



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:48 PM UTC

PDB ID : 7M1L / pdb_00007m1l
Title : Crystal structure of Pseudomonas aeruginosa ClpP2
Authors : Hall, B.M.; Grant, R.A.; Baker, T.A.; Sauer, R.T.
Deposited on : 2021-03-13
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

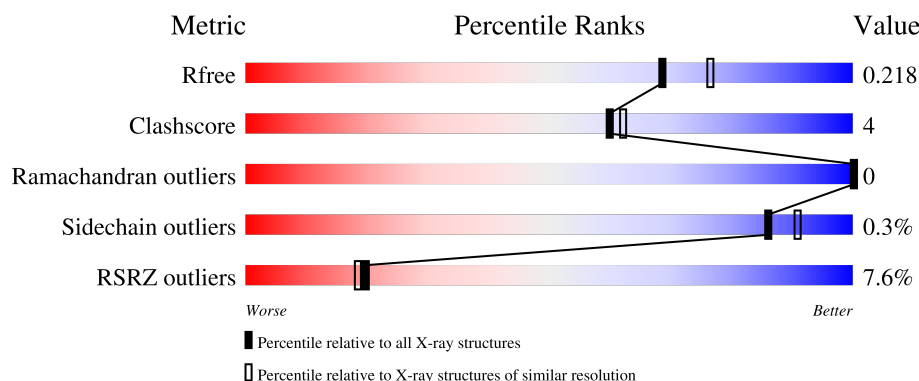
1 Overall quality at a glance

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	211	5% 79% 7% 13%
1	B	211	9% 75% 9% 16%
1	C	211	4% 82% 7% 12%
1	D	211	4% 72% 12% 16%
1	E	211	5% 81% 8% 12%

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Mol	Chain	Length	Quality of chain
1	F	211	
1	G	211	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 20210 atoms, of which 10021 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 ATP-dependent Clp protease proteolytic subunit.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	183	Total	C	H	N	O	S	0	0	0
			2861	905	1436	247	267	6			
1	B	178	Total	C	H	N	O	S	0	0	0
			2806	888	1410	241	261	6			
1	C	186	Total	C	H	N	O	S	0	1	0
			2907	918	1461	250	272	6			
1	D	178	Total	C	H	N	O	S	0	0	0
			2806	888	1410	241	261	6			
1	E	186	Total	C	H	N	O	S	0	0	0
			2899	916	1456	250	271	6			
1	F	181	Total	C	H	N	O	S	0	0	0
			2842	899	1428	244	265	6			
1	G	180	Total	C	H	N	O	S	0	0	0
			2827	894	1420	243	264	6			

There are 70 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	202	SER	-	expression tag	UNP A0A0A8RGC1
A	203	GLY	-	expression tag	UNP A0A0A8RGC1
A	204	TRP	-	expression tag	UNP A0A0A8RGC1
A	205	SER	-	expression tag	UNP A0A0A8RGC1
A	206	HIS	-	expression tag	UNP A0A0A8RGC1
A	207	PRO	-	expression tag	UNP A0A0A8RGC1
A	208	GLN	-	expression tag	UNP A0A0A8RGC1
A	209	PHE	-	expression tag	UNP A0A0A8RGC1
A	210	GLU	-	expression tag	UNP A0A0A8RGC1
A	211	LYS	-	expression tag	UNP A0A0A8RGC1
B	202	SER	-	expression tag	UNP A0A0A8RGC1
B	203	GLY	-	expression tag	UNP A0A0A8RGC1
B	204	TRP	-	expression tag	UNP A0A0A8RGC1
B	205	SER	-	expression tag	UNP A0A0A8RGC1
B	206	HIS	-	expression tag	UNP A0A0A8RGC1

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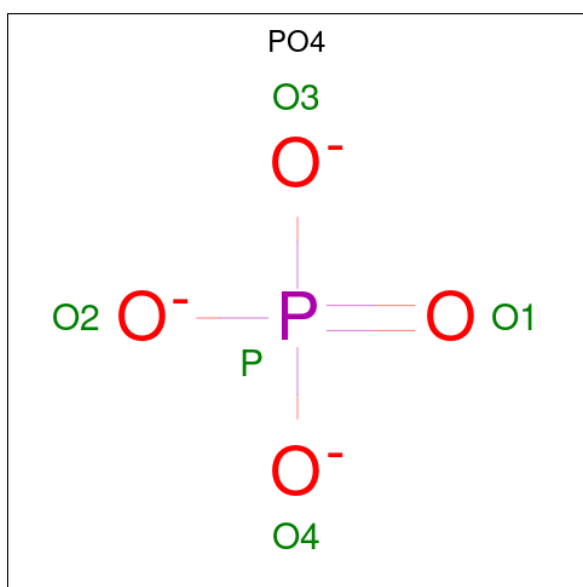
Chain	Residue	Modelled	Actual	Comment	Reference
B	207	PRO	-	expression tag	UNP A0A0A8RGC1
B	208	GLN	-	expression tag	UNP A0A0A8RGC1
B	209	PHE	-	expression tag	UNP A0A0A8RGC1
B	210	GLU	-	expression tag	UNP A0A0A8RGC1
B	211	LYS	-	expression tag	UNP A0A0A8RGC1
C	202	SER	-	expression tag	UNP A0A0A8RGC1
C	203	GLY	-	expression tag	UNP A0A0A8RGC1
C	204	TRP	-	expression tag	UNP A0A0A8RGC1
C	205	SER	-	expression tag	UNP A0A0A8RGC1
C	206	HIS	-	expression tag	UNP A0A0A8RGC1
C	207	PRO	-	expression tag	UNP A0A0A8RGC1
C	208	GLN	-	expression tag	UNP A0A0A8RGC1
C	209	PHE	-	expression tag	UNP A0A0A8RGC1
C	210	GLU	-	expression tag	UNP A0A0A8RGC1
C	211	LYS	-	expression tag	UNP A0A0A8RGC1
D	202	SER	-	expression tag	UNP A0A0A8RGC1
D	203	GLY	-	expression tag	UNP A0A0A8RGC1
D	204	TRP	-	expression tag	UNP A0A0A8RGC1
D	205	SER	-	expression tag	UNP A0A0A8RGC1
D	206	HIS	-	expression tag	UNP A0A0A8RGC1
D	207	PRO	-	expression tag	UNP A0A0A8RGC1
D	208	GLN	-	expression tag	UNP A0A0A8RGC1
D	209	PHE	-	expression tag	UNP A0A0A8RGC1
D	210	GLU	-	expression tag	UNP A0A0A8RGC1
D	211	LYS	-	expression tag	UNP A0A0A8RGC1
E	202	SER	-	expression tag	UNP A0A0A8RGC1
E	203	GLY	-	expression tag	UNP A0A0A8RGC1
E	204	TRP	-	expression tag	UNP A0A0A8RGC1
E	205	SER	-	expression tag	UNP A0A0A8RGC1
E	206	HIS	-	expression tag	UNP A0A0A8RGC1
E	207	PRO	-	expression tag	UNP A0A0A8RGC1
E	208	GLN	-	expression tag	UNP A0A0A8RGC1
E	209	PHE	-	expression tag	UNP A0A0A8RGC1
E	210	GLU	-	expression tag	UNP A0A0A8RGC1
E	211	LYS	-	expression tag	UNP A0A0A8RGC1
F	202	SER	-	expression tag	UNP A0A0A8RGC1
F	203	GLY	-	expression tag	UNP A0A0A8RGC1
F	204	TRP	-	expression tag	UNP A0A0A8RGC1
F	205	SER	-	expression tag	UNP A0A0A8RGC1
F	206	HIS	-	expression tag	UNP A0A0A8RGC1
F	207	PRO	-	expression tag	UNP A0A0A8RGC1
F	208	GLN	-	expression tag	UNP A0A0A8RGC1

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Chain	Residue	Modelled	Actual	Comment	Reference
F	209	PHE	-	expression tag	UNP A0A0A8RGC1
F	210	GLU	-	expression tag	UNP A0A0A8RGC1
F	211	LYS	-	expression tag	UNP A0A0A8RGC1
G	202	SER	-	expression tag	UNP A0A0A8RGC1
G	203	GLY	-	expression tag	UNP A0A0A8RGC1
G	204	TRP	-	expression tag	UNP A0A0A8RGC1
G	205	SER	-	expression tag	UNP A0A0A8RGC1
G	206	HIS	-	expression tag	UNP A0A0A8RGC1
G	207	PRO	-	expression tag	UNP A0A0A8RGC1
G	208	GLN	-	expression tag	UNP A0A0A8RGC1
G	209	PHE	-	expression tag	UNP A0A0A8RGC1
G	210	GLU	-	expression tag	UNP A0A0A8RGC1
G	211	LYS	-	expression tag	UNP A0A0A8RGC1

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	O	P	0	0
			5	4	1		
2	E	1	Total	O	P	0	0
			5	4	1		
2	F	1	Total	O	P	0	0
			5	4	1		

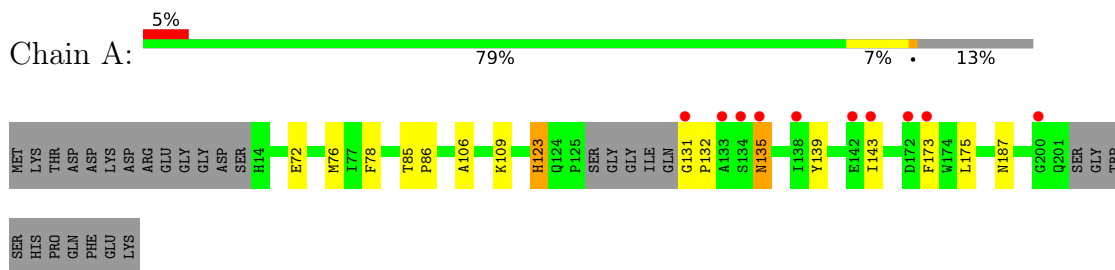
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	58	Total 58	O 58	0	0
3	B	32	Total 32	O 32	0	0
3	C	43	Total 43	O 43	0	0
3	D	35	Total 35	O 35	0	0
3	E	38	Total 38	O 38	0	0
3	F	29	Total 29	O 29	0	0
3	G	12	Total 12	O 12	0	0

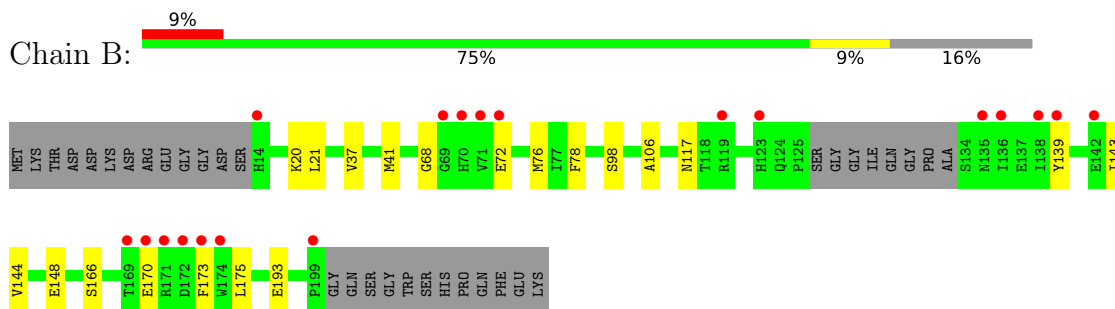
3 Residue-property plots [i](#)

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.

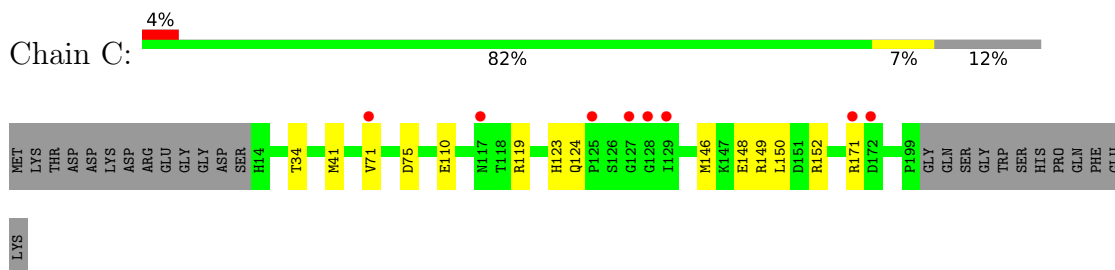
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



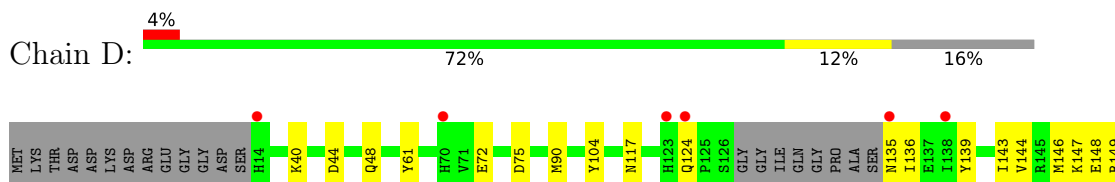
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

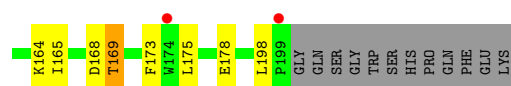


- Molecule 1: ATP-dependent Clp protease proteolytic subunit

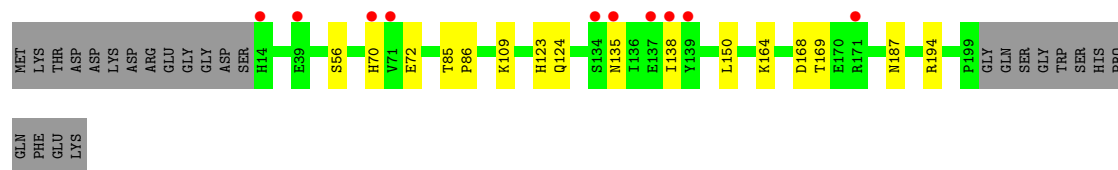
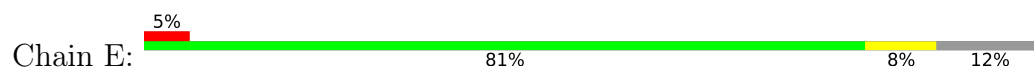


- Molecule 1: ATP-dependent Clp protease proteolytic subunit

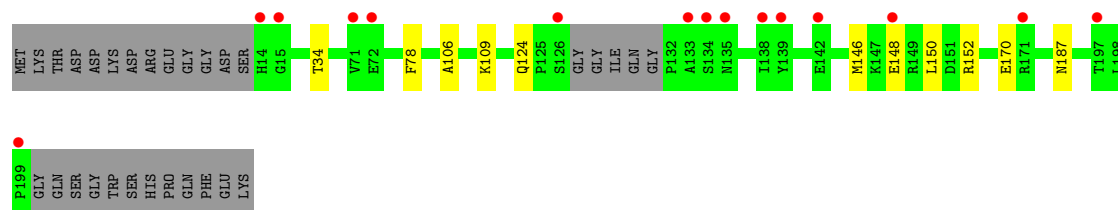
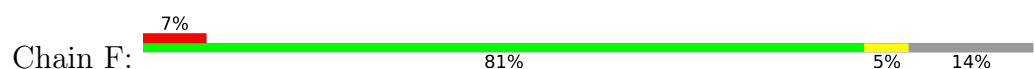




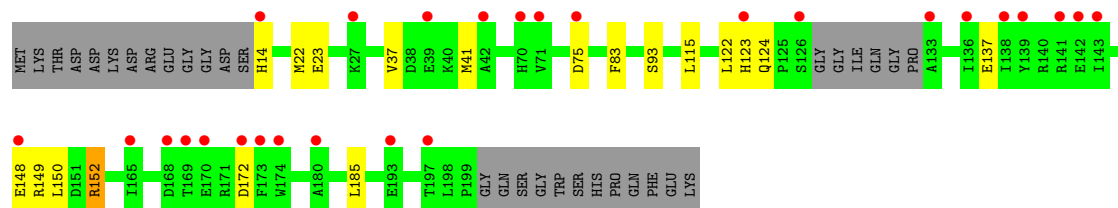
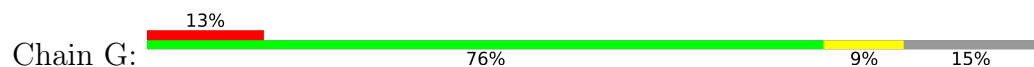
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



- Molecule 1: ATP-dependent Clp protease proteolytic subunit



- Molecule 1: ATP-dependent Clp protease proteolytic subunit



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	124.37Å 147.44Å 99.34Å 90.00° 121.73° 90.00°	Depositor
Resolution (Å)	19.97 – 2.00 19.97 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.5 (19.97-2.00) 99.6 (19.97-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.56 (at 2.01Å)	Xtriage
Refinement program	PHENIX 1.17.1	Depositor
R, R_{free}	0.197 , 0.217 0.197 , 0.218	Depositor DCC
R_{free} test set	5040 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	35.2	Xtriage
Anisotropy	0.488	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 45.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	20210	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.23% 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

5.1 Standard geometry

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	0.47	3/1450 (0.2%)	0.64	1/1957 (0.1%)
1	B	0.36	0/1420	0.52	0/1916
1	C	0.39	1/1475 (0.1%)	0.56	0/1992
1	D	0.38	0/1420	0.55	0/1916
1	E	0.35	0/1469	0.50	0/1984
1	F	0.41	0/1439	0.57	0/1942
1	G	0.38	0/1431	0.54	1/1931 (0.1%)
All	All	0.39	4/10104 (0.0%)	0.56	2/13638 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	135	ASN	CB-CG	-6.38	1.36	1.52
1	A	131	GLY	C-N	5.35	1.46	1.33
1	A	131	GLY	N-CA	5.06	1.53	1.45
1	C	41	MET	SD-CE	5.04	1.92	1.79

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	135	ASN	CB-CG-ND2	-6.74	106.29	116.40
1	G	152	ARG	NE-CZ-NH1	-6.08	115.42	121.50

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	1425	1436	1436	10	0
1	B	1396	1410	1410	16	0
1	C	1446	1461	1461	14	0
1	D	1396	1410	1410	16	1
1	E	1443	1456	1456	14	1
1	F	1414	1428	1428	9	1
1	G	1407	1420	1420	17	1
2	C	5	0	0	0	0
2	E	5	0	0	0	0
2	F	5	0	0	0	0
3	A	58	0	0	0	0
3	B	32	0	0	0	0
3	C	43	0	0	3	0
3	D	35	0	0	0	0
3	E	38	0	0	0	0
3	F	29	0	0	1	0
3	G	12	0	0	0	0
All	All	10189	10021	10021	86	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (86) 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:C:110:GLU:OE1	3:C:401:HOH:O	1.81	0.97
1:F:170:GLU:OE2	3:F:401:HOH:O	1.85	0.94
1:B:37:VAL:HG22	1:B:41:MET:HE1	1.50	0.93
1:B:20:LYS:HE2	1:G:23:GLU:HB2	1.58	0.86
1:G:122:LEU:HD21	1:G:185:LEU:HD22	1.65	0.79
1:G:75:ASP:OD1	1:G:149:ARG:NH1	2.20	0.75
1:A:76:MET:HE1	1:C:34:THR:HG23	1.71	0.72
1:D:135:ASN:OD1	1:D:136:ILE:N	2.23	0.71
1:D:124:GLN:OE1	1:D:147:LYS:HG3	1.91	0.69
1:B:20:LYS:NZ	1:G:23:GLU:OE1	2.25	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:148:GLU:OE2	1:G:152:ARG:NH1	2.28	0.66
1:B:76:MET:HE1	1:F:34:THR:HG23	1.78	0.66
1:G:37:VAL:HG22	1:G:41:MET:HE1	1.77	0.66
1:A:173:PHE:CZ	1:A:175:LEU:HD21	2.33	0.64
1:G:122:LEU:HD21	1:G:185:LEU:CD2	2.28	0.63
1:B:173:PHE:CZ	1:B:175:LEU:HD21	2.34	0.62
1:D:139:TYR:CE2	1:D:143:ILE:HD11	2.35	0.62
1:A:139:TYR:CE2	1:A:143:ILE:HD11	2.35	0.61
1:E:135:ASN:HB2	1:E:138:ILE:HD13	1.82	0.61
1:F:146:MET:HE3	1:F:150:LEU:CG	2.31	0.61
1:B:76:MET:HE1	1:F:34:THR:CG2	2.31	0.60
1:F:146:MET:HE3	1:F:150:LEU:HG	1.83	0.60
1:C:124:GLN:HG3	1:C:150:LEU:HD13	1.82	0.60
1:D:124:GLN:HG2	1:D:169:THR:O	2.01	0.60
1:B:139:TYR:CE2	1:B:143:ILE:HD11	2.37	0.59
1:E:135:ASN:CB	1:E:138:ILE:HD13	2.33	0.59
1:A:72:GLU:OE1	1:A:72:GLU:N	2.33	0.59
1:A:76:MET:HE1	1:C:34:THR:CG2	2.32	0.58
1:D:75:ASP:OD1	1:D:149:ARG:NH1	2.35	0.58
1:D:124:GLN:NE2	1:D:169:THR:OG1	2.37	0.57
1:G:37:VAL:HG13	1:G:41:MET:CE	2.34	0.56
1:F:148:GLU:OE2	1:F:152:ARG:NH1	2.39	0.55
1:E:124:GLN:HG3	1:E:150:LEU:HD13	1.88	0.55
1:B:37:VAL:HG13	1:B:41:MET:HE2	1.88	0.55
1:D:40:LYS:HD2	1:G:14:HIS:CD2	2.43	0.54
1:B:166:SER:O	1:B:170:GLU:HG3	2.07	0.53
1:D:173:PHE:CZ	1:D:175:LEU:HD21	2.43	0.53
1:G:93:SER:HB2	1:G:115:LEU:HD12	1.90	0.53
1:C:146:MET:HE3	1:C:150:LEU:HG	1.90	0.53
1:A:132:PRO:O	1:A:135:ASN:OD1	2.27	0.53
1:B:21:LEU:HD21	1:G:22:MET:SD	2.49	0.53
1:D:165:ILE:O	1:D:169:THR:OG1	2.26	0.51
1:C:146:MET:HE3	1:C:150:LEU:CG	2.41	0.51
1:E:123:HIS:HA	1:E:169:THR:HG23	1.92	0.51
1:E:169:THR:HG22	1:E:169:THR:O	2.10	0.50
1:C:75:ASP:OD1	1:C:149:ARG:NH1	2.36	0.50
1:E:138:ILE:HD12	1:E:138:ILE:H	1.77	0.50
1:G:124:GLN:HG3	1:G:150:LEU:HD13	1.93	0.49
1:C:71:VAL:CG1	1:C:146:MET:HE2	2.41	0.49
1:C:123:HIS:NE2	1:C:171:ARG:HG2	2.27	0.49
1:G:37:VAL:HG13	1:G:41:MET:HE2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:164:LYS:HE3	1:E:168:ASP:OD2	2.13	0.48
1:A:123:HIS:HD1	1:A:123:HIS:C	2.22	0.48
1:D:164:LYS:HE3	1:D:168:ASP:OD2	2.14	0.47
1:E:109:LYS:O	1:E:187:ASN:HB2	2.13	0.47
1:B:117:ASN:HD22	1:G:149:ARG:NH2	2.12	0.46
1:E:135:ASN:CA	1:E:138:ILE:HD13	2.45	0.46
1:D:72:GLU:OE2	1:D:146:MET:HE1	2.15	0.46
1:E:135:ASN:HA	1:E:138:ILE:HD13	1.97	0.46
1:E:70:HIS:CD2	1:E:72:GLU:H	2.35	0.45
1:E:70:HIS:CE1	1:E:72:GLU:HB2	2.51	0.45
1:C:152:ARG:NH2	3:C:403:HOH:O	2.28	0.45
1:F:124:GLN:HG3	1:F:150:LEU:HD13	1.99	0.45
1:D:61:TYR:OH	1:D:198:LEU:HD21	2.18	0.44
1:E:70:HIS:NE2	1:E:72:GLU:HB2	2.33	0.44
1:G:14:HIS:O	1:G:14:HIS:CG	2.69	0.44
1:F:78:PHE:CD2	1:F:106:ALA:HB2	2.52	0.44
1:D:144:VAL:O	1:D:148:GLU:HG3	2.18	0.44
1:B:68:GLY:HA2	1:B:98:SER:HB3	2.00	0.43
1:B:193:GLU:HB3	1:G:83:PHE:CE2	2.54	0.43
1:A:85:THR:N	1:A:86:PRO:CD	2.83	0.42
1:B:78:PHE:CD2	1:B:106:ALA:HB2	2.54	0.42
1:C:148:GLU:HG3	1:C:152:ARG:NH1	2.35	0.42
1:E:85:THR:N	1:E:86:PRO:CD	2.83	0.42
1:D:90:MET:HG3	1:D:104:TYR:CD1	2.55	0.42
1:F:109:LYS:O	1:F:187:ASN:HB2	2.19	0.41
1:A:78:PHE:CD2	1:A:106:ALA:HB2	2.56	0.41
1:C:71:VAL:HG12	1:C:146:MET:HE2	2.01	0.41
1:G:123:HIS:HD2	1:G:172:ASP:OD1	2.04	0.41
1:C:119:ARG:NE	3:C:402:HOH:O	2.21	0.41
1:A:109:LYS:O	1:A:187:ASN:HB2	2.21	0.40
1:D:117:ASN:OD1	1:D:117:ASN:N	2.45	0.40
1:B:144:VAL:O	1:B:148:GLU:HG3	2.21	0.40
1:D:44:ASP:O	1:D:48:GLN:HG3	2.22	0.40
1:B:72:GLU:OE1	1:B:72:GLU:N	2.52	0.40
1:C:71:VAL:O	1:C:75:ASP:HB2	2.22	0.40

All (2) 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)
1:E:194:ARG:NH1	1:F:187:ASN:OD1[4_556]	2.18	0.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:178:GLU:OE1	1:G:137:GLU:OE2[4_455]	2.19	0.01

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	179/211 (85%)	175 (98%)	4 (2%)	0	100	100
1	B	174/211 (82%)	169 (97%)	5 (3%)	0	100	100
1	C	185/211 (88%)	181 (98%)	4 (2%)	0	100	100
1	D	174/211 (82%)	169 (97%)	5 (3%)	0	100	100
1	E	184/211 (87%)	180 (98%)	4 (2%)	0	100	100
1	F	177/211 (84%)	171 (97%)	6 (3%)	0	100	100
1	G	176/211 (83%)	171 (97%)	5 (3%)	0	100	100
All	All	1249/1477 (85%)	1216 (97%)	33 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	151/174 (87%)	150 (99%)	1 (1%)	76	82
1	B	149/174 (86%)	149 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	154/174 (88%)	154 (100%)	0	100	100
1	D	149/174 (86%)	148 (99%)	1 (1%)	76	82
1	E	153/174 (88%)	152 (99%)	1 (1%)	76	82
1	F	151/174 (87%)	151 (100%)	0	100	100
1	G	150/174 (86%)	150 (100%)	0	100	100
All	All	1057/1218 (87%)	1054 (100%)	3 (0%)	86	91

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	123	HIS
1	D	169	THR
1	E	56	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	GLN
1	B	123	HIS
1	C	50	HIS
1	D	48	GLN
1	E	48	GLN
1	E	70	HIS
1	F	47	GLN
1	G	48	GLN
1	G	187	ASN

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 [i](#)

There are no oligosaccharides 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	PO4	C	301	-	4,4,4	0.89	0	6,6,6	0.53	0
2	PO4	F	301	-	4,4,4	0.88	0	6,6,6	0.41	0
2	PO4	E	301	-	4,4,4	0.98	0	6,6,6	0.52	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	183/211 (86%)	-0.01	10 (5%) 30 29	32, 48, 93, 118	0
1	B	178/211 (84%)	0.31	19 (10%) 11 10	34, 57, 113, 139	0
1	C	186/211 (88%)	0.03	8 (4%) 40 39	29, 50, 83, 142	1 (0%)
1	D	178/211 (84%)	0.02	8 (4%) 38 37	33, 50, 91, 120	0
1	E	186/211 (88%)	0.10	10 (5%) 31 30	33, 52, 98, 122	0
1	F	181/211 (85%)	0.12	15 (8%) 17 16	30, 50, 100, 126	0
1	G	180/211 (85%)	0.86	27 (15%) 5 5	41, 77, 131, 149	0
All	All	1272/1477 (86%)	0.20	97 (7%) 20 18	29, 54, 106, 149	1 (0%)

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	128	GLY	5.8
1	G	169	THR	5.4
1	F	71	VAL	5.3
1	B	173	PHE	5.2
1	B	136	ILE	5.0
1	C	129	ILE	4.7
1	G	71	VAL	4.6
1	G	133	ALA	4.6
1	B	14	HIS	4.2
1	D	135	ASN	4.0
1	E	138	ILE	3.7
1	F	134	SER	3.7
1	G	123	HIS	3.6
1	B	138	ILE	3.5
1	F	72	GLU	3.5
1	A	135	ASN	3.5
1	G	14	HIS	3.4

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Mol	Chain	Res	Type	RSRZ
1	G	136	ILE	3.4
1	A	133	ALA	3.4
1	B	135	ASN	3.3
1	A	172	ASP	3.3
1	G	193	GLU	3.3
1	D	199	PRO	3.2
1	G	170	GLU	3.2
1	G	70	HIS	3.1
1	G	142	GLU	3.1
1	F	126	SER	3.1
1	G	197	THR	3.1
1	G	138	ILE	3.1
1	F	139	TYR	3.1
1	G	75	ASP	3.0
1	G	126	SER	3.0
1	D	70	HIS	3.0
1	F	199	PRO	3.0
1	B	70	HIS	3.0
1	A	134	SER	3.0
1	E	71	VAL	3.0
1	B	142	GLU	2.9
1	D	124	GLN	2.9
1	G	172	ASP	2.8
1	F	138	ILE	2.8
1	A	131	GLY	2.8
1	E	70	HIS	2.7
1	B	72	GLU	2.7
1	B	199	PRO	2.7
1	A	173	PHE	2.7
1	B	71	VAL	2.7
1	E	134	SER	2.6
1	F	133	ALA	2.6
1	B	170	GLU	2.6
1	F	142	GLU	2.5
1	G	148	GLU	2.5
1	C	171	ARG	2.5
1	E	139	TYR	2.5
1	G	139	TYR	2.4
1	E	14	HIS	2.4
1	C	71	VAL	2.4
1	B	172	ASP	2.4
1	G	174	TRP	2.4

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Mol	Chain	Res	Type	RSRZ
1	G	180	ALA	2.4
1	G	39	GLU	2.4
1	B	174	TRP	2.4
1	E	39	GLU	2.3
1	E	137	GLU	2.3
1	C	127	GLY	2.3
1	E	135	ASN	2.3
1	F	15	GLY	2.3
1	D	123	HIS	2.3
1	D	174	TRP	2.3
1	B	119	ARG	2.3
1	E	171	ARG	2.3
1	F	14	HIS	2.3
1	G	168	ASP	2.3
1	D	14	HIS	2.2
1	G	165	ILE	2.2
1	B	171	ARG	2.2
1	A	138	ILE	2.2
1	B	69	GLY	2.2
1	C	117	ASN	2.2
1	G	143	ILE	2.2
1	G	173	PHE	2.2
1	C	125	PRO	2.1
1	A	200	GLY	2.1
1	G	27	LYS	2.1
1	F	197	THR	2.1
1	B	123	HIS	2.1
1	G	42	ALA	2.1
1	F	135	ASN	2.1
1	D	138	ILE	2.1
1	A	142	GLU	2.1
1	B	139	TYR	2.1
1	C	172	ASP	2.0
1	F	171	ARG	2.0
1	G	141	ARG	2.0
1	A	143	ILE	2.0
1	F	148	GLU	2.0
1	B	169	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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	PO4	C	301	5/5	0.79	0.11	106,106,107,108	0
2	PO4	F	301	5/5	0.86	0.14	86,87,90,90	0
2	PO4	E	301	5/5	0.91	0.18	108,109,109,109	0

6.5 Other polymers [i](#)

There are no such residues in this entry.