



Full wwPDB X-ray Structure Validation Report ⓘ

May 7, 2026 – 08:13 AM EDT

PDB ID : 2FFI / pdb_00002ffi
Title : Crystal Structure of Putative 2-Pyrone-4,6-Dicarboxylic Acid Hydrolase from *Pseudomonas putida*, Northeast Structural Genomics Target PpR23.
Authors : Forouhar, F.; Su, M.; Jayaraman, S.; Conover, K.; Xiao, R.; Acton, T.B.; Montelione, G.T.; Hunt, J.F.; Tong, L.; Northeast Structural Genomics Consortium (NESG)
Deposited on : 2005-12-19
Resolution : 2.61 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

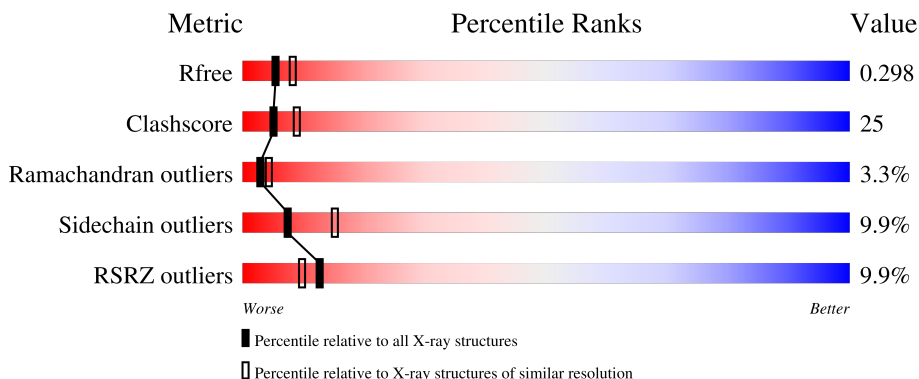
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.61 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	4951 (2.64-2.60)
Clashscore	190562	5303 (2.64-2.60)
Ramachandran outliers	187476	5217 (2.64-2.60)
Sidechain outliers	187428	5217 (2.64-2.60)
RSRZ outliers	180081	4950 (2.64-2.60)

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	288	 8% 49% 37% 7% • 5%
1	B	288	 10% 51% 35% 7% • 5%

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 4331 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 2-pyrone-4,6-dicarboxylic acid hydrolase, putative.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	273	2133	1347	394	385	2	5	0	0	0
1	B	273	2133	1347	394	385	2	5	0	0	0

There are 30 discrepancies between the modelled and reference sequences:

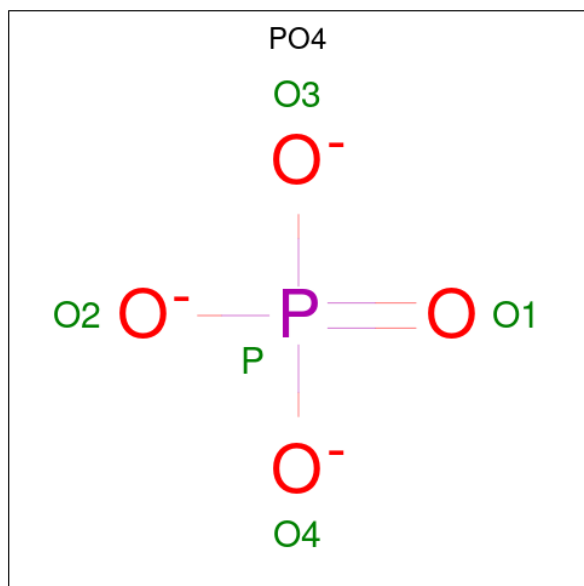
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	modified residue	UNP Q88M75
A	4	MSE	MET	modified residue	UNP Q88M75
A	88	MSE	MET	modified residue	UNP Q88M75
A	101	MSE	MET	modified residue	UNP Q88M75
A	114	MSE	MET	modified residue	UNP Q88M75
A	118	MSE	MET	modified residue	UNP Q88M75
A	232	MSE	MET	modified residue	UNP Q88M75
A	281	LEU	-	cloning artifact	UNP Q88M75
A	282	GLU	-	cloning artifact	UNP Q88M75
A	283	HIS	-	expression tag	UNP Q88M75
A	284	HIS	-	expression tag	UNP Q88M75
A	285	HIS	-	expression tag	UNP Q88M75
A	286	HIS	-	expression tag	UNP Q88M75
A	287	HIS	-	expression tag	UNP Q88M75
A	288	HIS	-	expression tag	UNP Q88M75
B	1	MSE	MET	modified residue	UNP Q88M75
B	4	MSE	MET	modified residue	UNP Q88M75
B	88	MSE	MET	modified residue	UNP Q88M75
B	101	MSE	MET	modified residue	UNP Q88M75
B	114	MSE	MET	modified residue	UNP Q88M75
B	118	MSE	MET	modified residue	UNP Q88M75
B	232	MSE	MET	modified residue	UNP Q88M75
B	281	LEU	-	cloning artifact	UNP Q88M75
B	282	GLU	-	cloning artifact	UNP Q88M75
B	283	HIS	-	expression tag	UNP Q88M75

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Chain	Residue	Modelled	Actual	Comment	Reference
B	284	HIS	-	expression tag	UNP Q88M75
B	285	HIS	-	expression tag	UNP Q88M75
B	286	HIS	-	expression tag	UNP Q88M75
B	287	HIS	-	expression tag	UNP Q88M75
B	288	HIS	-	expression tag	UNP Q88M75

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	26	26	26	0	0
3	B	29	29	29	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	43.39Å 46.29Å 64.08Å 80.86° 76.86° 80.61°	Depositor
Resolution (Å)	28.91 – 2.61 28.91 – 2.61	Depositor EDS
% Data completeness (in resolution range)	78.4 (28.91-2.61) 91.8 (28.91-2.61)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.93 (at 2.61Å)	Xtrriage
Refinement program	CNS 1.1, XTALVIEW	Depositor
R, R_{free}	0.228 , 0.287 0.249 , 0.298	Depositor DCC
R_{free} test set	2620 reflections (9.39%)	wwPDB-VP
Wilson B-factor (Å ²)	27.0	Xtrriage
Anisotropy	0.249	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 41.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	4331	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.27% 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: PO4

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	0.52	1/2177 (0.0%)	0.87	2/2944 (0.1%)
1	B	0.53	2/2177 (0.1%)	0.87	2/2944 (0.1%)
All	All	0.53	3/4354 (0.1%)	0.87	4/5888 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	114	MSE	SE-CE	-6.28	1.76	1.95
1	B	114	MSE	CG-SE	-5.89	1.77	1.95
1	B	114	MSE	SE-CE	-5.76	1.78	1.95

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	15	ILE	N-CA-C	6.71	117.55	107.75
1	A	15	ILE	N-CA-C	6.60	117.39	107.75
1	A	246	VAL	N-CA-C	5.49	117.30	108.85
1	B	246	VAL	N-CA-C	5.08	116.68	108.85

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	2133	0	2095	107	0
1	B	2133	0	2095	103	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
3	A	26	0	0	2	0
3	B	29	0	0	2	0
All	All	4331	0	4190	210	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 25.

All (210) 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:229:GLU:HG3	3:A:322:HOH:O	1.72	0.87
1:B:12:LEU:HD21	1:B:274:ARG:HD3	1.65	0.78
1:A:12:LEU:HD21	1:A:274:ARG:HD3	1.67	0.76
1:A:173:ALA:HB2	1:A:204:LEU:HB3	1.67	0.76
1:B:110:ARG:HD3	1:B:112:ASN:HB2	1.69	0.75
1:A:110:ARG:HD3	1:A:112:ASN:HB2	1.70	0.73
1:B:173:ALA:HB2	1:B:204:LEU:HB3	1.69	0.73
1:B:153:VAL:HG11	1:B:188:LEU:HD21	1.72	0.70
1:B:91:ARG:HD2	1:B:125:GLN:O	1.92	0.69
1:A:153:VAL:HG11	1:A:188:LEU:HD21	1.72	0.69
1:A:91:ARG:HD2	1:A:125:GLN:O	1.92	0.69
1:B:103:ARG:HD2	3:B:308:HOH:O	1.92	0.67
1:A:35:ALA:N	1:A:36:PRO:HD3	2.10	0.67
1:B:35:ALA:N	1:B:36:PRO:HD3	2.10	0.66
1:B:88:MSE:HE3	1:B:111:LEU:O	1.95	0.66
1:B:61:GLN:OE1	1:B:62:PRO:HD2	1.97	0.65
1:A:46:LEU:HD21	1:A:79:VAL:HG11	1.78	0.65
1:A:61:GLN:OE1	1:A:62:PRO:HD2	1.97	0.64
1:B:175:ARG:HB3	1:B:179:GLN:HG2	1.79	0.64
1:B:101:MSE:HB3	1:B:106:VAL:CG1	2.28	0.63
1:B:46:LEU:HD21	1:B:79:VAL:HG11	1.81	0.63
1:B:120:ASP:OD2	1:B:122:THR:HG22	2.00	0.62
1:B:157:GLN:N	1:B:158:PRO:HD2	2.14	0.62
1:B:143:HIS:HE1	1:B:170:ARG:HE	1.47	0.62
1:A:157:GLN:N	1:A:158:PRO:HD2	2.15	0.61
1:A:13:THR:HG22	1:A:55:SER:HB3	1.83	0.61
1:A:88:MSE:HE3	1:A:111:LEU:O	1.99	0.61
1:A:120:ASP:OD2	1:A:122:THR:HG22	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:LEU:H	1:A:113:LEU:HD22	1.65	0.61
1:B:15:ILE:HD13	1:B:279:PHE:CD2	2.35	0.61
1:B:12:LEU:HD11	1:B:15:ILE:HD11	1.84	0.60
1:A:110:ARG:HG3	1:A:141:GLU:HB3	1.85	0.59
1:A:175:ARG:HB3	1:A:179:GLN:HG2	1.84	0.59
1:A:101:MSE:HB3	1:A:106:VAL:CG1	2.32	0.59
1:B:113:LEU:HD22	1:B:113:LEU:H	1.68	0.59
1:A:15:ILE:HD13	1:A:279:PHE:CD2	2.36	0.59
1:A:143:HIS:HE1	1:A:170:ARG:HE	1.48	0.58
1:A:12:LEU:HD11	1:A:15:ILE:HD11	1.85	0.58
1:A:59:LEU:O	1:A:85:GLY:HA2	2.03	0.58
1:A:23:SER:HA	1:A:39:ASP:OD2	2.03	0.58
1:A:237:TRP:CG	1:A:238:PRO:HA	2.39	0.58
1:B:88:MSE:HG2	1:B:110:ARG:O	2.04	0.58
1:B:23:SER:HA	1:B:39:ASP:OD2	2.04	0.58
1:B:267:ALA:HA	1:B:271:ASP:HB2	1.86	0.58
1:A:88:MSE:HG2	1:A:110:ARG:O	2.04	0.57
1:B:227:GLY:O	1:B:231:LEU:HD13	2.03	0.57
1:A:168:PHE:CZ	1:A:198:VAL:HG23	2.39	0.57
1:B:219:LEU:HD12	1:B:258:LEU:HD13	1.85	0.57
1:B:59:LEU:O	1:B:85:GLY:HA2	2.04	0.57
1:B:110:ARG:HG3	1:B:141:GLU:HB3	1.85	0.57
1:A:219:LEU:HD12	1:A:258:LEU:HD13	1.87	0.57
1:A:267:ALA:HA	1:A:271:ASP:HB2	1.87	0.57
1:B:13:THR:HG22	1:B:55:SER:HB3	1.87	0.56
1:A:59:LEU:O	1:A:85:GLY:CA	2.53	0.56
1:A:227:GLY:O	1:A:231:LEU:HD13	2.04	0.56
1:B:42:LEU:HG	1:B:75:ALA:HB1	1.87	0.56
1:A:63:SER:OG	1:A:112:ASN:ND2	2.39	0.56
1:A:72:LEU:C	1:A:72:LEU:HD23	2.31	0.55
1:B:72:LEU:C	1:B:72:LEU:HD23	2.32	0.55
1:B:63:SER:OG	1:B:112:ASN:ND2	2.39	0.55
1:A:140:VAL:HG11	1:A:156:LEU:HD13	1.87	0.55
1:B:101:MSE:HB3	1:B:106:VAL:HG11	1.89	0.55
1:A:113:LEU:HD22	1:A:113:LEU:N	2.22	0.54
1:A:42:LEU:HG	1:A:75:ALA:HB1	1.88	0.54
1:B:140:VAL:HG11	1:B:156:LEU:HD13	1.90	0.54
1:B:237:TRP:CG	1:B:238:PRO:HA	2.42	0.54
1:A:67:THR:HG22	1:A:67:THR:O	2.08	0.54
1:B:264:LEU:HD22	1:B:268:LEU:HG	1.87	0.54
1:B:59:LEU:O	1:B:85:GLY:CA	2.55	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:ALA:N	1:A:36:PRO:CD	2.71	0.54
1:A:26:LEU:HG	3:A:327:HOH:O	2.06	0.54
1:B:168:PHE:CZ	1:B:198:VAL:HG23	2.43	0.53
1:A:13:THR:HG22	1:A:55:SER:CB	2.39	0.53
1:A:255:PHE:CZ	1:A:269:LEU:HD21	2.43	0.53
1:B:13:THR:HG22	1:B:55:SER:CB	2.39	0.53
1:B:35:ALA:N	1:B:36:PRO:CD	2.71	0.53
1:A:33:ARG:HH21	1:A:33:ARG:HG3	1.73	0.53
1:A:264:LEU:HD22	1:A:268:LEU:HG	1.90	0.53
1:B:113:LEU:HD22	1:B:113:LEU:N	2.24	0.52
1:A:230:ARG:C	1:A:231:LEU:HD12	2.35	0.52
1:B:33:ARG:HH21	1:B:33:ARG:HG3	1.75	0.52
1:A:18:HIS:HB2	1:A:197:LYS:HZ2	1.74	0.52
1:A:101:MSE:HB3	1:A:106:VAL:HG11	1.91	0.52
1:B:94:GLU:CD	1:B:97:THR:HG23	2.34	0.52
1:A:133:ILE:HD11	1:A:161:LEU:HD22	1.91	0.51
1:B:45:TYR:HB2	1:B:237:TRP:CZ3	2.45	0.51
1:B:67:THR:HG22	1:B:67:THR:O	2.10	0.51
1:A:231:LEU:O	1:A:268:LEU:HD23	2.09	0.51
1:B:218:ALA:O	1:B:222:LEU:HB2	2.10	0.51
1:B:255:PHE:CZ	1:B:269:LEU:HD21	2.46	0.51
1:A:175:ARG:HH21	1:A:180:PRO:HD3	1.75	0.51
1:B:53:GLY:O	1:B:54:PHE:C	2.54	0.51
1:A:77:GLN:HE21	1:A:104:LEU:HD22	1.76	0.51
1:A:172:ASP:HB3	1:A:175:ARG:HB2	1.92	0.50
1:B:230:ARG:C	1:B:231:LEU:HD12	2.36	0.50
1:B:101:MSE:HB3	1:B:106:VAL:HG13	1.94	0.50
1:A:146:VAL:HG22	1:A:181:GLY:C	2.36	0.50
1:B:133:ILE:HD11	1:B:161:LEU:HD22	1.92	0.50
1:B:146:VAL:HG22	1:B:181:GLY:C	2.37	0.49
1:A:45:TYR:HB2	1:A:237:TRP:CZ3	2.48	0.49
1:B:62:PRO:HG2	1:B:65:LEU:HD12	1.93	0.49
1:B:198:VAL:HG22	1:B:198:VAL:O	2.12	0.49
1:A:218:ALA:O	1:A:222:LEU:HB2	2.12	0.49
1:A:222:LEU:HB3	1:A:231:LEU:HD21	1.95	0.49
1:A:265:ARG:O	1:A:269:LEU:HG	2.13	0.49
1:B:172:ASP:HB3	1:B:175:ARG:HB2	1.93	0.49
1:B:175:ARG:HH21	1:B:180:PRO:HD3	1.77	0.49
1:B:24:ARG:H	1:B:39:ASP:CG	2.21	0.49
1:B:237:TRP:CD1	1:B:238:PRO:HA	2.47	0.49
1:B:248:PHE:O	1:B:252:VAL:HG23	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:LEU:HG	1:A:270:LEU:HD11	1.95	0.48
1:A:94:GLU:CD	1:A:97:THR:HG23	2.39	0.48
1:B:60:VAL:HG13	1:B:86:VAL:CG2	2.43	0.48
1:A:77:GLN:HE21	1:A:104:LEU:CD2	2.26	0.48
1:A:237:TRP:CD1	1:A:238:PRO:HA	2.48	0.48
1:A:53:GLY:O	1:A:54:PHE:C	2.57	0.47
1:B:85:GLY:O	1:B:106:VAL:HA	2.14	0.47
1:A:60:VAL:HG13	1:A:86:VAL:CG2	2.44	0.47
1:A:85:GLY:O	1:A:106:VAL:HA	2.14	0.47
1:A:274:ARG:HG2	1:A:274:ARG:HH21	1.79	0.47
1:B:132:ARG:HA	1:B:132:ARG:NE	2.29	0.47
1:A:60:VAL:HG22	1:A:86:VAL:HG22	1.96	0.47
1:A:198:VAL:O	1:A:198:VAL:HG22	2.13	0.47
1:B:222:LEU:HB3	1:B:231:LEU:HD21	1.96	0.47
1:A:48:GLN:HE21	1:A:248:PHE:HB2	1.80	0.47
1:A:279:PHE:O	1:A:281:LEU:N	2.48	0.47
1:B:265:ARG:O	1:B:269:LEU:HG	2.15	0.47
1:B:113:LEU:O	1:B:114:MSE:C	2.57	0.47
1:B:231:LEU:O	1:B:268:LEU:HD23	2.15	0.47
1:B:196:VAL:HG13	1:B:231:LEU:HG	1.97	0.46
1:B:62:PRO:CG	1:B:65:LEU:HD12	2.45	0.46
1:A:132:ARG:NE	1:A:132:ARG:HA	2.31	0.46
1:A:223:GLU:O	1:A:223:GLU:HG2	2.16	0.46
1:A:248:PHE:O	1:A:252:VAL:HG23	2.16	0.46
1:B:13:THR:HG22	1:B:55:SER:OG	2.16	0.46
1:B:129:LEU:O	1:B:133:ILE:HG23	2.15	0.46
1:A:129:LEU:O	1:A:133:ILE:HG23	2.15	0.46
1:B:179:GLN:HB3	1:B:180:PRO:HD2	1.97	0.45
1:A:201:ILE:C	1:A:203:ARG:H	2.24	0.45
1:B:175:ARG:HB3	1:B:179:GLN:CG	2.45	0.45
1:A:113:LEU:O	1:A:114:MSE:C	2.60	0.45
1:B:77:GLN:HE21	1:B:104:LEU:CD2	2.30	0.45
1:A:231:LEU:HD12	1:A:231:LEU:N	2.32	0.44
1:A:101:MSE:HB3	1:A:106:VAL:HG13	1.99	0.44
1:B:12:LEU:HG	1:B:270:LEU:HD11	1.98	0.44
1:B:77:GLN:HE21	1:B:104:LEU:HD22	1.81	0.44
1:B:155:ALA:HB2	3:B:326:HOH:O	2.16	0.44
1:B:100:GLU:O	1:B:104:LEU:HG	2.18	0.44
1:A:196:VAL:HG13	1:A:231:LEU:HG	1.99	0.44
1:B:18:HIS:HB2	1:B:197:LYS:HZ2	1.81	0.44
1:B:274:ARG:HG2	1:B:274:ARG:HH21	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:VAL:HG23	1:A:79:VAL:O	2.17	0.43
1:B:76:LEU:HD21	1:B:84:ARG:O	2.18	0.43
1:B:16:ASP:OD2	1:B:16:ASP:C	2.61	0.43
1:A:24:ARG:H	1:A:39:ASP:CG	2.25	0.43
1:A:139:HIS:CD2	1:A:164:VAL:HG21	2.52	0.43
1:A:144:ARG:HH12	1:A:145:GLN:HE22	1.66	0.43
1:B:146:VAL:HG13	1:B:181:GLY:HA3	1.99	0.43
1:B:252:VAL:O	1:B:255:PHE:HB3	2.18	0.43
1:A:146:VAL:HG13	1:A:181:GLY:HA3	2.00	0.43
1:B:14:ALA:HB3	1:B:54:PHE:HA	2.01	0.43
1:B:231:LEU:HD12	1:B:231:LEU:N	2.34	0.42
1:B:279:PHE:O	1:B:281:LEU:N	2.52	0.42
1:A:16:ASP:OD2	1:A:16:ASP:C	2.63	0.42
1:B:42:LEU:HD22	1:B:46:LEU:HD13	2.00	0.42
1:B:94:GLU:OE2	1:B:94:GLU:N	2.45	0.42
1:A:95:GLN:HE21	1:A:95:GLN:HA	1.85	0.42
1:B:15:ILE:HG12	1:B:56:HIS:HB2	2.02	0.42
1:B:139:HIS:HB3	1:B:162:ASP:HB2	2.01	0.42
1:A:142:LEU:HD12	1:A:142:LEU:HA	1.92	0.42
1:B:139:HIS:CD2	1:B:164:VAL:HG21	2.55	0.42
1:A:76:LEU:HD21	1:A:84:ARG:O	2.19	0.42
1:B:201:ILE:O	1:B:204:LEU:HD22	2.19	0.42
1:A:14:ALA:HB3	1:A:54:PHE:HA	2.02	0.42
1:B:127:ARG:N	1:B:128:PRO:CD	2.83	0.41
1:B:201:ILE:C	1:B:203:ARG:H	2.27	0.41
1:A:15:ILE:HG12	1:A:56:HIS:HB2	2.02	0.41
1:A:94:GLU:OE2	1:A:94:GLU:N	2.42	0.41
1:A:42:LEU:HD22	1:A:46:LEU:HD13	2.01	0.41
1:A:139:HIS:HB3	1:A:162:ASP:HB2	2.02	0.41
1:A:201:ILE:HG13	1:A:202:TYR:N	2.35	0.41
1:A:255:PHE:CE2	1:A:269:LEU:HD21	2.55	0.41
1:B:60:VAL:HG22	1:B:86:VAL:HG22	2.01	0.41
1:A:17:SER:OG	1:A:232:MSE:HG3	2.20	0.41
1:A:62:PRO:HG2	1:A:65:LEU:HD12	2.01	0.41
1:A:33:ARG:HG3	1:A:33:ARG:NH2	2.35	0.41
1:A:76:LEU:HD12	1:A:76:LEU:HA	1.84	0.41
1:A:127:ARG:N	1:A:128:PRO:CD	2.83	0.41
1:A:170:ARG:HH21	1:A:170:ARG:HG3	1.85	0.41
1:A:195:TRP:CE2	1:A:276:LEU:HD13	2.55	0.41
1:A:201:ILE:O	1:A:204:LEU:HD22	2.21	0.41
1:B:33:ARG:HG3	1:B:33:ARG:NH2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:154:ARG:HA	1:B:157:GLN:HB2	2.02	0.41
1:B:144:ARG:HH12	1:B:145:GLN:HE22	1.67	0.41
1:A:167:HIS:C	1:A:169:GLY:H	2.28	0.41
1:A:176:GLY:O	1:A:179:GLN:HG3	2.21	0.41
1:A:240:THR:O	1:A:241:GLN:HB2	2.20	0.41
1:B:79:VAL:HG23	1:B:79:VAL:O	2.21	0.41
1:B:223:GLU:O	1:B:223:GLU:HG2	2.19	0.41
1:A:60:VAL:HA	1:A:86:VAL:HG22	2.03	0.41
1:A:100:GLU:O	1:A:104:LEU:HG	2.21	0.41
1:B:195:TRP:CE2	1:B:276:LEU:HD13	2.56	0.41
1:B:233:TRP:CH2	1:B:235:SER:HB3	2.55	0.41
1:B:176:GLY:O	1:B:179:GLN:HG3	2.20	0.40
1:B:255:PHE:CE2	1:B:269:LEU:HD21	2.57	0.40
1:B:17:SER:O	1:B:234:GLY:HA2	2.20	0.40
1:A:233:TRP:CH2	1:A:235:SER:HB3	2.56	0.40
1:A:167:HIS:C	1:A:169:GLY:N	2.78	0.40
1:A:252:VAL:O	1:A:256:GLU:HG2	2.21	0.40
1:B:157:GLN:N	1:B:158:PRO:CD	2.83	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	271/288 (94%)	229 (84%)	33 (12%)	9 (3%)	3	4
1	B	271/288 (94%)	231 (85%)	31 (11%)	9 (3%)	3	4
All	All	542/576 (94%)	460 (85%)	64 (12%)	18 (3%)	3	4

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	34	TYR
1	A	280	GLU
1	B	34	TYR
1	B	114	MSE
1	B	280	GLU
1	A	54	PHE
1	A	114	MSE
1	B	54	PHE
1	B	85	GLY
1	A	31	GLN
1	A	36	PRO
1	A	85	GLY
1	B	36	PRO
1	A	204	LEU
1	B	31	GLN
1	B	204	LEU
1	A	112	ASN
1	B	112	ASN

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	217/224 (97%)	196 (90%)	21 (10%)	8	16
1	B	217/224 (97%)	195 (90%)	22 (10%)	7	14
All	All	434/448 (97%)	391 (90%)	43 (10%)	7	15

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	ARG
1	A	36	PRO
1	A	42	LEU
1	A	46	LEU
1	A	76	LEU
1	A	86	VAL

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Mol	Chain	Res	Type
1	A	106	VAL
1	A	113	LEU
1	A	133	ILE
1	A	140	VAL
1	A	142	LEU
1	A	145	GLN
1	A	161	LEU
1	A	172	ASP
1	A	194	VAL
1	A	198	VAL
1	A	204	LEU
1	A	219	LEU
1	A	222	LEU
1	A	245	GLU
1	A	264	LEU
1	B	33	ARG
1	B	36	PRO
1	B	42	LEU
1	B	46	LEU
1	B	76	LEU
1	B	86	VAL
1	B	106	VAL
1	B	113	LEU
1	B	133	ILE
1	B	140	VAL
1	B	142	LEU
1	B	145	GLN
1	B	161	LEU
1	B	172	ASP
1	B	194	VAL
1	B	198	VAL
1	B	204	LEU
1	B	205	GLN
1	B	219	LEU
1	B	222	LEU
1	B	245	GLU
1	B	264	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	HIS

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Mol	Chain	Res	Type
1	A	48	GLN
1	A	77	GLN
1	A	82	GLN
1	A	112	ASN
1	A	116	GLN
1	A	143	HIS
1	A	217	GLN
1	A	239	HIS
1	A	254	GLN
1	B	11	HIS
1	B	18	HIS
1	B	27	ASN
1	B	48	GLN
1	B	77	GLN
1	B	112	ASN
1	B	116	GLN
1	B	143	HIS
1	B	217	GLN
1	B	254	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 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	PO4	B	302	-	4,4,4	1.88	2 (50%)	6,6,6	0.46	0
2	PO4	A	301	-	4,4,4	1.78	2 (50%)	6,6,6	0.47	0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	302	PO4	P-O3	-2.25	1.48	1.54
2	B	302	PO4	P-O2	-2.14	1.48	1.54
2	A	301	PO4	P-O3	-2.07	1.48	1.54
2	A	301	PO4	P-O4	-2.01	1.48	1.54

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	268/288 (93%)	0.71	24 (8%) 15 12	5, 23, 47, 51	0
1	B	268/288 (93%)	0.81	29 (10%) 11 8	4, 24, 48, 54	0
All	All	536/576 (93%)	0.76	53 (9%) 13 10	4, 24, 48, 54	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	25	GLY	9.1
1	B	39	ASP	5.4
1	B	30	SER	4.9
1	A	26	LEU	4.5
1	B	28	LEU	4.2
1	B	26	LEU	4.0
1	A	91	ARG	3.8
1	B	24	ARG	3.8
1	B	36	PRO	3.7
1	B	27	ASN	3.7
1	B	32	ARG	3.6
1	A	29	ALA	3.5
1	A	35	ALA	3.5
1	B	35	ALA	3.4
1	A	34	TYR	3.3
1	B	23	SER	3.2
1	B	29	ALA	3.1
1	A	175	ARG	3.0
1	B	34	TYR	3.0
1	A	25	GLY	3.0
1	A	112	ASN	2.9
1	A	282	GLU	2.9
1	A	36	PRO	2.9
1	B	280	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	281	LEU	2.8
1	B	117	ASP	2.7
1	A	281	LEU	2.7
1	A	33	ARG	2.6
1	B	85	GLY	2.5
1	B	189	SER	2.4
1	B	37	ASN	2.3
1	B	119	PRO	2.3
1	B	229	GLU	2.2
1	A	85	GLY	2.2
1	A	39	ASP	2.2
1	A	81	GLY	2.2
1	A	116	GLN	2.2
1	B	31	GLN	2.2
1	B	79	VAL	2.2
1	A	229	GLU	2.1
1	A	190	GLY	2.1
1	B	262	ALA	2.1
1	A	180	PRO	2.1
1	A	259	GLY	2.1
1	A	125	GLN	2.1
1	B	123	GLY	2.1
1	A	224	ALA	2.1
1	B	38	TYR	2.1
1	A	216	ARG	2.0
1	A	266	GLN	2.0
1	B	10	LEU	2.0
1	B	115	GLY	2.0
1	B	282	GLU	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(Å ²)	Q<0.9
2	PO4	B	302	5/5	0.96	0.07	15,18,18,21	0
2	PO4	A	301	5/5	0.97	0.07	15,16,17,18	0

6.5 Other polymers [i](#)

There are no such residues in this entry.