



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:32 PM GMT

PDB ID : 1U2X
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
<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

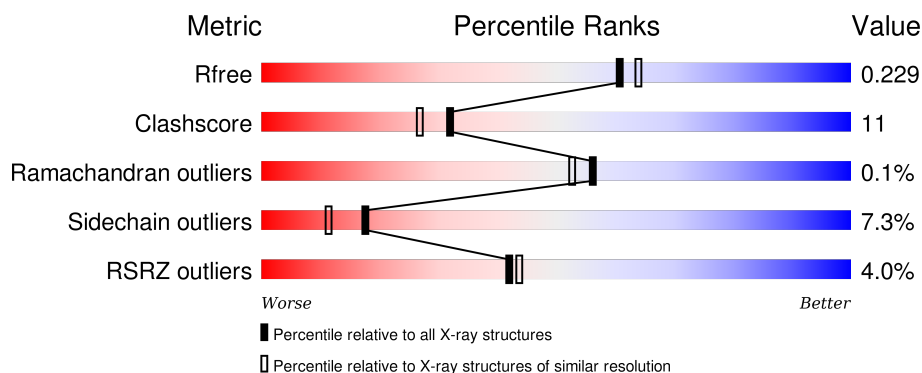
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



The reported resolution of this entry is 2.00 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}	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (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 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	474	
1	B	474	

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 (three-letter code: SO4) (formula: O₄S).



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

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 39.81 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.7 (39.84-2.00) 98.7 (39.81-2.00)	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	3496 reflections (5.32%)	DCC
Wilson B-factor (Å ²)	25.2	Xtriage
Anisotropy	0.308	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 56.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 69479 reflections (0.001%)	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.*

¹ Intensities estimated from amplitudes.

² Theoretical 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

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	1.19	5/3724 (0.1%)	1.09	21/5016 (0.4%)
1	B	1.19	3/3724 (0.1%)	1.12	21/5016 (0.4%)
All	All	1.19	8/7448 (0.1%)	1.11	42/10032 (0.4%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	261	TYR	CD2-CE2	9.57	1.53	1.39
1	A	332	TYR	CE2-CZ	-6.16	1.30	1.38
1	A	302	PHE	CE2-CZ	-6.16	1.25	1.37
1	B	277	VAL	CA-CB	-6.03	1.42	1.54
1	B	343	MSE	CG-SE	5.37	2.13	1.95
1	A	467	GLU	CG-CD	5.34	1.59	1.51
1	B	383	PHE	CE1-CZ	5.29	1.47	1.37
1	A	101	MSE	SE-CE	-5.03	1.65	1.95

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	442	ARG	NE-CZ-NH2	-9.70	115.45	120.30
1	B	442	ARG	NE-CZ-NH1	9.54	125.07	120.30
1	A	223	ARG	NE-CZ-NH1	9.21	124.91	120.30
1	B	225	ASP	CB-CG-OD2	9.07	126.47	118.30
1	B	334	ARG	NE-CZ-NH1	-8.98	115.81	120.30
1	A	288	ASP	CB-CG-OD2	8.18	125.67	118.30
1	B	398	ARG	NE-CZ-NH1	7.79	124.20	120.30
1	B	398	ARG	NE-CZ-NH2	-7.77	116.42	120.30
1	B	133	ARG	NE-CZ-NH1	7.47	124.03	120.30
1	B	288	ASP	CB-CG-OD2	7.46	125.02	118.30
1	A	257	ASP	CB-CG-OD1	7.33	124.90	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	177	ASP	CB-CG-OD2	6.96	124.57	118.30
1	A	238	ASP	CB-CG-OD2	6.90	124.51	118.30
1	A	57	ASP	CB-CG-OD2	6.88	124.49	118.30
1	A	396	ASP	CB-CG-OD2	6.69	124.32	118.30
1	A	59	ASP	CB-CG-OD2	6.62	124.26	118.30
1	A	402	ASP	CB-CG-OD2	6.60	124.24	118.30
1	B	133	ARG	NE-CZ-NH2	-6.25	117.17	120.30
1	B	366	THR	OG1-CB-CG2	-6.23	95.67	110.00
1	A	276	ASP	CB-CG-OD2	6.22	123.90	118.30
1	A	223	ARG	NE-CZ-NH2	-6.13	117.24	120.30
1	B	347	ASP	CB-CG-OD2	5.97	123.67	118.30
1	A	219	ARG	NE-CZ-NH2	5.95	123.28	120.30
1	A	133	ARG	NE-CZ-NH1	5.95	123.27	120.30
1	B	275	LYS	CD-CE-NZ	-5.93	98.07	111.70
1	A	268	ASP	CB-CG-OD2	5.78	123.50	118.30
1	B	432	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	B	334	ARG	NE-CZ-NH2	5.75	123.18	120.30
1	B	134	LYS	CD-CE-NZ	5.75	124.93	111.70
1	A	106	ASP	CB-CG-OD2	5.74	123.47	118.30
1	A	289	ARG	NE-CZ-NH1	-5.57	117.52	120.30
1	B	432	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	A	289	ARG	CG-CD-NE	-5.42	100.41	111.80
1	A	249	ARG	NE-CZ-NH1	-5.39	117.61	120.30
1	B	57	ASP	CB-CG-OD2	5.39	123.15	118.30
1	A	369	ASP	CB-CG-OD2	5.37	123.14	118.30
1	A	177	ASP	CB-CG-OD2	5.30	123.07	118.30
1	B	369	ASP	CB-CG-OD2	5.26	123.04	118.30
1	A	197	ASP	CB-CG-OD2	5.25	123.03	118.30
1	B	442	ARG	CD-NE-CZ	5.23	130.92	123.60
1	A	313	ILE	CB-CA-C	-5.13	101.34	111.60
1	B	115	ARG	NE-CZ-NH2	-5.00	117.80	120.30

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	83	0
1	B	3658	0	3730	76	0
2	A	5	0	0	0	0
2	B	10	0	0	0	0
3	A	400	0	0	26	1
3	B	412	0	0	38	0
All	All	8143	0	7460	156	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 (156) 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:B:302:PHE:CE2	3:B:1398:HOH:O	2.22	0.93
1:A:446:ASN:O	1:B:445:GLN:NE2	2.01	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: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:445:GLN:H	1:B:445:GLN:CD	1.80	0.85
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:B:251:LYS:NZ	3:B:1296:HOH:O	2.12	0.82
1:A:451:VAL:HG23	3:A:1291:HOH:O	1.77	0.82
1:B:133:ARG:HD3	3:B:1080:HOH:O	1.80	0.82
1:A:45:ASN:HD22	1:A:45:ASN:C	1.85	0.78
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: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: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:445:GLN:HG2	3:B:1392:HOH:O	1.88	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: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: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:446:ASN:O	3:B:1412:HOH:O	2.15	0.63
1:B:398:ARG:HD3	1:B:402:ASP:OD2	1.99	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:A:445:GLN:CD	1:A:445:GLN:H	2.04	0.60
1:B:170:GLN:H	1:B:170:GLN:NE2	1.99	0.60
1:A:453:LEU:CD2	3:A:1358:HOH:O	2.44	0.59
1:B:73:ASN:C	1:B:101:MSE:HE1	2.22	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: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:353:ILE:HD12	1:B:366:THR:HG22	1.88	0.56
1:B:287:GLN:NE2	3:B:1289:HOH:O	2.39	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:274:GLU:OE2	1:B:275:LYS:HE3	2.09	0.52
1:A:392:ALA:CB	1:A:444:VAL:HG21	2.39	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:A:160:GLU:OE1	1:A:167:LYS:HE3	2.09	0.52
1:B:264:ARG:HG3	3:B:1399:HOH:O	2.09	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:394:LEU:CD2	1:B:394:LEU:HD23	2.39	0.52
1:A:328:ARG:HH21	1:A:334:ARG:HH22	1.56	0.52
1:B:74:GLU:N	1:B:101:MSE:HE1	2.25	0.52
1:A:26:GLU:OE1	3:A:1368:HOH:O	2.19	0.52
1:B:273:LYS:CD	3:B:1163:HOH:O	2.58	0.51
1:A:45:ASN:ND2	1:A:45:ASN:C	2.61	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: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:B:235:LYS:NZ	3:B:1300:HOH:O	2.20	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:B:447:PRO:HA	3:B:1032:HOH:O	2.14	0.48
1:A:53:ILE:HG22	3:A:1247:HOH:O	2.12	0.48
1:A:45:ASN:HD21	1:A:48:THR:H	1.61	0.47
1:B:170:GLN:HE21	1:B:170:GLN:H	1.61	0.47
1:A:41:ILE:HG12	1:A:184:ILE:HB	1.96	0.47
1:A:414:ARG:CD	3:A:1137:HOH:O	2.61	0.47
1:A:256:LYS:HD3	1:A:260:TYR:CE2	2.49	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:420:LEU:C	1:A:420:LEU:HD23	2.35	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:LYS:NZ	3:A:1403:HOH:O	2.47	0.46
1:A:23:MSE:N	3:A:1176:HOH:O	2.49	0.46
1:A:426:LYS:HA	1:A:431:MSE:HE1	1.98	0.46
1:A:63:ARG:O	1:A:67:GLU:HG2	2.15	0.46
1:A:444:VAL:HG22	3:A:1382:HOH:O	2.16	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:B:392:ALA:HB3	1:B:444:VAL:HG21	1.97	0.45
1:A:96:LEU:HD22	1:A:98:ASN:H	1.82	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:96:LEU:HD21	1:B:101:MSE:HB3	1.99	0.44
1:B:64:ARG:HA	1:B:67:GLU:HG3	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:361:TYR:C	1:B:361:TYR:CD1	2.92	0.43
1:A:324:GLU:HB2	3:A:1376:HOH:O	2.18	0.42
1:B:98:ASN:HD22	1:B:98:ASN:C	2.22	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:B:133:ARG:HD2	3:B:1080:HOH:O	2.13	0.41
1:A:254:ASP:HA	3:A:1108:HOH:O	2.19	0.41
1:A:25:PRO:HG2	1:A:463:LEU:HG	2.02	0.41
1:A:420:LEU:CD2	1:A:424:GLU:OE2	2.65	0.41
1:B:290:LYS:NZ	3:B:1152:HOH:O	2.41	0.41
1:A:313:ILE:O	1:A:313:ILE:HG22	2.17	0.41
1:B:43:LYS:HE2	1:B:112:GLU:HG2	2.02	0.41
1:A:87:LYS:NZ	3:A:1333:HOH:O	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	52	48
1	B	448/474 (94%)	439 (98%)	9 (2%)	0	100	100
All	All	896/948 (94%)	868 (97%)	27 (3%)	1 (0%)	56	53

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	396	ASP

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	393/407 (97%)	360 (92%)	33 (8%)	14	8
1	B	393/407 (97%)	369 (94%)	24 (6%)	23	17
All	All	786/814 (97%)	729 (93%)	57 (7%)	17	11

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	MSE
1	A	26	GLU
1	A	44	LEU
1	A	45	ASN
1	A	49	ILE
1	A	63	ARG
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	134	LYS
1	A	139	THR
1	A	170	GLN
1	A	201	GLU
1	A	204	ASN
1	A	207	ARG
1	A	213	ARG
1	A	273	LYS
1	A	290	LYS
1	A	302	PHE
1	A	421	ARG
1	A	427	SER
1	A	430	ARG
1	A	431	MSE
1	A	432	ARG
1	A	433	GLU
1	A	443	LEU
1	A	445	GLN

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Mol	Chain	Res	Type
1	B	26	GLU
1	B	67	GLU
1	B	85	THR
1	B	90	LYS
1	B	96	LEU
1	B	98	ASN
1	B	133	ARG
1	B	139	THR
1	B	163	GLU
1	B	170	GLN
1	B	194	LYS
1	B	204	ASN
1	B	223	ARG
1	B	398	ARG
1	B	408	LYS
1	B	413	GLU
1	B	420	LEU
1	B	427	SER
1	B	431	MSE
1	B	443	LEU
1	B	444	VAL
1	B	445	GLN
1	B	467	GLU
1	B	470	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) 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	98	ASN
1	A	170	GLN
1	A	182	ASN
1	A	259	ASN
1	A	280	HIS
1	A	315	GLN
1	A	355	GLN
1	A	472	HIS
1	B	50	GLN

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Mol	Chain	Res	Type
1	B	51	ASN
1	B	54	ASN
1	B	98	ASN
1	B	165	GLN
1	B	170	GLN
1	B	182	ASN
1	B	259	ASN
1	B	280	HIS
1	B	315	GLN
1	B	355	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](#)

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	1.15	0	6,6,6	0.77	0
2	SO4	B	1001	-	4,4,4	0.73	0	6,6,6	0.46	0
2	SO4	B	1002	-	4,4,4	0.55	0	6,6,6	0.56	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	A	1003	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1001	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1002	-	-	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.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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%)	0.02	31 (6%) 19 21	13, 27, 65, 87	0
1	B	445/474 (93%)	-0.25	5 (1%) 82 83	13, 28, 46, 60	0
All	All	890/948 (93%)	-0.11	36 (4%) 42 44	13, 27, 56, 87	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	190	GLY	5.9
1	A	66	GLU	4.8
1	A	201	GLU	4.4
1	A	68	TYR	4.4
1	A	202	ILE	4.4
1	A	196	GLY	4.3
1	A	197	ASP	4.3
1	A	191	LEU	4.1
1	A	90	LYS	4.1
1	A	83	VAL	3.7
1	B	68	TYR	3.6
1	A	70	ARG	3.5
1	A	69	PRO	3.5
1	A	192	LYS	3.5
1	A	87	LYS	3.3
1	A	84	HIS	3.2
1	B	197	ASP	3.1
1	A	204	ASN	3.1
1	A	65	ILE	3.0
1	B	70	ARG	2.9
1	B	66	GLU	2.8
1	A	198	GLU	2.6
1	B	446	ASN	2.6
1	A	63	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	188	ARG	2.5
1	A	189	LYS	2.5
1	A	92	ALA	2.4
1	A	194	LYS	2.4
1	A	67	GLU	2.2
1	A	89	GLY	2.2
1	A	88	LEU	2.2
1	A	199	THR	2.2
1	A	200	ILE	2.2
1	A	446	ASN	2.1
1	A	110	ARG	2.1
1	A	195	LEU	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(\AA^2)	Q<0.9
2	SO4	B	1002	5/5	0.96	0.15	1.15	54,54,58,61	0
2	SO4	B	1001	5/5	0.99	0.08	-1.10	22,23,26,29	0
2	SO4	A	1003	5/5	0.99	0.07	-2.78	22,24,24,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.