:GLN:HE22	1:A:194:LYS:H	1.14	0.90
1:B:445:GLN:H	1:B:445:GLN:CD	1.80	0.90
1:B:107:LYS:HD2	3:B:1283:HOH:O	1.72	0.88
1:B:302:PHE:CZ	3:B:1398:HOH:O	2.27	0.88
1:B:174:ARG:HD3	3:B:1388:HOH:O	1.75	0.86
1:B:276:ASP:HB3	3:B:1407:HOH:O	1.73	0.85
1:A:453:LEU:HD22	3:A:1358:HOH:O	1.76	0.84
1:B:165:GLN:NE2	3:B:1079:HOH:O	2.11	0.83
1:A:451:VAL:HG23	3:A:1291:HOH:O	1.77	0.82
1:B:251:LYS:NZ	3:B:1296:HOH:O	2.12	0.82
1:B:133:ARG:HD3	3:B:1080:HOH:O	1.80	0.82
1:A:45:ASN:C	1:A:45:ASN:HD22	1.85	0.81
1:B:310:GLU:HG3	1:B:358:THR:HG22	1.65	0.78
1:B:414:ARG:HD2	3:B:1333:HOH:O	1.85	0.76
1:A:45:ASN:O	1:A:49:ILE:HG22	1.86	0.75
1:B:274:GLU:OE1	3:B:1219:HOH:O	2.05	0.74
1:B:235:LYS:NZ	3:B:1300:HOH:O	2.20	0.74
1:B:23:MSE:N	3:B:1406:HOH:O	2.21	0.73
1:B:133:ARG:CD	3:B:1080:HOH:O	2.36	0.73
1:A:445:GLN:HG2	3:B:1392:HOH:O	1.88	0.73
1:B:50:GLN:HE22	1:B:194:LYS:N	1.80	0.73
1:B:223:ARG:NH1	3:B:1054:HOH:O	2.21	0.73
1:A:289:ARG:NH1	1:A:318:SER:OG	2.22	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:ASN:HD22	1:A:212:ALA:H	1.36	0.71
1:B:213:ARG:HD3	3:B:1195:HOH:O	1.91	0.70
1:B:53:ILE:HD11	1:B:83:VAL:CG2	2.22	0.70
1:A:445:GLN:HG3	3:A:1141:HOH:O	1.92	0.69
1:B:182:ASN:ND2	1:B:212:ALA:H	1.91	0.69
1:A:74:GLU:CA	1:A:101:MSE:HE1	2.23	0.68
1:A:394:LEU:HD21	1:B:394:LEU:HD23	1.76	0.68
1:B:175:GLU:OE2	3:B:1358:HOH:O	2.13	0.67
1:A:182:ASN:ND2	1:A:212:ALA:H	1.93	0.66
1:A:194:LYS:NZ	3:A:1336:HOH:O	2.13	0.65
1:A:280:HIS:HD2	1:A:305:SER:OG	1.80	0.65
1:B:50:GLN:NE2	1:B:194:LYS:H	1.81	0.65
1:A:27:HIS:NE2	3:A:1259:HOH:O	2.17	0.65
1:A:445:GLN:CD	1:A:445:GLN:H	2.04	0.65
1:B:73:ASN:C	1:B:101:MSE:HE1	2.22	0.64
1:B:280:HIS:HD2	1:B:305:SER:OG	1.78	0.64
1:A:274:GLU:OE2	3:A:1395:HOH:O	2.15	0.64
1:B:432:ARG:NH2	3:B:1360:HOH:O	2.28	0.63
1:A:328:ARG:NH2	1:A:334:ARG:HH22	1.96	0.63
1:B:398:ARG:HD3	1:B:402:ASP:OD2	1.99	0.63
1:B:446:ASN:O	3:B:1412:HOH:O	2.15	0.63
1:A:74:GLU:HA	1:A:101:MSE:HE1	1.81	0.63
1:B:224:GLU:HG2	3:B:1339:HOH:O	1.99	0.63
1:A:420:LEU:HD21	1:A:424:GLU:OE2	1.99	0.62
1:B:182:ASN:HD22	1:B:212:ALA:H	1.48	0.61
1:A:50:GLN:HE22	1:A:194:LYS:N	1.92	0.61
1:A:302:PHE:CG	3:A:1375:HOH:O	2.42	0.61
1:B:170:GLN:NE2	1:B:170:GLN:H	1.99	0.60
1:A:453:LEU:CD2	3:A:1358:HOH:O	2.44	0.59
1:B:444:VAL:HG23	3:B:1386:HOH:O	2.02	0.59
1:A:280:HIS:HE1	1:A:282:GLU:OE1	1.85	0.58
1:A:432:ARG:HD2	3:A:1099:HOH:O	2.04	0.57
1:B:43:LYS:CE	1:B:112:GLU:HG2	2.34	0.57
1:A:45:ASN:C	1:A:45:ASN:ND2	2.61	0.57
1:B:43:LYS:HE3	1:B:112:GLU:HG2	1.87	0.57
1:A:65:ILE:HD11	1:A:83:VAL:CG2	2.35	0.56
1:B:430:ARG:O	1:B:431:MSE:HE2	2.06	0.56
1:B:287:GLN:NE2	3:B:1289:HOH:O	2.39	0.56
1:B:353:ILE:HD12	1:B:366:THR:HG22	1.88	0.56
1:B:445:GLN:NE2	3:B:1411:HOH:O	2.38	0.56
1:B:160:GLU:OE1	1:B:167:LYS:HD2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:273:LYS:HD3	3:B:1163:HOH:O	2.05	0.55
1:B:433:GLU:HG2	3:B:1404:HOH:O	2.06	0.54
1:B:264:ARG:CG	3:B:1399:HOH:O	2.55	0.54
1:B:76:ILE:HA	1:B:79:VAL:HG12	1.90	0.54
1:A:276:ASP:OD1	3:A:1343:HOH:O	2.19	0.53
1:B:432:ARG:NE	3:B:1265:HOH:O	2.27	0.53
1:A:414:ARG:NH2	3:A:1137:HOH:O	2.42	0.52
1:A:392:ALA:CB	1:A:444:VAL:HG21	2.39	0.52
1:B:274:GLU:OE2	1:B:275:LYS:HE3	2.09	0.52
1:A:160:GLU:OE1	1:A:167:LYS:HE3	2.09	0.52
1:B:280:HIS:HE1	1:B:282:GLU:OE1	1.91	0.52
1:B:446:ASN:HB3	3:B:1412:HOH:O	2.08	0.52
1:B:264:ARG:HG3	3:B:1399:HOH:O	2.09	0.52
1:B:290:LYS:NZ	3:B:1152:HOH:O	2.41	0.52
1:A:27:HIS:CE1	3:A:1259:HOH:O	2.61	0.52
1:A:184:ILE:HD13	1:A:209:ILE:HG23	1.90	0.52
1:A:328:ARG:HH21	1:A:334:ARG:HH22	1.56	0.52
1:A:394:LEU:CD2	1:B:394:LEU:HD23	2.39	0.52
1:A:26:GLU:OE1	3:A:1368:HOH:O	2.19	0.52
1:B:74:GLU:N	1:B:101:MSE:HE1	2.25	0.52
1:B:273:LYS:CD	3:B:1163:HOH:O	2.58	0.51
1:A:170:GLN:NE2	1:A:170:GLN:H	2.08	0.51
1:A:414:ARG:HG2	3:B:1295:HOH:O	2.10	0.51
1:A:45:ASN:ND2	1:A:48:THR:H	2.09	0.51
1:A:414:ARG:NH1	3:A:1400:HOH:O	2.45	0.50
1:A:420:LEU:C	1:A:420:LEU:HD23	2.35	0.50
1:B:445:GLN:CD	1:B:445:GLN:N	2.60	0.50
1:A:414:ARG:HD2	3:A:1137:HOH:O	2.12	0.50
1:A:274:GLU:OE2	1:A:275:LYS:HE3	2.13	0.49
1:A:417:TYR:O	1:A:421:ARG:HG2	2.12	0.49
1:B:96:LEU:HD22	1:B:98:ASN:H	1.77	0.49
1:A:160:GLU:OE1	1:A:167:LYS:CE	2.61	0.48
1:B:72:ILE:HG22	1:B:101:MSE:HE3	1.96	0.48
1:A:451:VAL:HG22	3:A:1380:HOH:O	2.13	0.48
1:A:53:ILE:HG22	3:A:1247:HOH:O	2.12	0.48
1:B:447:PRO:HA	3:B:1032:HOH:O	2.14	0.48
1:A:45:ASN:HD21	1:A:48:THR:H	1.61	0.47
1:A:41:ILE:HG12	1:A:184:ILE:HB	1.96	0.47
1:B:170:GLN:H	1:B:170:GLN:HE21	1.61	0.47
1:B:361:TYR:CD1	1:B:361:TYR:C	2.92	0.47
1:A:256:LYS:HD3	1:A:260:TYR:CE2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:414:ARG:CD	3:A:1137:HOH:O	2.61	0.47
1:B:355:GLN:NE2	1:B:357:HIS:ND1	2.53	0.47
1:A:398:ARG:HD2	3:A:1383:HOH:O	2.14	0.47
1:A:23:MSE:N	3:A:1176:HOH:O	2.49	0.46
1:A:63:ARG:O	1:A:67:GLU:HG2	2.15	0.46
1:A:426:LYS:HA	1:A:431:MSE:HE1	1.98	0.46
1:B:98:ASN:C	1:B:98:ASN:HD22	2.22	0.46
1:A:444:VAL:HG22	3:A:1382:HOH:O	2.16	0.45
1:A:235:LYS:NZ	3:A:1155:HOH:O	2.50	0.45
1:A:328:ARG:CZ	1:A:334:ARG:HH22	2.29	0.45
1:B:74:GLU:CA	1:B:101:MSE:HE1	2.46	0.45
1:B:263:ARG:O	1:B:267:GLU:HG3	2.16	0.45
1:A:429:LEU:O	1:A:431:MSE:CE	2.64	0.45
1:A:429:LEU:O	1:A:431:MSE:HE1	2.16	0.45
1:B:273:LYS:HE3	1:B:302:PHE:O	2.17	0.45
1:A:96:LEU:HD22	1:A:98:ASN:H	1.82	0.45
1:B:392:ALA:HB3	1:B:444:VAL:HG21	1.97	0.45
1:A:313:ILE:HD13	1:A:313:ILE:HG21	1.68	0.44
1:A:70:ARG:NE	1:A:70:ARG:H	2.16	0.44
1:B:64:ARG:HA	1:B:67:GLU:HG3	1.99	0.44
1:B:96:LEU:HD21	1:B:101:MSE:HB3	1.99	0.44
1:A:144:LYS:HE2	1:A:148:GLU:OE2	2.18	0.43
1:B:191:LEU:HB2	1:B:202:ILE:HD12	2.00	0.43
1:A:362:LEU:HD11	1:A:385:THR:HB	2.01	0.43
1:B:414:ARG:NH1	3:B:1333:HOH:O	2.41	0.43
1:A:74:GLU:N	1:A:101:MSE:HE1	2.33	0.43
1:B:264:ARG:HG2	3:B:1399:HOH:O	2.17	0.43
1:A:282:GLU:OE2	1:A:357:HIS:HE1	2.01	0.43
1:B:446:ASN:HB2	3:B:1384:HOH:O	2.19	0.43
1:B:134:LYS:NZ	1:B:236:GLU:O	2.43	0.43
1:A:324:GLU:HB2	3:A:1376:HOH:O	2.18	0.42
1:A:73:ASN:C	1:A:101:MSE:HE1	2.45	0.42
1:B:98:ASN:C	1:B:98:ASN:ND2	2.76	0.42
1:B:446:ASN:C	3:B:1412:HOH:O	2.62	0.42
1:A:417:TYR:CZ	1:A:421:ARG:HD3	2.54	0.42
1:B:392:ALA:HB1	1:B:447:PRO:HB3	2.02	0.42
1:A:64:ARG:HA	1:A:67:GLU:HG3	2.02	0.41
1:A:445:GLN:CG	3:B:1392:HOH:O	2.59	0.41
1:A:31:TYR:O	1:A:240:ALA:HA	2.20	0.41
1:A:25:PRO:HG2	1:A:463:LEU:HG	2.02	0.41
1:A:254:ASP:HA	3:A:1108:HOH:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:ARG:HD2	3:B:1080:HOH:O	2.13	0.41
1:A:420:LEU:CD2	1:A:424:GLU:OE2	2.65	0.41
1:A:87:LYS:NZ	3:A:1333:HOH:O	2.54	0.41
1:B:43:LYS:HE2	1:B:112:GLU:HG2	2.02	0.41
1:A:395:GLY:O	1:A:396:ASP:HB2	2.19	0.41
1:B:280:HIS:HA	1:B:305:SER:O	2.20	0.40
1:A:170:GLN:H	1:A:170:GLN:HE21	1.68	0.40
1:B:223:ARG:NH1	1:B:223:ARG:HB2	2.37	0.40
1:A:444:VAL:HG23	1:A:444:VAL:O	2.21	0.40

All (1) 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)
3:A:1093:HOH:O	3:A:1386:HOH:O[2_556]	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	448/474 (94%)	429 (96%)	18 (4%)	1 (0%)	43	42
1	B	448/474 (94%)	439 (98%)	9 (2%)	0	100	100
All	All	896/948 (94%)	868 (97%)	27 (3%)	1 (0%)	48	46

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	396	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	393/407 (97%)	359 (91%)	34 (9%)	9	6
1	B	393/407 (97%)	371 (94%)	22 (6%)	19	16
All	All	786/814 (97%)	730 (93%)	56 (7%)	13	10

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	GLU
1	A	44	LEU
1	A	45	ASN
1	A	49	ILE
1	A	63	ARG
1	A	65	ILE
1	A	67	GLU
1	A	70	ARG
1	A	76	ILE
1	A	85	THR
1	A	87	LYS
1	A	90	LYS
1	A	96	LEU
1	A	112	GLU
1	A	116	LEU
1	A	139	THR
1	A	170	GLN
1	A	194	LYS
1	A	201	GLU
1	A	207	ARG
1	A	213	ARG
1	A	273	LYS
1	A	302	PHE
1	A	313	ILE
1	A	334	ARG
1	A	420	LEU
1	A	421	ARG

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Mol	Chain	Res	Type
1	A	427	SER
1	A	430	ARG
1	A	431	MSE
1	A	433	GLU
1	A	443	LEU
1	A	445	GLN
1	A	446	ASN
1	B	26	GLU
1	B	67	GLU
1	B	85	THR
1	B	90	LYS
1	B	96	LEU
1	B	133	ARG
1	B	139	THR
1	B	163	GLU
1	B	170	GLN
1	B	194	LYS
1	B	223	ARG
1	B	273	LYS
1	B	398	ARG
1	B	408	LYS
1	B	413	GLU
1	B	420	LEU
1	B	431	MSE
1	B	443	LEU
1	B	444	VAL
1	B	445	GLN
1	B	467	GLU
1	B	470	LYS

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	45	ASN
1	A	46	GLN
1	A	50	GLN
1	A	51	ASN
1	A	54	ASN
1	A	84	HIS
1	A	98	ASN
1	A	170	GLN
1	A	182	ASN

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Mol	Chain	Res	Type
1	A	259	ASN
1	A	280	HIS
1	A	315	GLN
1	A	333	ASN
1	A	355	GLN
1	A	472	HIS
1	B	50	GLN
1	B	51	ASN
1	B	54	ASN
1	B	84	HIS
1	B	98	ASN
1	B	165	GLN
1	B	170	GLN
1	B	182	ASN
1	B	204	ASN
1	B	259	ASN
1	B	280	HIS
1	B	315	GLN
1	B	355	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 ⓘ

3 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	$\# Z > 2$
2	SO4	A	1003	-	4,4,4	0.85	0	6,6,6	0.72	0
2	SO4	B	1002	-	4,4,4	0.23	0	6,6,6	0.65	0
2	SO4	B	1001	-	4,4,4	0.47	0	6,6,6	0.35	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.

No monomer is involved in short contacts.

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	445/474 (93%)	0.01	20 (4%) 38 37	13, 27, 65, 87	0
1	B	445/474 (93%)	-0.21	2 (0%) 88 88	13, 28, 46, 60	0
All	All	890/948 (93%)	-0.10	22 (2%) 58 58	13, 27, 56, 87	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	190	GLY	4.7
1	A	191	LEU	3.9
1	A	448	VAL	3.9
1	A	202	ILE	3.6
1	A	200	ILE	3.4
1	A	446	ASN	3.1
1	A	449	LEU	2.9
1	A	195	LEU	2.8
1	A	199	THR	2.8
1	A	92	ALA	2.8
1	A	88	LEU	2.6
1	B	446	ASN	2.5
1	A	447	PRO	2.3
1	A	203	PRO	2.3
1	A	445	GLN	2.3
1	A	70	ARG	2.1
1	A	201	GLU	2.1
1	A	432	ARG	2.1
1	B	413	GLU	2.1
1	A	90	LYS	2.0
1	A	196	GLY	2.0
1	A	192	LYS	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
2	SO4	B	1002	5/5	0.92	0.10	54,54,58,61	0
2	SO4	B	1001	5/5	0.99	0.05	22,23,26,29	0
2	SO4	A	1003	5/5	0.99	0.04	22,24,24,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.