



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 03:43 pm BST

PDB ID : 5CDH
Title : Structure of Legionella pneumophila Histidine Acid Phosphatase complexed with L(+)-tartrate
Authors : Tanner, J.J.
Deposited on : 2015-07-04
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 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 : 2.11
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) : 2.11

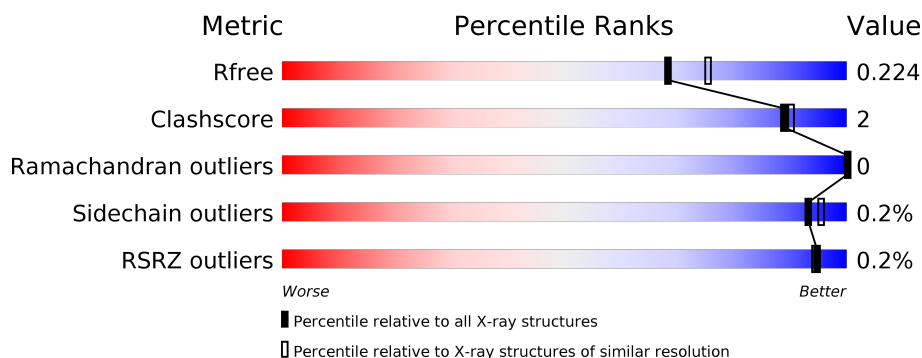
1 Overall quality at a glance

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 on 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	336	<div> <div>92%</div> <div>5% .</div> </div>
1	B	336	<div> <div>%</div> <div>93%</div> <div>. .</div> </div>
1	C	336	<div> <div>93%</div> <div>5% .</div> </div>
1	D	336	<div> <div>93%</div> <div>. .</div> </div>
1	E	336	<div> <div>92%</div> <div>5% .</div> </div>
1	F	336	<div> <div>94%</div> <div>. .</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	336	<div><div>%</div><div><div></div><div></div><div></div></div><div>93%</div><div><div></div><div></div><div></div></div><div>.</div><div>.</div></div>
1	H	336	<div><div></div><div></div><div></div></div> <div>92%</div> <div><div></div><div></div><div></div></div> <div>5%</div> <div>.</div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 21113 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 Major acid phosphatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	326	Total	C	N	O	S	0	0	0
			2542	1626	418	486	12			
1	B	325	Total	C	N	O	S	0	0	0
			2517	1614	410	481	12			
1	C	327	Total	C	N	O	S	0	1	0
			2528	1616	418	482	12			
1	D	327	Total	C	N	O	S	0	1	0
			2519	1617	413	477	12			
1	E	326	Total	C	N	O	S	0	0	0
			2542	1625	419	486	12			
1	F	327	Total	C	N	O	S	0	2	0
			2566	1642	425	487	12			
1	G	322	Total	C	N	O	S	0	0	0
			2459	1582	405	461	11			
1	H	325	Total	C	N	O	S	0	0	0
			2519	1609	415	483	12			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	25	MET	-	initiating methionine	UNP Q9APF7
A	26	VAL	-	expression tag	UNP Q9APF7
A	353	LEU	-	expression tag	UNP Q9APF7
A	354	GLU	-	expression tag	UNP Q9APF7
A	355	HIS	-	expression tag	UNP Q9APF7
A	356	HIS	-	expression tag	UNP Q9APF7
A	357	HIS	-	expression tag	UNP Q9APF7
A	358	HIS	-	expression tag	UNP Q9APF7
A	359	HIS	-	expression tag	UNP Q9APF7
A	360	HIS	-	expression tag	UNP Q9APF7
B	25	MET	-	initiating methionine	UNP Q9APF7
B	26	VAL	-	expression tag	UNP Q9APF7
B	353	LEU	-	expression tag	UNP Q9APF7

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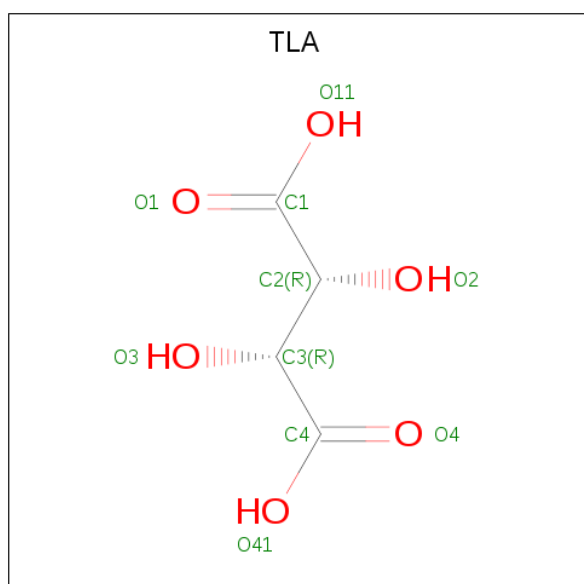
Chain	Residue	Modelled	Actual	Comment	Reference
B	354	GLU	-	expression tag	UNP Q9APF7
B	355	HIS	-	expression tag	UNP Q9APF7
B	356	HIS	-	expression tag	UNP Q9APF7
B	357	HIS	-	expression tag	UNP Q9APF7
B	358	HIS	-	expression tag	UNP Q9APF7
B	359	HIS	-	expression tag	UNP Q9APF7
B	360	HIS	-	expression tag	UNP Q9APF7
C	25	MET	-	initiating methionine	UNP Q9APF7
C	26	VAL	-	expression tag	UNP Q9APF7
C	353	LEU	-	expression tag	UNP Q9APF7
C	354	GLU	-	expression tag	UNP Q9APF7
C	355	HIS	-	expression tag	UNP Q9APF7
C	356	HIS	-	expression tag	UNP Q9APF7
C	357	HIS	-	expression tag	UNP Q9APF7
C	358	HIS	-	expression tag	UNP Q9APF7
C	359	HIS	-	expression tag	UNP Q9APF7
C	360	HIS	-	expression tag	UNP Q9APF7
D	25	MET	-	initiating methionine	UNP Q9APF7
D	26	VAL	-	expression tag	UNP Q9APF7
D	353	LEU	-	expression tag	UNP Q9APF7
D	354	GLU	-	expression tag	UNP Q9APF7
D	355	HIS	-	expression tag	UNP Q9APF7
D	356	HIS	-	expression tag	UNP Q9APF7
D	357	HIS	-	expression tag	UNP Q9APF7
D	358	HIS	-	expression tag	UNP Q9APF7
D	359	HIS	-	expression tag	UNP Q9APF7
D	360	HIS	-	expression tag	UNP Q9APF7
E	25	MET	-	initiating methionine	UNP Q9APF7
E	26	VAL	-	expression tag	UNP Q9APF7
E	353	LEU	-	expression tag	UNP Q9APF7
E	354	GLU	-	expression tag	UNP Q9APF7
E	355	HIS	-	expression tag	UNP Q9APF7
E	356	HIS	-	expression tag	UNP Q9APF7
E	357	HIS	-	expression tag	UNP Q9APF7
E	358	HIS	-	expression tag	UNP Q9APF7
E	359	HIS	-	expression tag	UNP Q9APF7
E	360	HIS	-	expression tag	UNP Q9APF7
F	25	MET	-	initiating methionine	UNP Q9APF7
F	26	VAL	-	expression tag	UNP Q9APF7
F	353	LEU	-	expression tag	UNP Q9APF7
F	354	GLU	-	expression tag	UNP Q9APF7
F	355	HIS	-	expression tag	UNP Q9APF7

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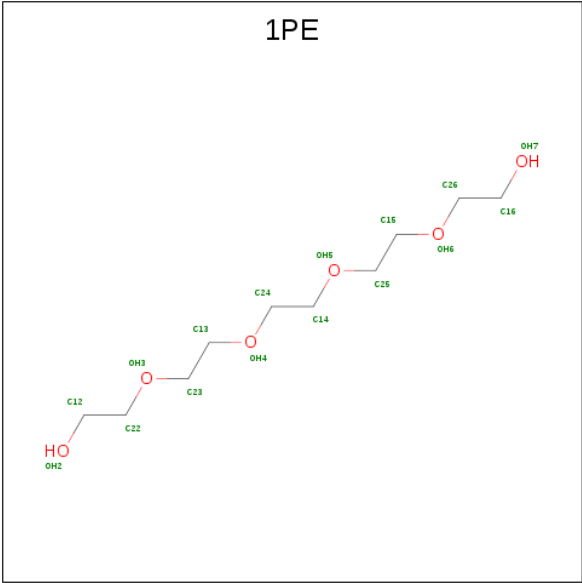
Chain	Residue	Modelled	Actual	Comment	Reference
F	356	HIS	-	expression tag	UNP Q9APF7
F	357	HIS	-	expression tag	UNP Q9APF7
F	358	HIS	-	expression tag	UNP Q9APF7
F	359	HIS	-	expression tag	UNP Q9APF7
F	360	HIS	-	expression tag	UNP Q9APF7
G	25	MET	-	initiating methionine	UNP Q9APF7
G	26	VAL	-	expression tag	UNP Q9APF7
G	353	LEU	-	expression tag	UNP Q9APF7
G	354	GLU	-	expression tag	UNP Q9APF7
G	355	HIS	-	expression tag	UNP Q9APF7
G	356	HIS	-	expression tag	UNP Q9APF7
G	357	HIS	-	expression tag	UNP Q9APF7
G	358	HIS	-	expression tag	UNP Q9APF7
G	359	HIS	-	expression tag	UNP Q9APF7
G	360	HIS	-	expression tag	UNP Q9APF7
H	25	MET	-	initiating methionine	UNP Q9APF7
H	26	VAL	-	expression tag	UNP Q9APF7
H	353	LEU	-	expression tag	UNP Q9APF7
H	354	GLU	-	expression tag	UNP Q9APF7
H	355	HIS	-	expression tag	UNP Q9APF7
H	356	HIS	-	expression tag	UNP Q9APF7
H	357	HIS	-	expression tag	UNP Q9APF7
H	358	HIS	-	expression tag	UNP Q9APF7
H	359	HIS	-	expression tag	UNP Q9APF7
H	360	HIS	-	expression tag	UNP Q9APF7

- Molecule 2 is L(+)-TARTARIC ACID (three-letter code: TLA) (formula: C₄H₆O₆).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 10 4 6	0	0
2	B	1	Total C O 10 4 6	0	0
2	C	1	Total C O 10 4 6	0	0
2	D	1	Total C O 10 4 6	0	0
2	E	1	Total C O 10 4 6	0	0
2	F	1	Total C O 10 4 6	0	0
2	G	1	Total C O 10 4 6	0	0
2	H	1	Total C O 10 4 6	0	0

- Molecule 3 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: C₁₀H₂₂O₆).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 16 10 6	0	0
3	A	1	Total C O 16 10 6	0	0
3	A	1	Total C O 13 8 5	0	0
3	A	1	Total C O 7 4 3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			16	10	6		
3	B	1	Total	C	O	0	0
			13	8	5		
3	C	1	Total	C	O	0	0
			16	10	6		
3	D	1	Total	C	O	0	0
			10	6	4		
3	E	1	Total	C	O	0	0
			16	10	6		
3	E	1	Total	C	O	0	0
			13	8	5		
3	E	1	Total	C	O	0	0
			13	8	5		
3	F	1	Total	C	O	0	0
			16	10	6		
3	H	1	Total	C	O	0	0
			16	10	6		


- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	107	Total	O	0	0
			107	107		
4	B	67	Total	O	0	0
			67	67		
4	C	54	Total	O	0	0
			54	54		
4	D	63	Total	O	0	0
			63	63		
4	E	106	Total	O	0	0
			106	106		
4	F	128	Total	O	0	0
			128	128		
4	G	47	Total	O	0	0
			47	47		
4	H	88	Total	O	0	0
			88	88		

Chain F:  94% . .



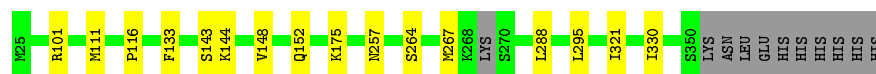
- Molecule 1: Major acid phosphatase

Chain G:  93% . .



- Molecule 1: Major acid phosphatase

Chain H:  92% 5% .



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	217.89Å 134.27Å 135.78Å 90.00° 127.46° 90.00°	Depositor
Resolution (Å)	42.88 – 2.00 42.88 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.4 (42.88-2.00) 99.3 (42.88-2.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.38 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.186 , 0.224 0.188 , 0.224	Depositor DCC
R_{free} test set	10421 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	24.5	Xtriage
Anisotropy	0.588	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 43.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.100 for -h+k-l,-l,-k 0.039 for -h-k-l,l,k 0.036 for -h-2*l,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	21113	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.95% 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: TLA, 1PE

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	0.38	0/2606	0.49	0/3557
1	B	0.33	0/2580	0.47	0/3523
1	C	0.33	0/2595	0.48	0/3546
1	D	0.34	0/2586	0.46	0/3533
1	E	0.39	0/2606	0.49	0/3557
1	F	0.41	0/2636	0.51	0/3593
1	G	0.33	0/2521	0.47	0/3448
1	H	0.36	0/2582	0.49	0/3527
All	All	0.36	0/20712	0.48	0/28284

There are no bond length outliers.

There are no bond angle outliers.

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	2542	0	2459	12	0
1	B	2517	0	2419	8	0
1	C	2528	0	2428	13	0
1	D	2519	0	2423	8	0
1	E	2542	0	2462	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2566	0	2509	9	0
1	G	2459	0	2358	6	0
1	H	2519	0	2415	12	0
2	A	10	0	4	0	0
2	B	10	0	4	0	0
2	C	10	0	4	0	0
2	D	10	0	4	0	0
2	E	10	0	4	0	0
2	F	10	0	4	1	0
2	G	10	0	4	0	0
2	H	10	0	4	1	0
3	A	52	0	70	5	0
3	B	29	0	39	4	0
3	C	16	0	22	4	0
3	D	10	0	13	2	0
3	E	42	0	56	3	0
3	F	16	0	22	2	0
3	H	16	0	22	2	0
4	A	107	0	0	0	0
4	B	67	0	0	1	0
4	C	54	0	0	0	0
4	D	63	0	0	0	0
4	E	106	0	0	0	0
4	F	128	0	0	0	0
4	G	47	0	0	0	0
4	H	88	0	0	1	0
All	All	21113	0	19749	76	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 2.

All (76) 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:F:169:THR:HG22	1:F:172:TRP:H	1.34	0.92
1:D:169:THR:HG22	1:D:172:TRP:H	1.55	0.71
1:F:282:THR:HB	3:F:402:1PE:H142	1.73	0.70
1:C:175:LYS:HZ2	3:C:402:1PE:H261	1.56	0.69
1:A:320:LYS:HD2	3:A:404:1PE:H142	1.79	0.65
1:E:116:PRO:HG3	1:E:133:PHE:CE1	2.32	0.64
1:H:116:PRO:HG3	1:H:133:PHE:CE1	2.34	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:47:ASN:HD21	1:E:46:VAL:HA	1.63	0.62
1:H:321:ILE:HD12	1:H:330:ILE:HD11	1.80	0.62
1:H:175:LYS:HD3	3:H:402:1PE:H122	1.82	0.61
1:D:252:SER:HB2	1:D:351:LYS:HB2	1.83	0.60
1:G:169:THR:HG22	1:G:171:GLU:H	1.66	0.60
1:A:175:LYS:HE2	3:A:402:1PE:H262	1.82	0.60
1:B:175:LYS:HB2	3:B:402:1PE:H121	1.85	0.59
1:E:175:LYS:HG3	3:E:402:1PE:H151	1.85	0.59
1:C:63:GLN:HG2	1:C:67:LYS:HE3	1.85	0.57
1:B:248:ASN:O	1:B:252:SER:HB2	2.04	0.57
1:A:167:PHE:O	1:A:173:GLN:NE2	2.36	0.57
1:A:205:HIS:HB2	3:A:403:1PE:H151	1.86	0.57
1:F:166:VAL:O	1:F:169:THR:HB	2.05	0.56
1:D:121:SER:HA	1:D:127:SER:HA	1.86	0.56
1:E:175:LYS:HA	3:E:402:1PE:H261	1.90	0.54
1:E:107:GLN:HE21	1:F:107:GLN:HE21	1.55	0.53
1:A:175:LYS:HG3	3:A:402:1PE:H122	1.90	0.53
1:B:282:THR:HB	3:B:403:1PE:H131	1.91	0.52
1:H:101:ARG:HH21	2:H:401:TLA:C1	2.23	0.51
1:C:175:LYS:NZ	3:C:402:1PE:H261	2.26	0.50
1:H:321:ILE:HD12	1:H:330:ILE:CD1	2.42	0.50
1:G:169:THR:HG22	1:G:171:GLU:N	2.25	0.50
1:D:158:ARG:HH22	3:D:402:1PE:H221	1.77	0.49
1:D:282:THR:HB	3:D:402:1PE:H141	1.93	0.49
1:H:288:LEU:HD13	1:H:295:LEU:HD21	1.95	0.49
1:C:121:SER:HA	1:C:127:SER:HA	1.95	0.48
1:H:144:LYS:HA	1:H:152:GLN:HG3	1.96	0.48
1:E:42:ALA:O	1:E:44:PRO:HD3	2.14	0.48
1:C:321:ILE:HD12	1:C:330:ILE:CD1	2.44	0.47
1:C:42:ALA:O	1:C:44:PRO:HD3	2.15	0.47
1:B:25:MET:N	4:B:603:HOH:O	2.48	0.47
1:H:264:SER:HA	1:H:267:MET:HE2	1.97	0.47
1:A:26:VAL:HG21	1:A:311:ASP:HB2	1.97	0.47
1:E:145:TYR:CD2	1:F:145:TYR:HB3	2.49	0.47
1:E:194:ILE:HG21	1:E:200:LEU:HD13	1.97	0.47
1:D:321:ILE:HD12	1:D:330:ILE:HD11	1.97	0.46
1:F:282:THR:OG1	3:F:402:1PE:H152	2.15	0.46
1:G:320:LYS:HG2	1:G:337:VAL:HG22	1.97	0.46
1:F:148:VAL:HA	1:F:257:ASN:ND2	2.31	0.46
1:F:101:ARG:HH21	2:F:401:TLA:C1	2.29	0.46
1:B:321:ILE:HD12	1:B:330:ILE:HD11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:143:SER:O	4:H:501:HOH:O	2.21	0.45
1:D:166:VAL:O	1:D:169:THR:HB	2.18	0.44
1:G:92:ILE:HG13	1:G:274:TYR:HD2	1.81	0.44
1:A:321:ILE:HD12	1:A:330:ILE:HD11	2.00	0.44
1:F:321:ILE:HD12	1:F:330:ILE:HD11	1.99	0.44
1:G:133:PHE:CD1	1:H:111:MET:HE1	2.52	0.44
1:E:144:LYS:HA	1:E:152:GLN:HG3	1.99	0.44
1:A:175:LYS:CE	3:A:402:1PE:H262	2.48	0.44
3:H:402:1PE:H151	3:H:402:1PE:H161	1.59	0.44
1:C:175:LYS:HE3	3:C:402:1PE:H241	1.98	0.44
1:B:121:SER:HA	1:B:127:SER:HA	2.00	0.44
1:G:234:GLU:HG3	1:G:298:SER:OG	2.17	0.44
1:A:74:LYS:NZ	1:A:79:GLU:OE2	2.51	0.43
1:E:320:LYS:HD2	3:E:404:1PE:H151	1.99	0.43
1:A:255:MET:HG3	1:A:290:PHE:CD2	2.54	0.43
1:C:111:MET:HE2	1:C:111:MET:HB2	1.74	0.43
1:C:194:ILE:HD11	1:C:203:VAL:HG21	2.02	0.42
1:H:148:VAL:HA	1:H:257:ASN:ND2	2.34	0.42
3:B:402:1PE:H242	3:B:402:1PE:H252	1.74	0.42
1:H:288:LEU:HA	1:H:288:LEU:HD23	1.90	0.42
1:A:43:LEU:HD13	1:A:218:PRO:HG3	2.01	0.42
1:B:175:LYS:HZ2	3:B:402:1PE:H252	1.84	0.42
1:B:43:LEU:HD13	1:B:218:PRO:HD3	2.03	0.41
1:C:235:TRP:CD1	3:C:402:1PE:H242	2.55	0.41
1:C:321:ILE:HD12	1:C:330:ILE:HD11	2.02	0.41
1:D:154:ASP:OD2	1:D:156:LYS:HB2	2.21	0.41
1:C:122:ILE:HG12	1:C:126:THR:O	2.20	0.41
1:A:122:ILE:HG23	1:A:128:ALA:HA	2.04	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	324/336 (96%)	320 (99%)	4 (1%)	0	100	100
1	B	321/336 (96%)	317 (99%)	4 (1%)	0	100	100
1	C	326/336 (97%)	320 (98%)	6 (2%)	0	100	100
1	D	326/336 (97%)	324 (99%)	2 (1%)	0	100	100
1	E	324/336 (96%)	322 (99%)	2 (1%)	0	100	100
1	F	327/336 (97%)	324 (99%)	3 (1%)	0	100	100
1	G	318/336 (95%)	314 (99%)	4 (1%)	0	100	100
1	H	321/336 (96%)	318 (99%)	3 (1%)	0	100	100
All	All	2587/2688 (96%)	2559 (99%)	28 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	274/294 (93%)	274 (100%)	0	100	100
1	B	268/294 (91%)	268 (100%)	0	100	100
1	C	270/294 (92%)	270 (100%)	0	100	100
1	D	266/294 (90%)	265 (100%)	1 (0%)	91	93
1	E	275/294 (94%)	272 (99%)	3 (1%)	73	78
1	F	279/294 (95%)	278 (100%)	1 (0%)	91	93
1	G	256/294 (87%)	256 (100%)	0	100	100
1	H	270/294 (92%)	270 (100%)	0	100	100
All	All	2158/2352 (92%)	2153 (100%)	5 (0%)	93	95

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	51	GLN
1	E	214	ASN

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Mol	Chain	Res	Type
1	E	312	ASN
1	E	315	ASN
1	F	169	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	107	GLN
1	H	173	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

21 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	TLA	B	401	-	3,9,9	0.94	0	6,12,12	2.08	2 (33%)
2	TLA	D	401	-	3,9,9	1.01	0	6,12,12	2.32	3 (50%)
2	TLA	F	401	-	3,9,9	1.05	0	6,12,12	2.14	2 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	1PE	A	404	-	12,12,15	0.64	0	11,11,14	0.93	0
2	TLA	H	401	-	3,9,9	0.99	0	6,12,12	2.02	2 (33%)
3	1PE	E	404	-	12,12,15	0.67	0	11,11,14	0.95	0
3	1PE	A	405	-	6,6,15	0.62	0	5,5,14	0.78	0
2	TLA	C	401	-	3,9,9	0.84	0	6,12,12	1.64	1 (16%)
3	1PE	E	402	-	15,15,15	0.63	0	14,14,14	0.80	0
2	TLA	G	401	-	3,9,9	1.02	0	6,12,12	1.99	2 (33%)
3	1PE	A	403	-	15,15,15	0.69	0	14,14,14	0.68	0
2	TLA	A	401	-	3,9,9	0.94	0	6,12,12	1.82	2 (33%)
3	1PE	F	402	-	15,15,15	0.58	0	14,14,14	0.90	1 (7%)
3	1PE	B	403	-	12,12,15	0.66	0	11,11,14	0.86	0
3	1PE	D	402	-	9,9,15	0.61	0	8,8,14	0.82	0
2	TLA	E	401	-	3,9,9	0.68	0	6,12,12	1.60	1 (16%)
3	1PE	B	402	-	15,15,15	0.65	0	14,14,14	0.86	0
3	1PE	C	402	-	15,15,15	0.63	0	14,14,14	0.81	0
3	1PE	A	402	-	15,15,15	0.63	0	14,14,14	0.85	0
3	1PE	H	402	-	15,15,15	0.63	0	14,14,14	0.94	1 (7%)
3	1PE	E	403	-	12,12,15	0.62	0	11,11,14	0.82	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TLA	B	401	-	-	0/4/12/12	-
2	TLA	D	401	-	-	0/4/12/12	-
2	TLA	F	401	-	-	0/4/12/12	-
3	1PE	A	404	-	-	5/10/10/13	-
2	TLA	H	401	-	-	4/4/12/12	-
3	1PE	E	404	-	-	2/10/10/13	-
3	1PE	A	405	-	-	3/4/4/13	-
2	TLA	C	401	-	-	0/4/12/12	-
3	1PE	E	402	-	-	7/13/13/13	-
2	TLA	G	401	-	-	0/4/12/12	-
3	1PE	A	403	-	-	4/13/13/13	-
2	TLA	A	401	-	-	0/4/12/12	-
3	1PE	F	402	-	-	11/13/13/13	-
3	1PE	B	403	-	-	7/10/10/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	1PE	D	402	-	-	5/7/7/13	-
2	TLA	E	401	-	-	0/4/12/12	-
3	1PE	B	402	-	-	5/13/13/13	-
3	1PE	C	402	-	-	7/13/13/13	-
3	1PE	A	402	-	-	10/13/13/13	-
3	1PE	H	402	-	-	7/13/13/13	-
3	1PE	E	403	-	-	4/10/10/13	-

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	TLA	C1-C2-C3	-4.59	103.23	113.11
2	F	401	TLA	C4-C3-C2	-4.53	103.35	113.11
2	H	401	TLA	C4-C3-C2	-4.21	104.05	113.11
2	B	401	TLA	C4-C3-C2	-4.13	104.22	113.11
2	G	401	TLA	C4-C3-C2	-3.91	104.69	113.11
2	C	401	TLA	C1-C2-C3	-3.64	105.27	113.11
2	A	401	TLA	C4-C3-C2	-3.27	106.06	113.11
2	E	401	TLA	C4-C3-C2	-3.25	106.11	113.11
2	B	401	TLA	C1-C2-C3	-2.60	107.51	113.11
2	G	401	TLA	C1-C2-C3	-2.58	107.55	113.11
2	A	401	TLA	C1-C2-C3	-2.45	107.83	113.11
2	F	401	TLA	C1-C2-C3	-2.38	107.97	113.11
3	F	402	1PE	C25-OH5-C14	2.22	122.91	113.29
2	D	401	TLA	O2-C2-C1	-2.17	105.87	111.10
2	D	401	TLA	C4-C3-C2	-2.16	108.46	113.11
2	H	401	TLA	C1-C2-C3	-2.15	108.47	113.11
3	H	402	1PE	C26-OH6-C15	2.07	122.25	113.29

There are no chirality outliers.

All (81) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	401	TLA	C1-C2-C3-C4
3	H	402	1PE	C16-C26-OH6-C15
3	B	402	1PE	C24-C14-OH5-C25
3	E	402	1PE	OH6-C15-C25-OH5
3	B	402	1PE	OH5-C14-C24-OH4
3	C	402	1PE	OH5-C14-C24-OH4

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Mol	Chain	Res	Type	Atoms
3	F	402	1PE	OH5-C14-C24-OH4
3	H	402	1PE	OH6-C15-C25-OH5
3	C	402	1PE	OH6-C15-C25-OH5
3	A	402	1PE	OH4-C13-C23-OH3
3	A	402	1PE	OH2-C12-C22-OH3
3	H	402	1PE	OH2-C12-C22-OH3
3	H	402	1PE	OH5-C14-C24-OH4
3	B	403	1PE	OH5-C14-C24-OH4
3	B	402	1PE	OH6-C15-C25-OH5
3	E	402	1PE	OH5-C14-C24-OH4
3	F	402	1PE	OH4-C13-C23-OH3
3	A	405	1PE	OH4-C13-C23-OH3
3	A	404	1PE	C15-C25-OH5-C14
3	B	403	1PE	OH6-C15-C25-OH5
3	A	402	1PE	OH6-C15-C25-OH5
3	E	403	1PE	OH5-C14-C24-OH4
3	A	403	1PE	OH7-C16-C26-OH6
3	H	402	1PE	OH7-C16-C26-OH6
3	D	402	1PE	OH4-C13-C23-OH3
3	A	402	1PE	OH5-C14-C24-OH4
3	A	404	1PE	OH6-C15-C25-OH5
3	B	403	1PE	OH7-C16-C26-OH6
3	E	403	1PE	OH6-C15-C25-OH5
3	F	402	1PE	OH2-C12-C22-OH3
2	H	401	TLA	O2-C2-C3-O3
3	A	404	1PE	OH5-C14-C24-OH4
3	C	402	1PE	OH7-C16-C26-OH6
3	A	402	1PE	OH7-C16-C26-OH6
3	E	402	1PE	OH7-C16-C26-OH6
3	A	404	1PE	OH4-C13-C23-OH3
3	E	404	1PE	OH4-C13-C23-OH3
3	B	403	1PE	C24-C14-OH5-C25
3	F	402	1PE	C16-C26-OH6-C15
3	D	402	1PE	C14-C24-OH4-C13
3	F	402	1PE	C23-C13-OH4-C24
3	A	403	1PE	C24-C14-OH5-C25
3	B	403	1PE	C25-C15-OH6-C26
3	B	403	1PE	C15-C25-OH5-C14
3	C	402	1PE	C15-C25-OH5-C14
3	A	402	1PE	C13-C23-OH3-C22
3	F	402	1PE	C14-C24-OH4-C13
3	A	402	1PE	C16-C26-OH6-C15

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Mol	Chain	Res	Type	Atoms
3	D	402	1PE	OH5-C14-C24-OH4
3	B	403	1PE	C16-C26-OH6-C15
3	A	402	1PE	C14-C24-OH4-C13
3	A	403	1PE	OH5-C14-C24-OH4
2	H	401	TLA	O2-C2-C3-C4
3	C	402	1PE	C24-C14-OH5-C25
3	E	402	1PE	C13-C23-OH3-C22
3	A	404	1PE	OH2-C12-C22-OH3
3	F	402	1PE	C15-C25-OH5-C14
3	A	403	1PE	C15-C25-OH5-C14
3	B	402	1PE	OH4-C13-C23-OH3
3	E	402	1PE	C16-C26-OH6-C15
3	A	402	1PE	C23-C13-OH4-C24
3	F	402	1PE	C12-C22-OH3-C23
3	B	402	1PE	C23-C13-OH4-C24
3	C	402	1PE	C25-C15-OH6-C26
3	E	402	1PE	C25-C15-OH6-C26
3	A	402	1PE	C24-C14-OH5-C25
3	E	404	1PE	C14-C24-OH4-C13
3	F	402	1PE	C13-C23-OH3-C22
3	A	405	1PE	C13-C23-OH3-C22
3	E	403	1PE	OH4-C13-C23-OH3
2	H	401	TLA	C1-C2-C3-O3
3	F	402	1PE	C24-C14-OH5-C25
3	A	405	1PE	OH2-C12-C22-OH3
3	E	402	1PE	C24-C14-OH5-C25
3	C	402	1PE	OH4-C13-C23-OH3
3	H	402	1PE	C23-C13-OH4-C24
3	D	402	1PE	C23-C13-OH4-C24
3	E	403	1PE	OH2-C12-C22-OH3
3	D	402	1PE	OH2-C12-C22-OH3
3	H	402	1PE	C15-C25-OH5-C14
3	F	402	1PE	OH6-C15-C25-OH5

There are no ring outliers.

13 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	401	TLA	1	0
3	A	404	1PE	1	0
2	H	401	TLA	1	0
3	E	404	1PE	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	402	1PE	2	0
3	A	403	1PE	1	0
3	F	402	1PE	2	0
3	B	403	1PE	1	0
3	D	402	1PE	2	0
3	B	402	1PE	3	0
3	C	402	1PE	4	0
3	A	402	1PE	3	0
3	H	402	1PE	2	0

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	326/336 (97%)	-0.62	0 100 100	19, 26, 45, 66	0
1	B	325/336 (96%)	-0.45	2 (0%) 89 88	22, 32, 54, 67	0
1	C	327/336 (97%)	-0.53	0 100 100	23, 32, 51, 71	0
1	D	327/336 (97%)	-0.41	1 (0%) 94 93	24, 34, 57, 72	0
1	E	326/336 (97%)	-0.57	0 100 100	13, 26, 44, 62	0
1	F	327/336 (97%)	-0.55	0 100 100	14, 23, 45, 58	0
1	G	322/336 (95%)	-0.40	2 (0%) 89 88	20, 35, 59, 70	0
1	H	325/336 (96%)	-0.62	0 100 100	18, 28, 44, 68	0
All	All	2605/2688 (96%)	-0.52	5 (0%) 95 94	13, 30, 52, 72	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	184	PRO	2.3
1	B	220	GLY	2.3
1	G	314	ALA	2.2
1	D	185	LEU	2.1
1	G	316	TYR	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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
3	1PE	F	402	16/16	0.78	0.18	36,51,57,60	0
3	1PE	H	402	16/16	0.82	0.14	48,52,54,57	0
3	1PE	B	402	16/16	0.84	0.16	54,62,70,70	0
3	1PE	B	403	13/16	0.84	0.16	42,45,53,55	0
3	1PE	E	402	16/16	0.86	0.13	44,50,62,62	0
3	1PE	E	404	13/16	0.88	0.17	39,49,57,57	0
3	1PE	C	402	16/16	0.88	0.11	39,47,54,55	0
2	TLA	H	401	10/10	0.88	0.19	21,34,53,63	0
2	TLA	C	401	10/10	0.89	0.10	26,32,45,47	0
2	TLA	G	401	10/10	0.89	0.14	37,40,57,57	0
3	1PE	D	402	10/16	0.89	0.13	33,44,49,52	0
2	TLA	F	401	10/10	0.90	0.15	22,24,41,44	0
2	TLA	D	401	10/10	0.90	0.16	31,35,44,44	0
3	1PE	E	403	13/16	0.90	0.13	31,45,49,51	0
3	1PE	A	402	16/16	0.91	0.11	32,42,55,55	0
3	1PE	A	403	16/16	0.91	0.12	37,43,51,51	0
3	1PE	A	404	13/16	0.91	0.12	36,43,54,57	0
2	TLA	E	401	10/10	0.92	0.11	20,27,40,41	0
2	TLA	A	401	10/10	0.93	0.10	21,25,32,34	0
2	TLA	B	401	10/10	0.94	0.12	25,31,42,43	0
3	1PE	A	405	7/16	0.94	0.10	34,38,42,43	0

6.5 Other polymers ⓘ

There are no such residues in this entry.