



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 9, 2023 – 10:58 PM EDT

PDB ID : 7M1L
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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35.1

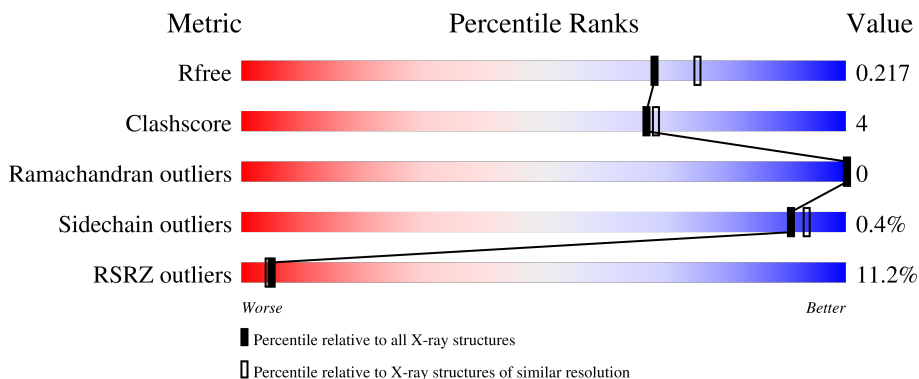
1 Overall quality at a glance

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.



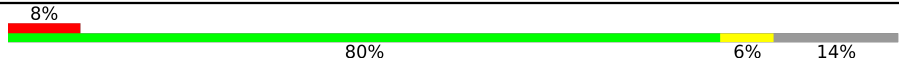

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	 6% 78% 8% 13%
1	B	211	 9% 75% 9% 16%
1	C	211	 7% 82% 6% 12%
1	D	211	 6% 72% 11% 16%
1	E	211	 11% 81% 8% 12%

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

2 Entry composition

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

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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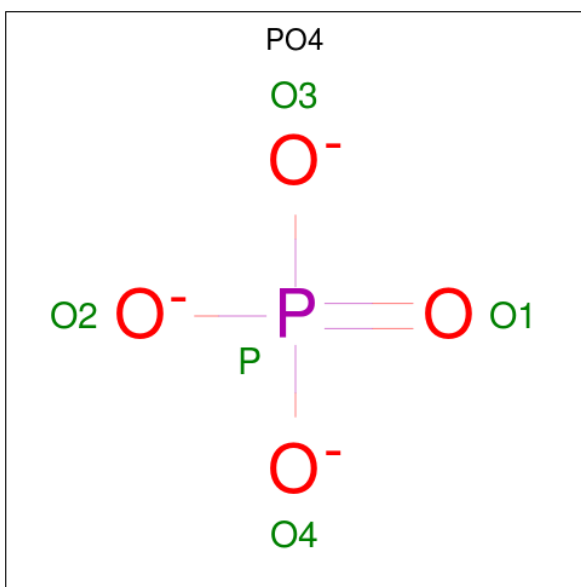
Chain	Residue	Modelled	Actual	Comment	Reference
B	207	PRO	-	expression tag	UNP A0A0A8RGC1
B	208	GLN	-	expression tag	UNP A0A0A8RGC1
B	209	PHE	-	expression tag	UNP A0A0A8RGC1
B	210	GLU	-	expression tag	UNP A0A0A8RGC1
B	211	LYS	-	expression tag	UNP A0A0A8RGC1
C	202	SER	-	expression tag	UNP A0A0A8RGC1
C	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 (three-letter code: 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		

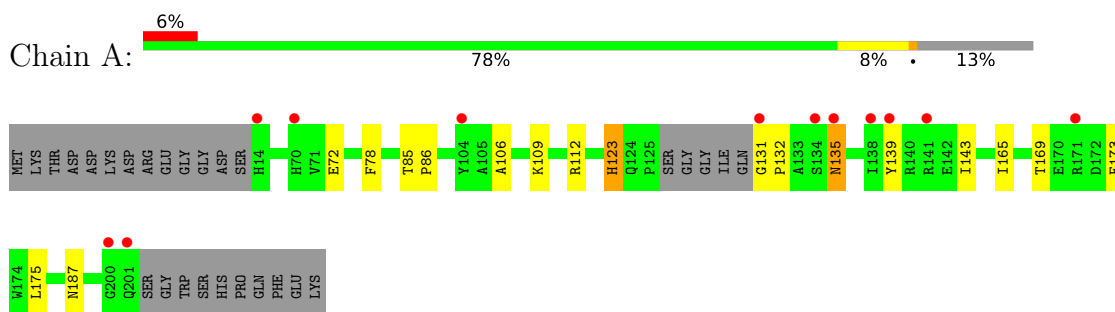
- Molecule 3 is water.

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

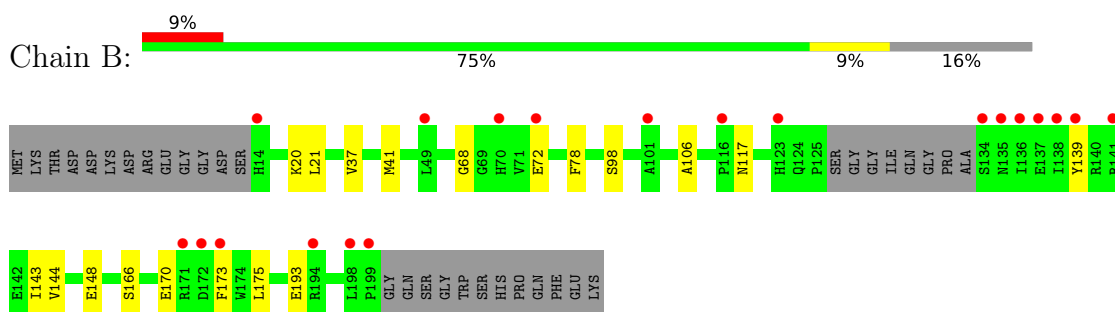
3 Residue-property plots [i](#)

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.

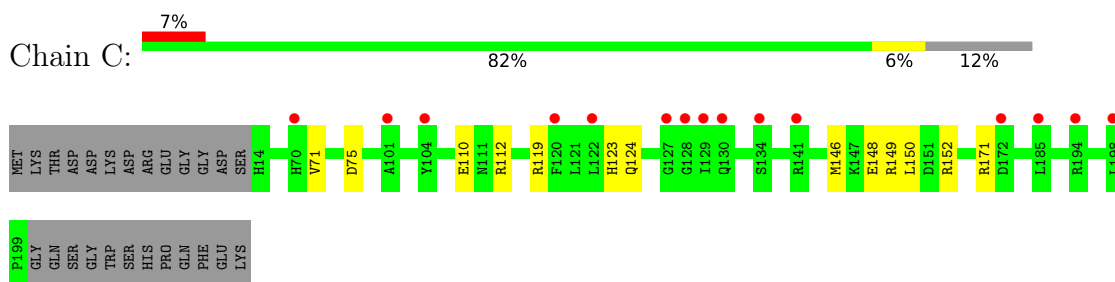
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



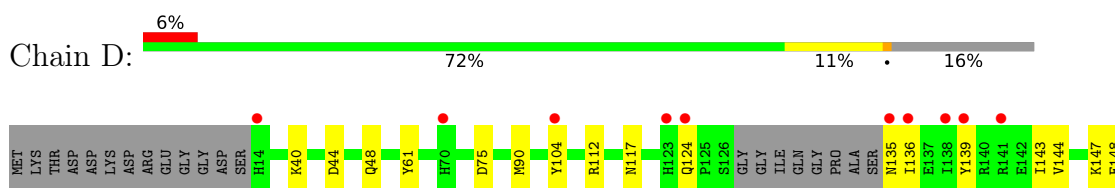
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



- Molecule 1: ATP-dependent Clp protease proteolytic subunit

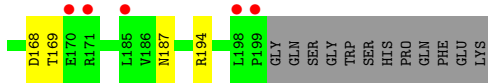
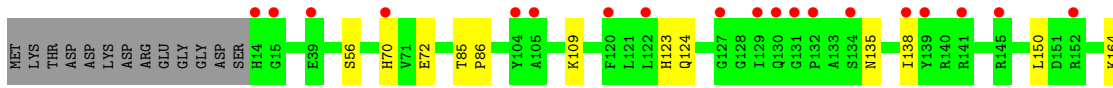
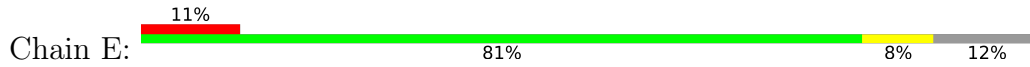


- Molecule 1: ATP-dependent Clp protease proteolytic subunit

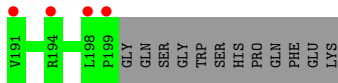
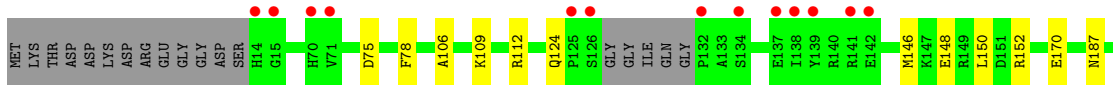
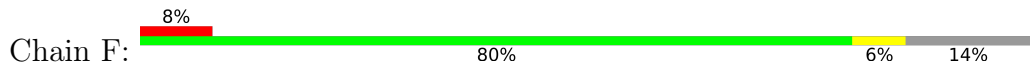




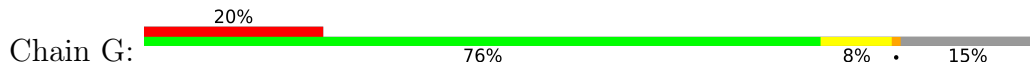
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



- 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)	Xtrriage
Refinement program	PHENIX 1.17.1	Depositor
R, R_{free}	0.197 , 0.217 0.196 , 0.217	Depositor DCC
R_{free} test set	5040 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	35.2	Xtrriage
Anisotropy	0.488	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.46 , 52.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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 [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	0.50	3/1450 (0.2%)	0.66	2/1957 (0.1%)
1	B	0.40	0/1420	0.58	0/1916
1	C	0.43	0/1475	0.62	2/1992 (0.1%)
1	D	0.43	0/1420	0.61	2/1916 (0.1%)
1	E	0.41	0/1469	0.55	0/1984
1	F	0.44	0/1439	0.64	2/1942 (0.1%)
1	G	0.47	1/1431 (0.1%)	0.66	3/1931 (0.2%)
All	All	0.44	4/10104 (0.0%)	0.62	11/13638 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	135	ASN	CB-CG	-6.50	1.36	1.51
1	A	131	GLY	C-N	6.37	1.46	1.34
1	G	148	GLU	CB-CG	-6.15	1.40	1.52
1	A	131	GLY	N-CA	5.07	1.53	1.46

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	152	ARG	NE-CZ-NH1	-9.76	115.42	120.30
1	A	112	ARG	NE-CZ-NH1	8.43	124.51	120.30
1	C	112	ARG	NE-CZ-NH2	-7.79	116.41	120.30
1	C	112	ARG	NE-CZ-NH1	7.57	124.08	120.30
1	F	112	ARG	NE-CZ-NH1	7.33	123.96	120.30
1	A	112	ARG	NE-CZ-NH2	-6.55	117.03	120.30
1	D	112	ARG	NE-CZ-NH2	-6.11	117.24	120.30
1	F	112	ARG	NE-CZ-NH2	-5.93	117.33	120.30
1	G	152	ARG	NE-CZ-NH2	5.55	123.08	120.30
1	G	149	ARG	NE-CZ-NH2	-5.46	117.57	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	178	GLU	OE1-CD-OE2	-5.31	116.93	123.30

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	1425	1436	1436	9	0
1	B	1396	1410	1410	14	0
1	C	1446	1461	1461	9	0
1	D	1396	1410	1410	15	1
1	E	1443	1456	1456	14	1
1	F	1414	1428	1428	6	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	78	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 (78) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:VAL:HG22	1:B:41:MET:HE1	1.54	0.90
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: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
1:G:148:GLU:OE2	1:G:152:ARG:NH1	2.28	0.66
1:A:173:PHE:CZ	1:A:175:LEU:HD21	2.33	0.64
1:G:37:VAL:HG22	1:G:41:MET:HE1	1.79	0.63
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: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: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:B:37:VAL:HG13	1:B:41:MET:HE2	1.85	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: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:F:146:MET:HE2	1:F:150:LEU:HD11	1.89	0.53
1:G:93:SER:HB2	1:G:115:LEU:HD12	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:G:37:VAL:HG13	1:G:41:MET:HE2	1.92	0.51
1:D:165:ILE:O	1:D:169:THR:OG1	2.26	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:146:MET:HE2	1:C:150:LEU:HD11	1.93	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:123:HIS:NE2	1:C:171:ARG:HG2	2.27	0.49
1:E:164:LYS:HE3	1:E:168:ASP:OD2	2.13	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: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:A:165:ILE:O	1:A:169:THR:OG1	2.28	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:A:123:HIS:HD1	1:A:123:HIS:C	2.22	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: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%)	84	88
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%)	84	88
1	E	153/174 (88%)	152 (99%)	1 (1%)	84	88
1	F	151/174 (87%)	150 (99%)	1 (1%)	84	88
1	G	150/174 (86%)	150 (100%)	0	100	100
All	All	1057/1218 (87%)	1053 (100%)	4 (0%)	91	93

All (4) 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
1	F	75	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	70	HIS

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 monosaccharides 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	F	301	-	4,4,4	0.84	0	6,6,6	0.38	0
2	PO4	E	301	-	4,4,4	0.94	0	6,6,6	0.49	0
2	PO4	C	301	-	4,4,4	0.84	0	6,6,6	0.49	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%)	0.26	12 (6%) 18 17	29, 43, 82, 107	0
1	B	178/211 (84%)	0.59	20 (11%) 5 4	31, 52, 105, 129	0
1	C	186/211 (88%)	0.35	15 (8%) 12 11	30, 46, 75, 131	0
1	D	178/211 (84%)	0.33	13 (7%) 15 14	30, 46, 82, 110	0
1	E	186/211 (88%)	0.55	24 (12%) 3 3	30, 47, 88, 111	0
1	F	181/211 (85%)	0.41	17 (9%) 8 8	27, 45, 91, 115	0
1	G	180/211 (85%)	1.16	42 (23%) 0 0	37, 69, 120, 138	0
All	All	1272/1477 (86%)	0.52	143 (11%) 5 4	27, 48, 96, 138	0

All (143) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	134	SER	9.7
1	G	136	ILE	8.6
1	C	128	GLY	6.9
1	G	170	GLU	6.7
1	G	134	SER	5.8
1	G	139	TYR	5.7
1	G	171	ARG	5.4
1	G	138	ILE	5.1
1	G	169	THR	5.0
1	B	173	PHE	4.8
1	B	70	HIS	4.8
1	E	199	PRO	4.7
1	D	198	LEU	4.7
1	G	71	VAL	4.7
1	E	134	SER	4.7
1	B	139	TYR	4.6
1	B	171	ARG	4.6

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Mol	Chain	Res	Type	RSRZ
1	G	70	HIS	4.5
1	D	141	ARG	4.4
1	B	135	ASN	4.4
1	G	185	LEU	4.3
1	G	122	LEU	4.3
1	G	182	GLN	4.2
1	A	135	ASN	4.1
1	G	194	ARG	4.0
1	G	119	ARG	4.0
1	G	135	ASN	3.9
1	A	171	ARG	3.9
1	D	139	TYR	3.9
1	A	141	ARG	3.9
1	F	139	TYR	3.9
1	B	138	ILE	3.8
1	E	138	ILE	3.7
1	D	135	ASN	3.7
1	F	141	ARG	3.6
1	B	136	ILE	3.5
1	C	129	ILE	3.4
1	G	140	ARG	3.4
1	F	134	SER	3.4
1	F	71	VAL	3.4
1	E	139	TYR	3.4
1	E	122	LEU	3.4
1	G	197	THR	3.3
1	G	137	GLU	3.3
1	G	154	PHE	3.3
1	E	70	HIS	3.3
1	D	138	ILE	3.3
1	G	148	GLU	3.2
1	E	39	GLU	3.2
1	G	125	PRO	3.2
1	E	130	GLN	3.2
1	F	15	GLY	3.1
1	G	141	ARG	3.1
1	F	199	PRO	3.1
1	C	130	GLN	3.1
1	E	127	GLY	3.1
1	D	199	PRO	3.1
1	G	163	GLU	3.1
1	C	141	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	199	PRO	3.0
1	G	126	SER	3.0
1	B	137	GLU	3.0
1	E	15	GLY	3.0
1	F	198	LEU	3.0
1	E	132	PRO	2.9
1	D	171	ARG	2.9
1	F	70	HIS	2.9
1	D	124	GLN	2.9
1	A	139	TYR	2.9
1	D	136	ILE	2.9
1	E	145	ARG	2.8
1	F	132	PRO	2.8
1	C	104	TYR	2.8
1	G	193	GLU	2.8
1	F	194	ARG	2.8
1	A	131	GLY	2.8
1	E	198	LEU	2.8
1	A	200	GLY	2.7
1	C	198	LEU	2.7
1	E	141	ARG	2.7
1	A	201	GLN	2.7
1	G	104	TYR	2.7
1	F	138	ILE	2.7
1	G	145	ARG	2.7
1	D	70	HIS	2.6
1	A	14	HIS	2.6
1	E	185	LEU	2.6
1	G	40	LYS	2.5
1	B	198	LEU	2.5
1	G	198	LEU	2.5
1	C	194	ARG	2.5
1	E	152	ARG	2.5
1	A	138	ILE	2.5
1	C	185	LEU	2.5
1	G	172	ASP	2.5
1	B	14	HIS	2.5
1	E	131	GLY	2.5
1	E	171	ARG	2.4
1	G	199	PRO	2.4
1	G	133	ALA	2.4
1	A	134	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	G	101	ALA	2.4
1	F	137	GLU	2.4
1	G	102	LEU	2.3
1	C	122	LEU	2.3
1	B	141	ARG	2.3
1	G	144	VAL	2.3
1	G	152	ARG	2.3
1	E	14	HIS	2.3
1	G	173	PHE	2.3
1	D	123	HIS	2.2
1	G	123	HIS	2.2
1	G	143	ILE	2.2
1	A	70	HIS	2.2
1	F	14	HIS	2.2
1	A	104	TYR	2.2
1	D	104	TYR	2.2
1	E	104	TYR	2.2
1	C	127	GLY	2.2
1	F	126	SER	2.2
1	C	70	HIS	2.2
1	C	101	ALA	2.2
1	F	125	PRO	2.2
1	B	194	ARG	2.2
1	B	172	ASP	2.2
1	G	75	ASP	2.2
1	E	120	PHE	2.2
1	E	170	GLU	2.2
1	E	105	ALA	2.1
1	G	116	PRO	2.1
1	F	191	VAL	2.1
1	C	134	SER	2.1
1	D	14	HIS	2.1
1	C	120	PHE	2.1
1	E	129	ILE	2.1
1	G	103	ILE	2.1
1	F	142	GLU	2.1
1	B	101	ALA	2.1
1	B	123	HIS	2.0
1	C	172	ASP	2.0
1	B	49	LEU	2.0
1	B	116	PRO	2.0
1	B	72	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 monosaccharides 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	C	301	5/5	0.81	0.17	106,106,107,108	0
2	PO4	F	301	5/5	0.86	0.24	86,87,90,90	0
2	PO4	E	301	5/5	0.88	0.27	108,109,109,109	0

6.5 Other polymers [i](#)

There are no such residues in this entry.