



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:27 PM UTC

PDB ID : 1QEZ / pdb_00001qez
Title : SULFOLOBUS ACIDOCALDARIUS INORGANIC PYROPHOSPHATASE:
AN ARCHAEL PYROPHOSPHATASE.
Authors : Leppanen, V.-M.; Nummelin, H.; Hansen, T.; Lahti, R.; Schafer, G.; Goldman, A.
Deposited on : 1999-04-06
Resolution : 2.70 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
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

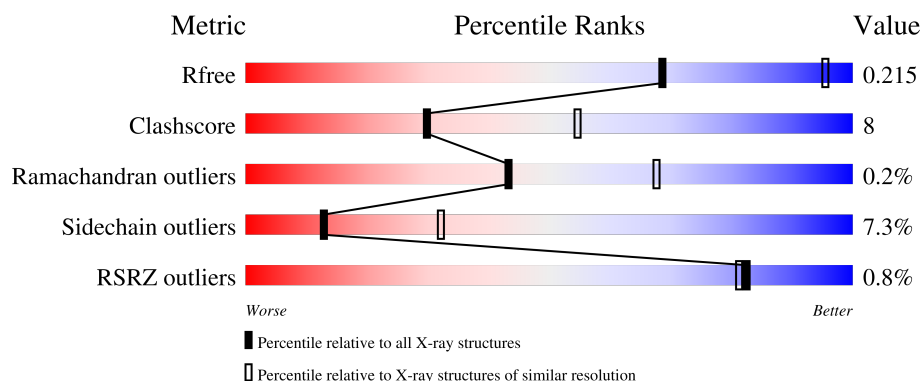
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	173	2% 76% 19% ..
1	B	173	2% 79% 17% ..
1	C	173	2% 76% 20% ..
1	D	173	73% 22% ..
1	E	173	2% 77% 19% ..

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Mol	Chain	Length	Quality of chain
1	F	173	% 74% 20% 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8028 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 PROTEIN (INORGANIC PYROPHOSPHATASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	170	Total	C	N	O	S	0	0	1
			1316	843	210	261	2			
1	B	170	Total	C	N	O	S	0	0	1
			1327	850	213	262	2			
1	C	170	Total	C	N	O	S	0	0	1
			1319	844	211	262	2			
1	D	170	Total	C	N	O	S	0	0	1
			1327	850	213	262	2			
1	E	170	Total	C	N	O	S	0	0	1
			1327	850	213	262	2			
1	F	170	Total	C	N	O	S	0	0	1
			1331	853	214	262	2			

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		
2	D	1	Total	Mg	0	0
			1	1		
2	E	1	Total	Mg	0	0
			1	1		
2	F	1	Total	Mg	0	0
			1	1		

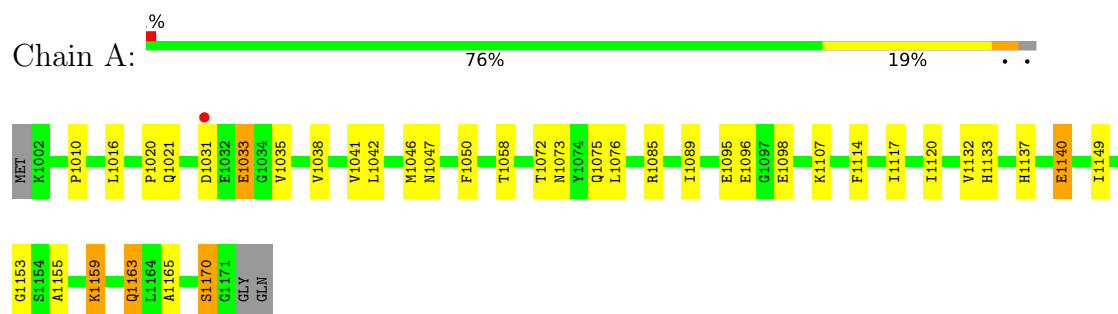
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	12	Total 12	O 12	0	0
3	B	13	Total 13	O 13	0	0
3	C	10	Total 10	O 10	0	0
3	D	14	Total 14	O 14	0	0
3	E	13	Total 13	O 13	0	0
3	F	13	Total 13	O 13	0	0

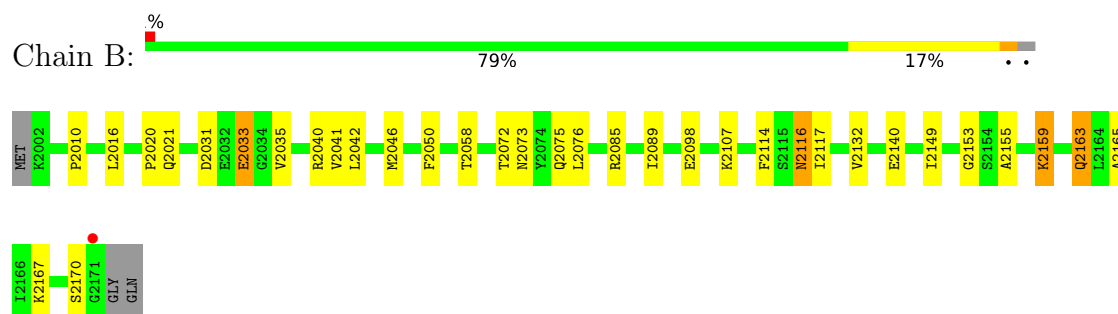
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

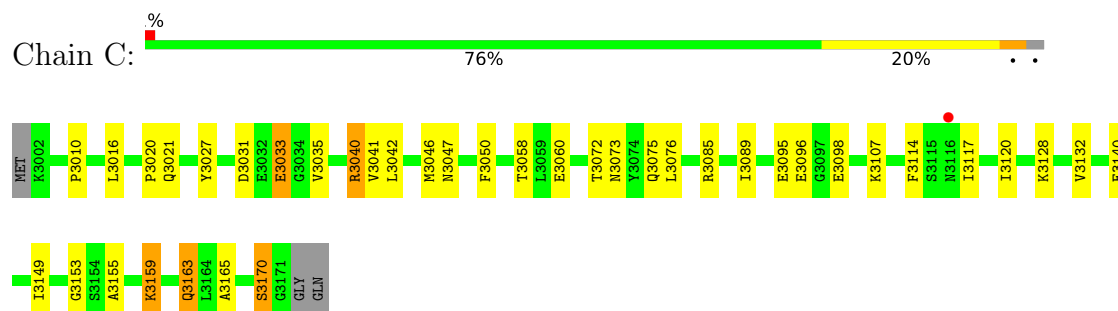
- Molecule 1: PROTEIN (INORGANIC PYROPHOSPHATASE)



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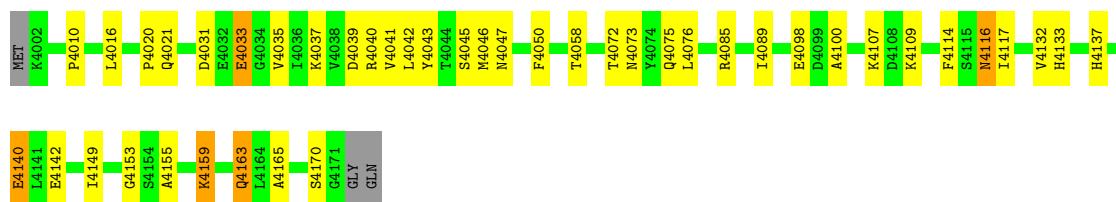


- Molecule 1: PROTEIN (INORGANIC PYROPHOSPHATASE)

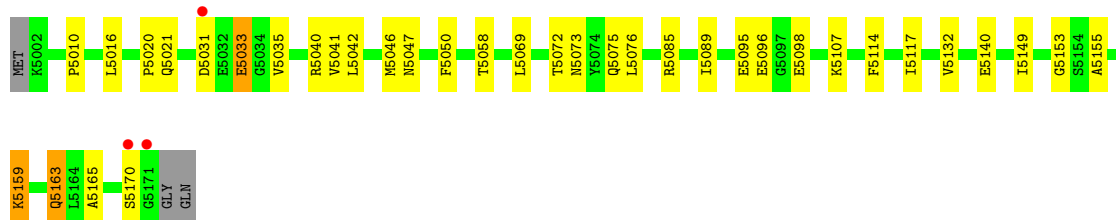
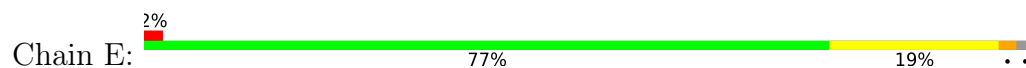


- Molecule 1: PROTEIN (INORGANIC PYROPHOSPHATASE)

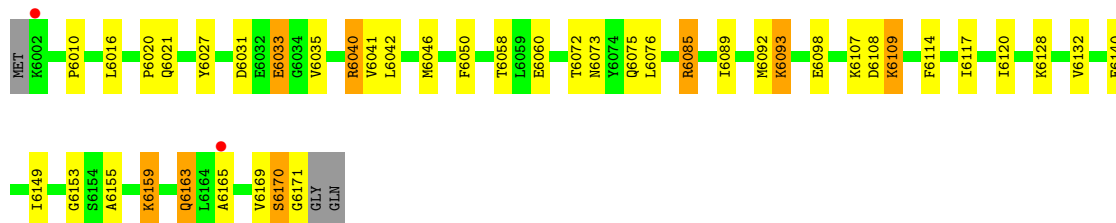
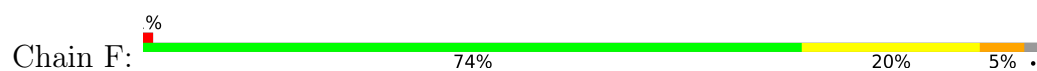




• Molecule 1: PROTEIN (INORGANIC PYROPHOSPHATASE)



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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	70.12Å 98.73Å 107.25Å 90.00° 78.01° 90.00°	Depositor
Resolution (Å)	8.00 – 2.70 8.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	92.2 (8.00-2.70) 90.7 (8.00-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.197 , 0.239 0.181 , 0.215	Depositor DCC
R_{free} test set	3790 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å ²)	(Not available)	Xtriage
Anisotropy	(Not available)	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 68.1	EDS
L-test for twinning ¹	$\langle L \rangle =$ (Not available), $\langle L^2 \rangle =$ (Not available)	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8028	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *(Not available)*

¹Theoretical 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG

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	0.45	1/1346 (0.1%)	0.81	0/1836
1	B	0.49	1/1357 (0.1%)	0.82	0/1848
1	C	0.46	1/1349 (0.1%)	0.81	0/1840
1	D	0.44	1/1357 (0.1%)	0.81	0/1848
1	E	0.47	1/1357 (0.1%)	0.81	0/1848
1	F	0.45	1/1361 (0.1%)	0.81	0/1852
All	All	0.46	6/8127 (0.1%)	0.81	0/11072

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	2170	SER	C-N	-7.09	1.23	1.33
1	E	5170	SER	C-N	-5.74	1.25	1.33
1	C	3170	SER	C-N	-5.72	1.25	1.33
1	F	6170	SER	C-N	-5.46	1.25	1.33
1	A	1170	SER	C-N	-5.40	1.25	1.33
1	D	4170	SER	C-N	-5.33	1.25	1.33

There are no bond angle outliers.

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	1316	0	1266	27	0
1	B	1327	0	1292	18	0
1	C	1319	0	1270	24	0
1	D	1327	0	1292	34	0
1	E	1327	0	1292	21	0
1	F	1331	0	1303	29	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	12	0	0	0	0
3	B	13	0	0	0	0
3	C	10	0	0	2	0
3	D	14	0	0	1	0
3	E	13	0	0	0	0
3	F	13	0	0	2	0
All	All	8028	0	7715	133	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 8.

All (133) 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:B:2116:ASN:HD22	1:B:2116:ASN:H	1.21	0.88
1:D:4109:LYS:HE3	1:E:5040:ARG:HH22	1.39	0.88
1:D:4116:ASN:ND2	1:D:4116:ASN:H	1.86	0.72
1:C:3163:GLN:HE21	1:C:3163:GLN:HA	1.53	0.72
1:D:4085:ARG:NH2	1:D:4117:ILE:O	2.24	0.70
1:A:1085:ARG:NH2	1:A:1117:ILE:O	2.26	0.69
1:D:4116:ASN:H	1:D:4116:ASN:HD22	1.41	0.69
1:D:4109:LYS:CE	1:E:5040:ARG:HH22	2.06	0.68
1:C:3085:ARG:NH2	1:C:3117:ILE:O	2.27	0.67
1:E:5085:ARG:NH2	1:E:5117:ILE:O	2.27	0.67
1:F:6109:LYS:HZ2	1:F:6109:LYS:H	1.41	0.67
1:F:6021:GLN:HE21	1:F:6050:PHE:HA	1.60	0.67
1:B:2085:ARG:NH2	1:B:2117:ILE:O	2.27	0.67
1:F:6085:ARG:NH2	1:F:6117:ILE:O	2.28	0.66
1:A:1021:GLN:HE21	1:A:1050:PHE:HA	1.60	0.65
1:C:3021:GLN:HE21	1:C:3050:PHE:HA	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2021:GLN:HE21	1:B:2050:PHE:HA	1.62	0.65
1:B:2116:ASN:HD22	1:B:2116:ASN:N	1.88	0.64
1:B:2163:GLN:HE21	1:B:2163:GLN:HA	1.62	0.64
1:E:5021:GLN:HE21	1:E:5050:PHE:HA	1.62	0.64
1:D:4039:ASP:OD2	1:D:4040:ARG:HG2	1.97	0.63
1:A:1163:GLN:HE21	1:A:1163:GLN:HA	1.64	0.63
1:D:4021:GLN:HE21	1:D:4050:PHE:HA	1.62	0.62
1:F:6163:GLN:HA	1:F:6163:GLN:HE21	1.63	0.62
1:E:5163:GLN:HA	1:E:5163:GLN:HE21	1.63	0.62
1:C:3132:VAL:HG13	1:C:3149:ILE:HG13	1.82	0.62
1:F:6027:TYR:OH	3:F:7020:HOH:O	2.16	0.62
1:F:6109:LYS:H	1:F:6109:LYS:NZ	1.98	0.62
1:A:1046:MET:HG2	1:D:4046:MET:HE3	1.81	0.61
1:D:4163:GLN:HE21	1:D:4163:GLN:HA	1.64	0.61
1:F:6132:VAL:HG13	1:F:6149:ILE:HG13	1.81	0.61
1:A:1132:VAL:HG13	1:A:1149:ILE:HG13	1.84	0.59
1:B:2046:MET:HE3	1:F:6046:MET:HG2	1.84	0.59
1:B:2116:ASN:H	1:B:2116:ASN:ND2	1.96	0.58
1:E:5132:VAL:HG13	1:E:5149:ILE:HG13	1.85	0.58
1:A:1046:MET:HE3	1:D:4046:MET:HG2	1.86	0.58
1:B:2132:VAL:HG13	1:B:2149:ILE:HG13	1.85	0.57
1:C:3010:PRO:HG3	1:C:3163:GLN:HG2	1.86	0.57
1:F:6010:PRO:HG3	1:F:6163:GLN:HG2	1.87	0.57
1:C:3033:GLU:HB2	1:C:3035:VAL:HG22	1.87	0.57
1:A:1046:MET:HE3	1:D:4046:MET:HE3	1.86	0.56
1:D:4132:VAL:HG13	1:D:4149:ILE:HG13	1.85	0.56
1:D:4010:PRO:HG3	1:D:4163:GLN:HG2	1.88	0.56
1:F:6033:GLU:HB2	1:F:6035:VAL:HG22	1.88	0.56
1:F:6040:ARG:HH11	1:F:6040:ARG:HG3	1.71	0.56
1:D:4033:GLU:HB2	1:D:4035:VAL:HG22	1.88	0.55
1:C:3046:MET:HG2	1:E:5046:MET:HE3	1.87	0.55
1:A:1033:GLU:HB2	1:A:1035:VAL:HG22	1.88	0.55
1:A:1010:PRO:HG3	1:A:1163:GLN:HG2	1.89	0.55
1:B:2033:GLU:HB2	1:B:2035:VAL:HG22	1.89	0.55
1:E:5033:GLU:HB2	1:E:5035:VAL:HG22	1.89	0.55
1:C:3046:MET:HE3	1:E:5046:MET:HG2	1.88	0.54
1:E:5010:PRO:HG3	1:E:5163:GLN:HG2	1.89	0.54
1:C:3027:TYR:OH	3:C:7026:HOH:O	2.18	0.54
1:F:6169:VAL:O	1:F:6171:GLY:N	2.41	0.53
1:B:2010:PRO:HG3	1:B:2163:GLN:HG2	1.91	0.52
1:F:6108:ASP:HB2	1:F:6109:LYS:HZ1	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4040:ARG:NE	1:D:4142:GLU:OE2	2.43	0.51
1:F:6040:ARG:HH11	1:F:6040:ARG:CG	2.23	0.51
1:F:6060:GLU:HB2	3:F:7015:HOH:O	2.11	0.50
1:A:1046:MET:HG2	1:D:4046:MET:CE	2.43	0.48
1:A:1046:MET:HA	1:D:4046:MET:HA	1.95	0.48
1:A:1089:ILE:CG2	1:A:1153:GLY:HA3	2.43	0.48
1:A:1155:ALA:O	1:A:1159:LYS:HD3	2.14	0.47
1:B:2046:MET:HG2	1:F:6046:MET:HE3	1.95	0.47
1:C:3060:GLU:HB2	3:C:7032:HOH:O	2.14	0.47
1:A:1137:HIS:CE1	1:D:4137:HIS:CE1	3.02	0.47
1:B:2041:VAL:O	1:B:2042:LEU:C	2.57	0.47
1:C:3041:VAL:O	1:C:3042:LEU:C	2.57	0.47
1:D:4045:SER:HB3	3:D:7053:HOH:O	2.14	0.47
1:E:5041:VAL:O	1:E:5042:LEU:C	2.57	0.47
1:C:3040:ARG:CZ	1:C:3040:ARG:CB	2.94	0.46
1:D:4089:ILE:CG2	1:D:4153:GLY:HA3	2.46	0.46
1:C:3020:PRO:HB3	1:C:3076:LEU:O	2.16	0.46
1:F:6041:VAL:O	1:F:6042:LEU:C	2.58	0.46
1:B:2089:ILE:CG2	1:B:2153:GLY:HA3	2.46	0.45
1:C:3155:ALA:O	1:C:3159:LYS:HD3	2.16	0.45
1:E:5155:ALA:O	1:E:5159:LYS:HD3	2.15	0.45
1:D:4020:PRO:HB3	1:D:4076:LEU:O	2.16	0.45
1:F:6093:LYS:HE2	1:F:6093:LYS:HB3	1.72	0.45
1:A:1016:LEU:HD23	1:A:1016:LEU:C	2.42	0.45
1:B:2020:PRO:HB3	1:B:2076:LEU:O	2.17	0.45
1:E:5020:PRO:HB3	1:E:5076:LEU:O	2.17	0.45
1:E:5089:ILE:CG2	1:E:5153:GLY:HA3	2.46	0.45
1:B:2155:ALA:O	1:B:2159:LYS:HD3	2.15	0.45
1:D:4016:LEU:C	1:D:4016:LEU:HD23	2.42	0.45
1:D:4155:ALA:O	1:D:4159:LYS:HD3	2.16	0.45
1:A:1046:MET:CE	1:D:4046:MET:HG2	2.47	0.45
1:C:3016:LEU:C	1:C:3016:LEU:HD23	2.42	0.45
1:B:2016:LEU:HD23	1:B:2016:LEU:C	2.42	0.45
1:A:1041:VAL:O	1:A:1042:LEU:C	2.59	0.45
1:C:3047:ASN:OD1	1:E:5047:ASN:OD1	2.35	0.44
1:D:4033:GLU:HG3	1:D:4037:LYS:HZ1	1.82	0.44
1:F:6089:ILE:CG2	1:F:6153:GLY:HA3	2.48	0.44
1:F:6020:PRO:HB3	1:F:6076:LEU:O	2.18	0.44
1:C:3089:ILE:CG2	1:C:3153:GLY:HA3	2.48	0.44
1:D:4041:VAL:O	1:D:4042:LEU:C	2.60	0.44
1:F:6155:ALA:O	1:F:6159:LYS:HD3	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4043:TYR:OH	1:F:6109:LYS:O	2.32	0.43
1:D:4072:THR:HA	1:D:4114:PHE:CZ	2.54	0.43
1:E:5016:LEU:C	1:E:5016:LEU:HD23	2.43	0.43
1:D:4109:LYS:HE2	1:D:4109:LYS:HB3	1.84	0.43
1:F:6040:ARG:CG	1:F:6040:ARG:NH1	2.82	0.43
1:A:1020:PRO:HB3	1:A:1076:LEU:O	2.19	0.43
1:C:3058:THR:HB	1:C:3165:ALA:HB1	2.00	0.42
1:C:3072:THR:HA	1:C:3114:PHE:CZ	2.54	0.42
1:A:1058:THR:HB	1:A:1165:ALA:HB1	2.01	0.42
1:B:2058:THR:HB	1:B:2165:ALA:HB1	2.01	0.42
1:A:1072:THR:HA	1:A:1114:PHE:CZ	2.55	0.42
1:D:4089:ILE:HD11	1:D:4100:ALA:HB1	2.01	0.42
1:F:6016:LEU:C	1:F:6016:LEU:HD23	2.44	0.42
1:E:5058:THR:HB	1:E:5165:ALA:HB1	2.01	0.42
1:D:4058:THR:HB	1:D:4165:ALA:HB1	2.02	0.41
1:A:1038:VAL:HG21	1:C:3076:LEU:HD22	2.03	0.41
1:A:1095:GLU:HG2	1:A:1096:GLU:HG2	2.02	0.41
1:F:6092:MET:HE2	1:F:6092:MET:HB3	1.97	0.41
1:F:6120:ILE:O	1:F:6128:LYS:HE2	2.20	0.41
1:B:2072:THR:HA	1:B:2114:PHE:CZ	2.55	0.41
1:A:1133:HIS:NE2	1:D:4140:GLU:OE1	2.53	0.41
1:A:1140:GLU:OE1	1:D:4133:HIS:NE2	2.53	0.41
1:F:6058:THR:HB	1:F:6165:ALA:HB1	2.01	0.41
1:C:3163:GLN:HE21	1:C:3163:GLN:CA	2.27	0.41
1:E:5072:THR:HA	1:E:5114:PHE:CZ	2.55	0.41
1:F:6163:GLN:HE21	1:F:6163:GLN:CA	2.32	0.41
1:A:1047:ASN:OD1	1:D:4047:ASN:OD1	2.38	0.41
1:C:3046:MET:HE3	1:E:5046:MET:HE3	2.03	0.41
1:E:5095:GLU:HG2	1:E:5096:GLU:HG2	2.03	0.41
1:C:3095:GLU:HG2	1:C:3096:GLU:HG2	2.03	0.40
1:F:6072:THR:HA	1:F:6114:PHE:CZ	2.56	0.40
1:A:1089:ILE:HG22	1:A:1153:GLY:HA3	2.02	0.40
1:A:1120:ILE:HD12	1:A:1120:ILE:HA	1.95	0.40
1:E:5050:PHE:CE1	1:E:5069:LEU:HG	2.56	0.40
1:C:3120:ILE:O	1:C:3128:LYS:HE2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	168/173 (97%)	165 (98%)	3 (2%)	0	100	100
1	B	168/173 (97%)	163 (97%)	5 (3%)	0	100	100
1	C	168/173 (97%)	164 (98%)	3 (2%)	1 (1%)	21	44
1	D	168/173 (97%)	164 (98%)	4 (2%)	0	100	100
1	E	168/173 (97%)	164 (98%)	4 (2%)	0	100	100
1	F	168/173 (97%)	164 (98%)	3 (2%)	1 (1%)	21	44
All	All	1008/1038 (97%)	984 (98%)	22 (2%)	2 (0%)	43	68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	6170	SER
1	C	3170	SER

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	143/152 (94%)	133 (93%)	10 (7%)	14	34
1	B	146/152 (96%)	134 (92%)	12 (8%)	10	27
1	C	144/152 (95%)	134 (93%)	10 (7%)	14	34
1	D	146/152 (96%)	136 (93%)	10 (7%)	14	35
1	E	146/152 (96%)	137 (94%)	9 (6%)	16	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	147/152 (97%)	134 (91%)	13 (9%)	9	23
All	All	872/912 (96%)	808 (93%)	64 (7%)	13	32

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1031	ASP
1	A	1033	GLU
1	A	1073	ASN
1	A	1075	GLN
1	A	1098	GLU
1	A	1107	LYS
1	A	1140	GLU
1	A	1159	LYS
1	A	1163	GLN
1	A	1170	SER
1	B	2031	ASP
1	B	2033	GLU
1	B	2040	ARG
1	B	2073	ASN
1	B	2075	GLN
1	B	2098	GLU
1	B	2107	LYS
1	B	2116	ASN
1	B	2140	GLU
1	B	2159	LYS
1	B	2163	GLN
1	B	2167	LYS
1	C	3031	ASP
1	C	3033	GLU
1	C	3040	ARG
1	C	3073	ASN
1	C	3075	GLN
1	C	3098	GLU
1	C	3107	LYS
1	C	3140	GLU
1	C	3159	LYS
1	C	3163	GLN
1	D	4031	ASP
1	D	4033	GLU
1	D	4073	ASN
1	D	4075	GLN

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Mol	Chain	Res	Type
1	D	4098	GLU
1	D	4107	LYS
1	D	4116	ASN
1	D	4140	GLU
1	D	4159	LYS
1	D	4163	GLN
1	E	5031	ASP
1	E	5033	GLU
1	E	5073	ASN
1	E	5075	GLN
1	E	5098	GLU
1	E	5107	LYS
1	E	5140	GLU
1	E	5159	LYS
1	E	5163	GLN
1	F	6031	ASP
1	F	6033	GLU
1	F	6040	ARG
1	F	6073	ASN
1	F	6075	GLN
1	F	6085	ARG
1	F	6093	LYS
1	F	6098	GLU
1	F	6107	LYS
1	F	6109	LYS
1	F	6140	GLU
1	F	6159	LYS
1	F	6163	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1021	GLN
1	A	1024	ASN
1	A	1047	ASN
1	A	1160	ASN
1	A	1163	GLN
1	B	2021	GLN
1	B	2047	ASN
1	B	2116	ASN
1	B	2160	ASN
1	B	2163	GLN

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Mol	Chain	Res	Type
1	C	3021	GLN
1	C	3116	ASN
1	C	3160	ASN
1	C	3163	GLN
1	D	4021	GLN
1	D	4024	ASN
1	D	4116	ASN
1	D	4160	ASN
1	D	4163	GLN
1	E	5021	GLN
1	E	5047	ASN
1	E	5125	GLN
1	E	5160	ASN
1	E	5163	GLN
1	F	6021	GLN
1	F	6160	ASN
1	F	6163	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](#)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	170/173 (98%)	-0.39	1 (0%) 85 85	17, 37, 77, 100	0
1	B	170/173 (98%)	-0.66	1 (0%) 85 85	8, 23, 55, 95	0
1	C	170/173 (98%)	-0.52	1 (0%) 85 85	16, 35, 84, 100	0
1	D	170/173 (98%)	-0.38	0 100 100	19, 41, 89, 100	0
1	E	170/173 (98%)	-0.56	3 (1%) 67 65	11, 30, 79, 93	0
1	F	170/173 (98%)	-0.39	2 (1%) 76 75	11, 35, 73, 98	0
All	All	1020/1038 (98%)	-0.48	8 (0%) 82 81	8, 34, 82, 100	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2171	GLY	3.6
1	E	5171	GLY	3.1
1	E	5031	ASP	2.8
1	C	3116	ASN	2.6
1	F	6002	LYS	2.4
1	E	5170	SER	2.4
1	A	1031	ASP	2.2
1	F	6165	ALA	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	MG	D	4201	1/1	0.13	0.09	39,39,39,39	0
2	MG	C	3201	1/1	0.86	0.04	28,28,28,28	0
2	MG	A	1201	1/1	0.88	0.04	44,44,44,44	0
2	MG	F	6201	1/1	0.92	0.03	38,38,38,38	0
2	MG	B	2201	1/1	0.95	0.04	22,22,22,22	0
2	MG	E	5201	1/1	0.96	0.05	19,19,19,19	0

6.5 Other polymers [i](#)

There are no such residues in this entry.