Full wwPDB X-ray Structure Validation Report (i)

Feb 19, 2016 – 10:27 PM GMT

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)

The following versions of software and data (see references (i)) were used in the production of this report:

|		
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

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.
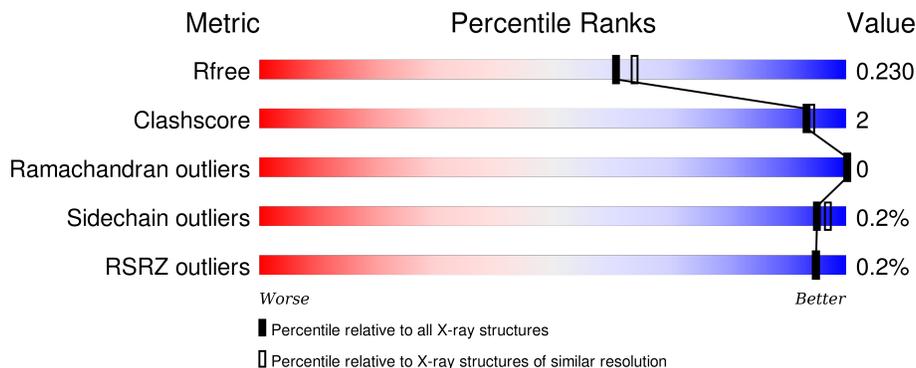

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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. 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 <=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	92% 5% ·
1	B	336	% 93% · ·
1	C	336	93% 5% ·
1	D	336	93% · ·
1	E	336	92% 5% ·
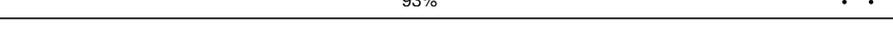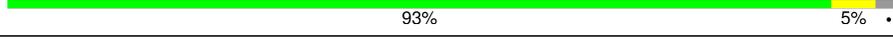
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Mol	Chain	Length	Quality of chain
1	F	336	94%
1	G	336	93%
1	H	336	92% 5%
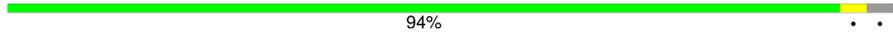
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	TLA	D	401	-	-	-	X
2	TLA	F	401	-	-	-	X
2	TLA	G	401	-	-	-	X
2	TLA	H	401	-	-	-	X
3	1PE	B	402	-	-	-	X
3	1PE	B	403	-	-	-	X
3	1PE	F	402	-	-	-	X

2 Entry composition (i)

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: $C_4H_6O_6$).

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

- Molecule 3 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).

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

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

- Molecule 4 is water.

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

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Major acid phosphatase
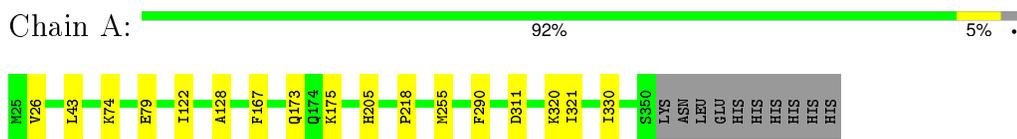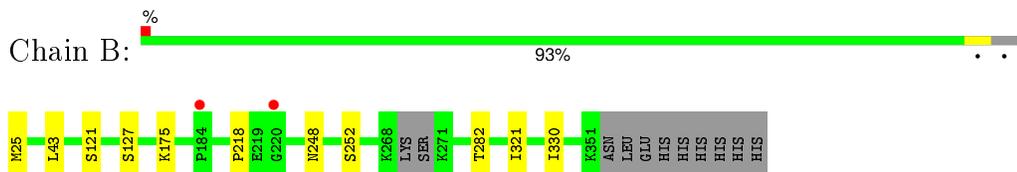
Chain A:

- Molecule 1: Major acid phosphatase

Chain B:

- Molecule 1: Major acid phosphatase

Chain C:

- Molecule 1: Major acid phosphatase

Chain D:

- Molecule 1: Major acid phosphatase

Chain E:

- Molecule 1: Major acid phosphatase

Chain F:

M25 R101 Q107 Y145 V148 V166 T169 W172 N257 T282 I321 I330 K351 ASN LEU GLU HIS HIS HIS HIS HIS HIS

• Molecule 1: Major acid phosphatase

Chain G:

93%

M25 I92 F133 T169 R170 E171 E234 S266 MET LYS LYS SER K271 Y274 S298 A314 N315 Y316 K320 V337 S350 LYS ASN LEU GLU HIS HIS HIS HIS HIS HIS

• Molecule 1: Major acid phosphatase

Chain H:

92%　　　　　　　　　　　　　　　　　　　　　　　5%

M25 R101 M111 P116 F133 S143 K144 V148 Q152 K175 N257 S264 M267 K268 LYS S270 L288 L295 I321 I330 S350 LYS ASN LEU GLU HIS HIS HIS HIS HIS HIS
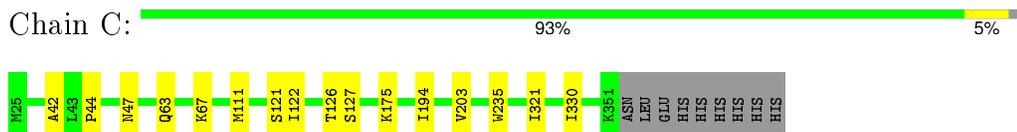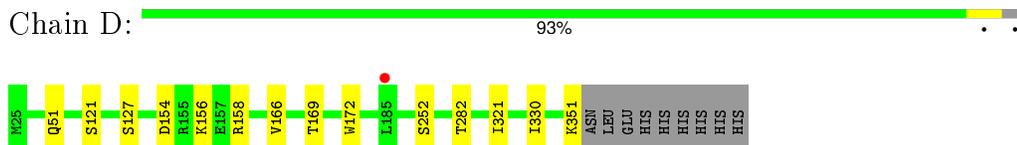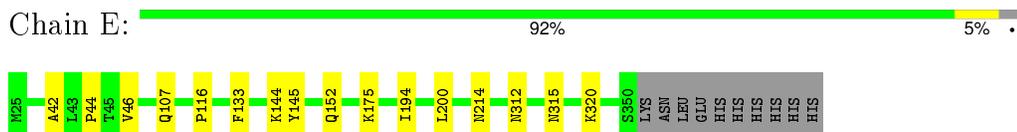
4 Data and refinement statistics (i)

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
$<I/\sigma(I)>$ [1]	2.38 (at 2.00Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.186 , 0.224 0.195 , 0.230	Depositor DCC
R_{free} test set	10421 reflections (5.30%)	DCC
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
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
L-test for twinning[2]	$<|L|>=0.50$, $<L^2>=0.33$	Xtriage
Outliers	0 of 207076 reflections	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.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $<|L|>$, $<L^2>$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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:G:169:THR:HG22	1:G:171:GLU:H	1.66	0.60
1:D:252:SER:HB2	1:D:351:LYS:HB2	1.83	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
3:H:402:1PE:H151	3:H:402:1PE:H161	1.59	0.44
1:A:175:LYS:CE	3:A:402:1PE:H262	2.48	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:C:235:TRP:CD1	3:C:402:1PE:H242	2.55	0.41
1:B:43:LEU:HD13	1:B:218:PRO:HD3	2.03	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 (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	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 (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	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%)	93	95
1	E	275/294 (94%)	272 (99%)	3 (1%)	80	83
1	F	279/294 (95%)	278 (100%)	1 (0%)	93	95
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%)	95	97

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 ⓘ

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 ⓘ

There are no carbohydrates in this entry.

5.6   Ligand geometry ⓘ

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	A	401	-	3,9,9	0.92	0	6,12,12	1.95	2 (33%)
3	1PE	A	402	-	15,15,15	0.65	0	14,14,14	0.86	0
3	1PE	A	403	-	15,15,15	0.70	0	14,14,14	0.69	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
3	1PE	A	404	-	12,12,15	0.65	0	11,11,14	0.95	0
3	1PE	A	405	-	6,6,15	0.62	0	5,5,14	0.80	0
2	TLA	B	401	-	3,9,9	0.92	0	6,12,12	2.24	2 (33%)
3	1PE	B	402	-	15,15,15	0.66	0	14,14,14	0.88	0
3	1PE	B	403	-	12,12,15	0.67	0	11,11,14	0.88	0
2	TLA	C	401	-	3,9,9	0.82	0	6,12,12	1.78	1 (16%)
3	1PE	C	402	-	15,15,15	0.64	0	14,14,14	0.82	0
2	TLA	D	401	-	3,9,9	0.98	0	6,12,12	2.46	3 (50%)
3	1PE	D	402	-	9,9,15	0.62	0	8,8,14	0.83	0
2	TLA	E	401	-	3,9,9	0.66	0	6,12,12	1.74	1 (16%)
3	1PE	E	402	-	15,15,15	0.65	0	14,14,14	0.81	0
3	1PE	E	403	-	12,12,15	0.63	0	11,11,14	0.83	0
3	1PE	E	404	-	12,12,15	0.68	0	11,11,14	0.97	0
2	TLA	F	401	-	3,9,9	1.03	0	6,12,12	2.32	2 (33%)
3	1PE	F	402	-	15,15,15	0.59	0	14,14,14	0.92	1 (7%)
2	TLA	G	401	-	3,9,9	0.99	0	6,12,12	2.14	2 (33%)
2	TLA	H	401	-	3,9,9	0.96	0	6,12,12	2.18	2 (33%)
3	1PE	H	402	-	15,15,15	0.64	0	14,14,14	0.95	1 (7%)

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	A	401	-	-	0/4/12/12	0/0/0/0
3	1PE	A	402	-	-	0/13/13/13	0/0/0/0
3	1PE	A	403	-	-	0/13/13/13	0/0/0/0
3	1PE	A	404	-	-	0/10/10/13	0/0/0/0
3	1PE	A	405	-	-	0/4/4/13	0/0/0/0
2	TLA	B	401	-	-	0/4/12/12	0/0/0/0
3	1PE	B	402	-	-	0/13/13/13	0/0/0/0
3	1PE	B	403	-	-	0/10/10/13	0/0/0/0
2	TLA	C	401	-	-	0/4/12/12	0/0/0/0
3	1PE	C	402	-	-	0/13/13/13	0/0/0/0
2	TLA	D	401	-	-	0/4/12/12	0/0/0/0
3	1PE	D	402	-	-	0/7/7/13	0/0/0/0
2	TLA	E	401	-	-	0/4/12/12	0/0/0/0
3	1PE	E	402	-	-	0/13/13/13	0/0/0/0
3	1PE	E	403	-	-	0/10/10/13	0/0/0/0
3	1PE	E	404	-	-	0/10/10/13	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TLA	F	401	-	-	0/4/12/12	0/0/0/0
3	1PE	F	402	-	-	0/13/13/13	0/0/0/0
2	TLA	G	401	-	-	0/4/12/12	0/0/0/0
2	TLA	H	401	-	-	0/4/12/12	0/0/0/0
3	1PE	H	402	-	-	0/13/13/13	0/0/0/0

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	401	TLA	C1-C2-C3	-4.93	103.23	113.35
2	F	401	TLA	C4-C3-C2	-4.88	103.35	113.35
2	H	401	TLA	C4-C3-C2	-4.54	104.05	113.35
2	B	401	TLA	C4-C3-C2	-4.45	104.22	113.35
2	G	401	TLA	C4-C3-C2	-4.23	104.69	113.35
2	C	401	TLA	C1-C2-C3	-3.94	105.27	113.35
2	A	401	TLA	C4-C3-C2	-3.56	106.06	113.35
2	E	401	TLA	C4-C3-C2	-3.53	106.11	113.35
2	B	401	TLA	C1-C2-C3	-2.85	107.51	113.35
2	G	401	TLA	C1-C2-C3	-2.83	107.55	113.35
2	A	401	TLA	C1-C2-C3	-2.69	107.83	113.35
2	F	401	TLA	C1-C2-C3	-2.62	107.97	113.35
2	D	401	TLA	C4-C3-C2	-2.38	108.46	113.35
2	H	401	TLA	C1-C2-C3	-2.38	108.47	113.35
2	D	401	TLA	O2-C2-C1	-2.11	105.87	111.12
3	H	402	1PE	C26-OH6-C15	2.09	122.25	113.31
3	F	402	1PE	C25-OH5-C14	2.25	122.91	113.31

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

13 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	402	1PE	3	0
3	A	403	1PE	1	0
3	A	404	1PE	1	0
3	B	402	1PE	3	0
3	B	403	1PE	1	0
3	C	402	1PE	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	402	1PE	2	0
3	E	402	1PE	2	0
3	E	404	1PE	1	0
2	F	401	TLA	1	0
3	F	402	1PE	2	0
2	H	401	TLA	1	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(Å²)	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%) 90	90	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	94	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%) 90	90	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	95	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	2.1
1	D	185	LEU	2.0
1	G	316	TYR	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å²)	Q<0.9
2	TLA	G	401	10/10	0.89	0.14	11.22	37,40,57,57	0
2	TLA	H	401	10/10	0.88	0.19	6.70	21,34,53,63	0
3	1PE	F	402	16/16	0.78	0.18	5.82	36,51,57,60	0
2	TLA	D	401	10/10	0.90	0.16	4.71	31,35,44,44	0
2	TLA	F	401	10/10	0.90	0.15	4.26	22,24,41,44	0
3	1PE	B	403	13/16	0.84	0.16	2.81	42,45,53,55	0
3	1PE	B	402	16/16	0.84	0.16	2.43	54,62,70,70	0
3	1PE	A	403	16/16	0.91	0.12	1.98	37,43,51,51	0
3	1PE	E	403	13/16	0.90	0.13	1.97	31,45,49,51	0
3	1PE	D	402	10/16	0.89	0.13	1.95	33,44,49,52	0
3	1PE	E	402	16/16	0.86	0.13	1.36	44,50,62,62	0
2	TLA	B	401	10/10	0.94	0.12	1.18	25,31,42,43	0
3	1PE	H	402	16/16	0.81	0.14	1.08	48,52,54,57	0
3	1PE	A	402	16/16	0.91	0.11	0.99	32,42,55,55	0
2	TLA	E	401	10/10	0.92	0.11	0.93	20,27,40,41	0
3	1PE	C	402	16/16	0.88	0.11	0.72	39,47,54,55	0
2	TLA	C	401	10/10	0.89	0.10	0.42	26,32,45,47	0
2	TLA	A	401	10/10	0.93	0.10	-0.10	21,25,32,34	0
3	1PE	A	405	7/16	0.94	0.10	-0.16	34,38,42,43	0
3	1PE	E	404	13/16	0.88	0.17	-	39,49,57,57	0
3	1PE	A	404	13/16	0.91	0.12	-	36,43,54,57	0

6.5 Other polymers (i)

There are no such residues in this entry.