Full wwPDB X-ray Structure Validation Report ⓘ

Jun 18, 2024 – 02:49 AM EDT

PDB ID	:	5UNM
Title	:	LarE, a sulfur transferase involved in synthesis of the cofactor for lactate racemase, substrate free form with flexible loop
Authors	:	Fellner, M.; Desguin, B.; Hausinger, R.P.; Hu, J.
Deposited on	:	2017-01-31
Resolution	:	2.58 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:

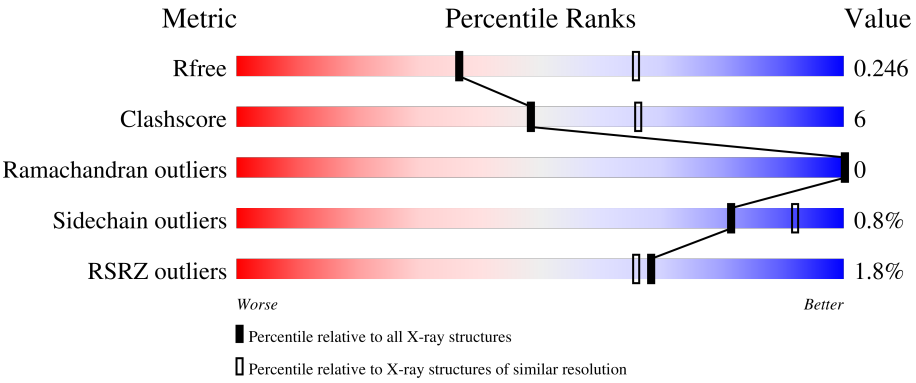
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.58 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	3676 (2.60-2.56)
Clashscore	141614	4049 (2.60-2.56)
Ramachandran outliers	138981	3979 (2.60-2.56)
Sidechain outliers	138945	3979 (2.60-2.56)
RSRZ outliers	127900	3614 (2.60-2.56)

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 <=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	286	2% 83% 11% 6%
1	B	286	2% 74% 16% 10%
1	C	286	77% 10% 12%
1	D	286	% 68% 15% 17%
1	E	286	3% 78% 13% 9%

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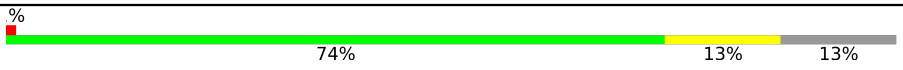
Mol	Chain	Length	Quality of chain
1	F	286	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 12024 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 ATP-utilizing enzyme of the PP-loopsuperfamily.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	269	Total	C	N	O	S	0	0	0
			2035	1283	355	391	6			
1	B	258	Total	C	N	O	S	0	1	0
			1982	1246	343	387	6			
1	C	251	Total	C	N	O	S	0	0	0
			1934	1221	339	368	6			
1	D	238	Total	C	N	O	S	0	0	0
			1802	1138	309	350	5			
1	E	261	Total	C	N	O	S	0	0	0
			1987	1257	338	385	7			
1	F	248	Total	C	N	O	S	0	0	0
			1901	1199	331	365	6			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	277	ALA	-	expression tag	UNP A0A0G9FES3
A	278	SER	-	expression tag	UNP A0A0G9FES3
A	279	TRP	-	expression tag	UNP A0A0G9FES3
A	280	SER	-	expression tag	UNP A0A0G9FES3
A	281	HIS	-	expression tag	UNP A0A0G9FES3
A	282	PRO	-	expression tag	UNP A0A0G9FES3
A	283	GLN	-	expression tag	UNP A0A0G9FES3
A	284	PHE	-	expression tag	UNP A0A0G9FES3
A	285	GLU	-	expression tag	UNP A0A0G9FES3
A	286	LYS	-	expression tag	UNP A0A0G9FES3
B	277	ALA	-	expression tag	UNP A0A0G9FES3
B	278	SER	-	expression tag	UNP A0A0G9FES3
B	279	TRP	-	expression tag	UNP A0A0G9FES3
B	280	SER	-	expression tag	UNP A0A0G9FES3
B	281	HIS	-	expression tag	UNP A0A0G9FES3
B	282	PRO	-	expression tag	UNP A0A0G9FES3
B	283	GLN	-	expression tag	UNP A0A0G9FES3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	284	PHE	-	expression tag	UNP A0A0G9FES3
B	285	GLU	-	expression tag	UNP A0A0G9FES3
B	286	LYS	-	expression tag	UNP A0A0G9FES3
C	277	ALA	-	expression tag	UNP A0A0G9FES3
C	278	SER	-	expression tag	UNP A0A0G9FES3
C	279	TRP	-	expression tag	UNP A0A0G9FES3
C	280	SER	-	expression tag	UNP A0A0G9FES3
C	281	HIS	-	expression tag	UNP A0A0G9FES3
C	282	PRO	-	expression tag	UNP A0A0G9FES3
C	283	GLN	-	expression tag	UNP A0A0G9FES3
C	284	PHE	-	expression tag	UNP A0A0G9FES3
C	285	GLU	-	expression tag	UNP A0A0G9FES3
C	286	LYS	-	expression tag	UNP A0A0G9FES3
D	277	ALA	-	expression tag	UNP A0A0G9FES3
D	278	SER	-	expression tag	UNP A0A0G9FES3
D	279	TRP	-	expression tag	UNP A0A0G9FES3
D	280	SER	-	expression tag	UNP A0A0G9FES3
D	281	HIS	-	expression tag	UNP A0A0G9FES3
D	282	PRO	-	expression tag	UNP A0A0G9FES3
D	283	GLN	-	expression tag	UNP A0A0G9FES3
D	284	PHE	-	expression tag	UNP A0A0G9FES3
D	285	GLU	-	expression tag	UNP A0A0G9FES3
D	286	LYS	-	expression tag	UNP A0A0G9FES3
E	277	ALA	-	expression tag	UNP A0A0G9FES3
E	278	SER	-	expression tag	UNP A0A0G9FES3
E	279	TRP	-	expression tag	UNP A0A0G9FES3
E	280	SER	-	expression tag	UNP A0A0G9FES3
E	281	HIS	-	expression tag	UNP A0A0G9FES3
E	282	PRO	-	expression tag	UNP A0A0G9FES3
E	283	GLN	-	expression tag	UNP A0A0G9FES3
E	284	PHE	-	expression tag	UNP A0A0G9FES3
E	285	GLU	-	expression tag	UNP A0A0G9FES3
E	286	LYS	-	expression tag	UNP A0A0G9FES3
F	277	ALA	-	expression tag	UNP A0A0G9FES3
F	278	SER	-	expression tag	UNP A0A0G9FES3
F	279	TRP	-	expression tag	UNP A0A0G9FES3
F	280	SER	-	expression tag	UNP A0A0G9FES3
F	281	HIS	-	expression tag	UNP A0A0G9FES3
F	282	PRO	-	expression tag	UNP A0A0G9FES3
F	283	GLN	-	expression tag	UNP A0A0G9FES3
F	284	PHE	-	expression tag	UNP A0A0G9FES3
F	285	GLU	-	expression tag	UNP A0A0G9FES3

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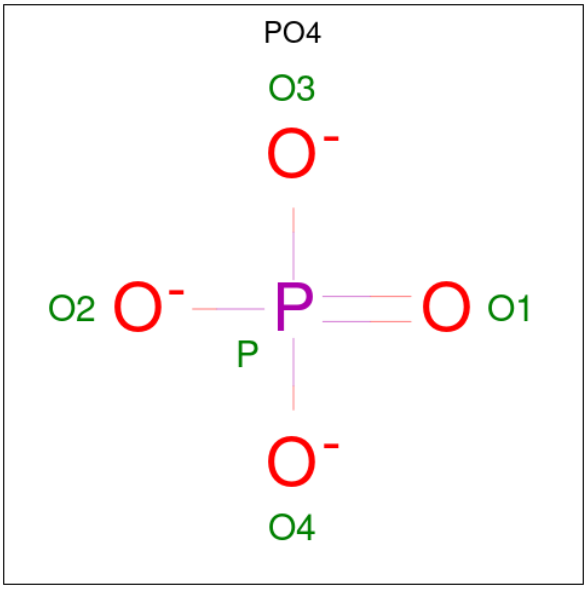
Chain	Residue	Modelled	Actual	Comment	Reference
F	286	LYS	-	expression tag	UNP A0A0G9FES3

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	46	Total O 46 46	0	0
3	B	56	Total O 56 56	0	0
3	C	84	Total O 84 84	0	0

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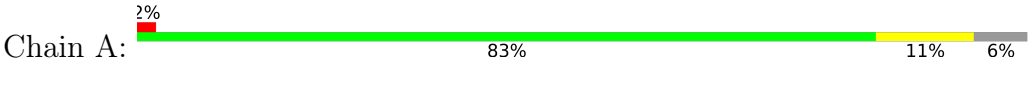
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	46	Total O 46 46	0	0
3	E	57	Total O 57 57	0	0
3	F	64	Total O 64 64	0	0

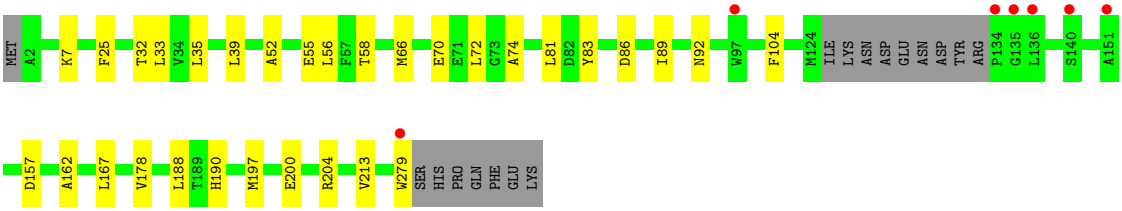
3 Residue-property plots (i)

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-utilizing enzyme of the PP-loopsuperfamily

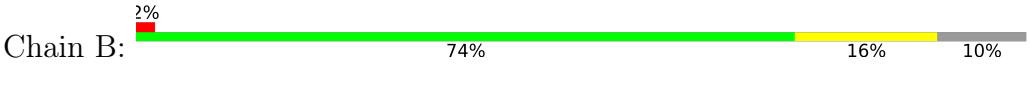
Chain A:

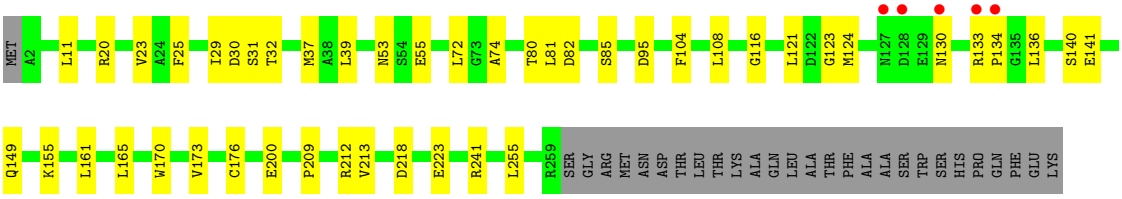




• Molecule 1: ATP-utilizing enzyme of the PP-loopsuperfamily

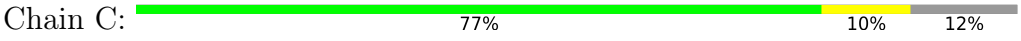
Chain B:

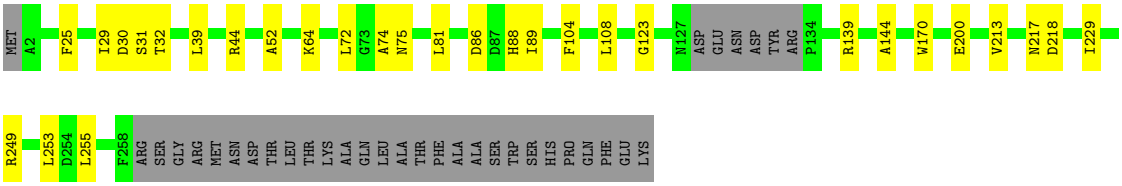




• Molecule 1: ATP-utilizing enzyme of the PP-loopsuperfamily

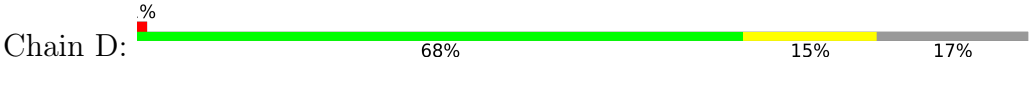
Chain C:

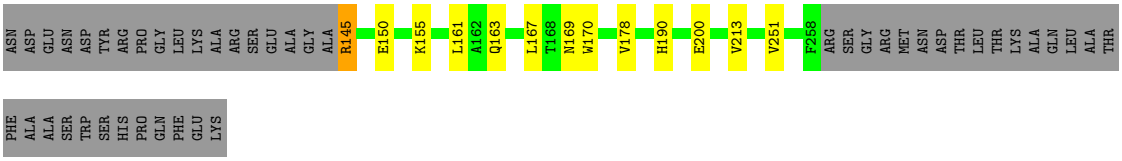




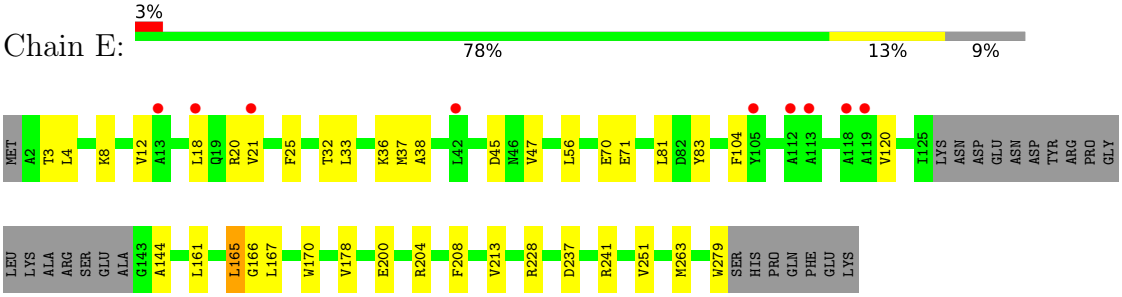
• Molecule 1: ATP-utilizing enzyme of the PP-loopsuperfamily

Chain D:

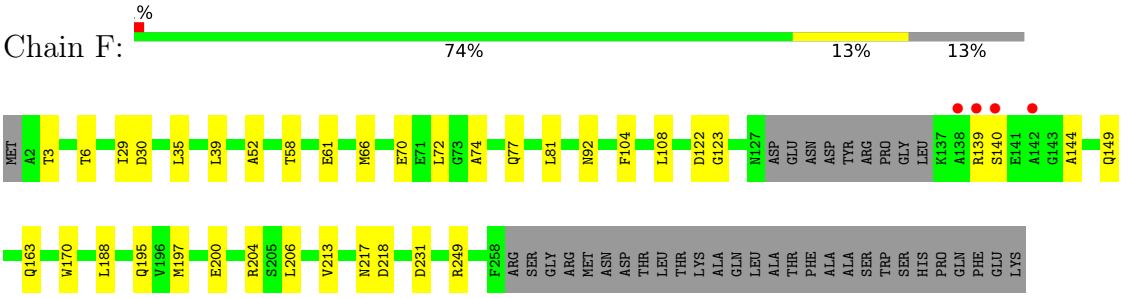




• Molecule 1: ATP-utilizing enzyme of the PP-loopsuperfamily



• Molecule 1: ATP-utilizing enzyme of the PP-loopsuperfamily



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 2 2	Depositor
Cell constants a, b, c, α, β, γ	107.34Å 107.34Å 318.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.83 – 2.58 48.83 – 2.58	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.83-2.58) 99.8 (48.83-2.58)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.93 (at 2.58Å)	Xtriage
Refinement program	PHENIX 1.11.1-2575	Depositor
R, R_{free}	0.189 , 0.243 0.194 , 0.246	Depositor DCC
R_{free} test set	2967 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	40.5	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 41.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	12024	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.04% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.35	0/2068	0.51	0/2806
1	B	0.38	0/2014	0.58	3/2733 (0.1%)
1	C	0.31	0/1964	0.51	0/2657
1	D	0.30	0/1830	0.49	0/2486
1	E	0.31	0/2019	0.54	0/2740
1	F	0.34	0/1930	0.54	1/2615 (0.0%)
All	All	0.33	0/11825	0.53	4/16037 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	204	ARG	NE-CZ-NH2	-6.34	117.13	120.30
1	B	136	LEU	N-CA-C	-5.55	96.00	111.00
1	B	95	ASP	CB-CG-OD1	5.31	123.08	118.30
1	B	140	SER	N-CA-C	5.01	124.53	111.00

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	2035	0	1971	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1982	0	1916	25	2
1	C	1934	0	1927	20	0
1	D	1802	0	1734	28	0
1	E	1987	0	1941	29	0
1	F	1901	0	1868	27	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
2	E	5	0	0	0	0
2	F	5	0	0	0	0
3	A	46	0	0	1	0
3	B	56	0	0	0	0
3	C	84	0	0	1	0
3	D	46	0	0	1	0
3	E	57	0	0	2	0
3	F	64	0	0	2	0
All	All	12024	0	11357	137	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 6.

All (137) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:ASN:HB3	1:B:133:ARG:O	1.80	0.81
1:F:218:ASP:HB2	1:F:249:ARG:HB3	1.66	0.77
1:B:124:MET:SD	1:B:149:GLN:NE2	2.58	0.76
1:C:44:ARG:NH1	1:C:75:ASN:OD1	2.22	0.72
1:E:33:LEU:HD12	1:E:33:LEU:O	1.91	0.70
1:B:141:GLU:HA	1:B:141:GLU:OE1	1.92	0.69
1:F:139:ARG:HG2	1:F:144:ALA:HB3	1.74	0.69
1:A:33:LEU:HD12	1:A:33:LEU:O	1.95	0.67
1:C:32:THR:HG23	1:C:72:LEU:HD11	1.77	0.66
1:F:231:ASP:OD1	3:F:401:HOH:O	2.13	0.66
1:B:82:ASP:OD2	1:B:85:SER:HB3	1.98	0.64
1:C:39:LEU:HD11	1:C:74:ALA:HB2	1.80	0.64
1:F:58:THR:HG22	1:F:197:MET:SD	2.38	0.64
1:E:204:ARG:NH2	3:E:404:HOH:O	2.30	0.63
1:B:39:LEU:HD11	1:B:74:ALA:HB2	1.80	0.63
1:D:58:THR:HG23	1:D:61:GLU:H	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:GLU:OE2	1:A:190:HIS:ND1	2.31	0.61
1:E:237:ASP:OD2	1:E:241:ARG:NH1	2.33	0.61
1:A:7:LYS:NZ	1:A:157:ASP:OD2	2.35	0.60
1:C:25:PHE:HA	1:C:31:SER:OG	2.02	0.59
1:A:32:THR:HG23	1:A:72:LEU:HD11	1.85	0.59
1:E:25:PHE:HE1	1:E:32:THR:HA	1.69	0.57
1:B:173:VAL:HG21	1:B:209:PRO:HB2	1.86	0.57
1:F:66:MET:O	1:F:70:GLU:HG3	2.04	0.57
1:C:30:ASP:HB3	1:C:123:GLY:O	2.04	0.57
1:F:39:LEU:HD11	1:F:74:ALA:HB2	1.86	0.56
1:B:200:GLU:HG2	1:B:213:VAL:HG23	1.87	0.56
1:C:139:ARG:HG2	1:C:144:ALA:HB3	1.87	0.56
1:A:204:ARG:NH1	3:A:401:HOH:O	2.35	0.55
1:F:139:ARG:HD3	1:F:144:ALA:O	2.06	0.55
1:E:81:LEU:HD23	1:E:83:TYR:CE1	2.42	0.55
1:C:217:ASN:ND2	3:C:407:HOH:O	2.40	0.54
1:E:4:LEU:HD11	1:E:161:LEU:HB2	1.89	0.54
1:A:39:LEU:HD11	1:A:74:ALA:HB2	1.90	0.53
1:B:32:THR:HG23	1:B:72:LEU:HD11	1.90	0.53
1:D:33:LEU:HD21	1:D:161:LEU:HD23	1.91	0.53
1:F:3:THR:HG23	1:F:6:THR:H	1.72	0.53
1:D:47:VAL:O	3:D:401:HOH:O	2.18	0.53
1:E:81:LEU:HD12	1:E:81:LEU:N	2.22	0.53
1:D:163:GLN:NE2	1:E:166:GLY:HA2	2.24	0.53
1:A:81:LEU:HD11	1:A:104:PHE:HD1	1.75	0.52
1:A:66:MET:O	1:A:70:GLU:HG3	2.09	0.52
1:A:56:LEU:HA	1:A:178:VAL:HG12	1.91	0.52
1:F:81:LEU:HD11	1:F:104:PHE:HD2	1.74	0.52
1:C:86:ASP:HB3	1:C:89:ILE:HD12	1.92	0.52
1:F:35:LEU:HD23	1:F:72:LEU:HD12	1.92	0.52
1:D:68:LEU:HD22	1:D:170:TRP:HA	1.93	0.51
1:B:25:PHE:HA	1:B:31:SER:OG	2.11	0.50
1:C:200:GLU:HG2	1:C:213:VAL:HG23	1.93	0.50
1:D:39:LEU:HD11	1:D:74:ALA:HB2	1.92	0.50
1:C:52:ALA:HB2	1:C:104:PHE:CE2	2.47	0.50
1:E:37:MET:SD	1:E:165:LEU:HD21	2.51	0.50
1:B:11:LEU:HD21	1:B:37:MET:HG3	1.94	0.49
1:F:122:ASP:OD2	1:F:139:ARG:HG3	2.12	0.49
1:B:81:LEU:HD11	1:B:104:PHE:HD1	1.77	0.49
1:F:3:THR:CG2	1:F:6:THR:H	2.25	0.49
1:E:200:GLU:HG2	1:E:213:VAL:HG23	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:139:ARG:NH1	1:F:140:SER:OG	2.46	0.49
1:D:163:GLN:HE21	1:E:166:GLY:HA2	1.77	0.49
1:E:120:VAL:HG23	1:E:144:ALA:HA	1.95	0.49
1:D:86:ASP:HB3	1:D:89:ILE:HD12	1.94	0.48
1:F:29:ILE:HD12	1:F:170:TRP:CZ2	2.48	0.48
1:A:279:TRP:CD2	1:F:249:ARG:HD2	2.48	0.48
1:A:162:ALA:HA	1:A:167:LEU:HD12	1.95	0.48
1:B:23:VAL:HG22	1:B:121:LEU:HD12	1.93	0.48
1:B:20:ARG:HD3	1:B:116:GLY:C	2.34	0.48
1:F:52:ALA:HB2	1:F:104:PHE:CE2	2.49	0.48
1:F:58:THR:N	1:F:61:GLU:OE1	2.44	0.48
1:C:249:ARG:HB2	1:E:279:TRP:CZ2	2.49	0.47
1:C:29:ILE:HD13	1:C:170:TRP:CZ2	2.49	0.47
1:D:21:VAL:HB	1:D:121:LEU:CD2	2.45	0.47
1:D:21:VAL:HB	1:D:121:LEU:HD23	1.96	0.47
1:A:25:PHE:HE2	1:A:32:THR:HA	1.80	0.47
1:D:53:ASN:HB2	1:D:62:PHE:CD1	2.50	0.47
1:E:21:VAL:CG2	1:E:47:VAL:HG22	2.45	0.47
1:D:50:VAL:HA	1:D:77:GLN:O	2.16	0.46
1:D:25:PHE:HE2	1:D:32:THR:HA	1.79	0.46
1:E:263:MET:HB3	1:F:206:LEU:HD23	1.98	0.46
1:F:200:GLU:HG2	1:F:213:VAL:HG23	1.98	0.46
1:D:3:THR:O	1:D:6:THR:HG22	2.15	0.46
1:A:52:ALA:HB2	1:A:104:PHE:CE1	2.51	0.45
1:B:29:ILE:HD12	1:B:170:TRP:CZ2	2.50	0.45
1:B:255:LEU:HD12	1:D:251:VAL:HG12	1.97	0.45
1:C:81:LEU:HD11	1:C:104:PHE:HD2	1.80	0.45
1:E:161:LEU:O	1:E:165:LEU:HD13	2.17	0.45
1:D:71:GLU:OE1	1:D:169:ASN:ND2	2.46	0.45
1:A:35:LEU:HD23	1:A:72:LEU:HD12	1.99	0.44
1:D:4:LEU:HD11	1:D:161:LEU:HB2	1.99	0.44
1:C:104:PHE:CZ	1:C:108:LEU:HD11	2.52	0.44
1:E:208:PHE:HE2	1:E:228:ARG:HB3	1.82	0.44
1:A:83:TYR:HB3	1:A:89:ILE:HG21	1.98	0.44
1:C:255:LEU:HD12	1:E:251:VAL:HG12	2.00	0.44
1:B:161:LEU:O	1:B:165:LEU:HG	2.18	0.44
1:D:145:ARG:NH2	1:D:150:GLU:OE1	2.51	0.44
1:E:56:LEU:HA	1:E:178:VAL:HG12	2.00	0.44
1:B:53:ASN:O	1:B:80:THR:HA	2.18	0.44
1:A:86:ASP:HB3	1:A:89:ILE:HD12	1.99	0.44
1:D:167:LEU:HD23	1:F:163:GLN:HG3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:104:PHE:CZ	1:F:108:LEU:HD11	2.53	0.44
1:A:200:GLU:HG2	1:A:213:VAL:HG23	1.99	0.44
1:C:218:ASP:HB2	1:C:249:ARG:HB3	1.99	0.43
1:B:25:PHE:HD2	1:B:31:SER:HG	1.65	0.43
1:B:104:PHE:CZ	1:B:108:LEU:HD11	2.53	0.43
1:C:86:ASP:OD1	1:C:88:HIS:HB2	2.18	0.43
1:F:217:ASN:ND2	3:F:402:HOH:O	2.21	0.43
1:B:241[B]:ARG:NH2	1:E:241:ARG:HH22	2.17	0.43
1:C:229:ILE:HG23	1:C:253:LEU:HD21	2.00	0.43
1:F:30:ASP:HB3	1:F:123:GLY:O	2.19	0.43
1:E:18:LEU:O	1:E:20:ARG:N	2.45	0.43
1:E:45:ASP:OD1	3:E:401:HOH:O	2.21	0.43
1:F:92:ASN:HB2	1:F:188:LEU:CD1	2.49	0.43
1:F:218:ASP:OD1	1:F:218:ASP:N	2.52	0.43
1:D:56:LEU:HA	1:D:178:VAL:HG12	2.00	0.42
1:E:38:ALA:HB1	1:E:47:VAL:HG21	2.01	0.42
1:D:2:ALA:HB3	1:E:70:GLU:OE2	2.20	0.42
1:E:8:LYS:O	1:E:12:VAL:HG23	2.20	0.42
1:B:155:LYS:HD2	1:B:155:LYS:HA	1.94	0.42
1:D:3:THR:N	1:D:6:THR:HG22	2.34	0.42
1:C:64:LYS:HA	1:C:64:LYS:HD2	1.84	0.41
1:E:81:LEU:HD21	1:E:104:PHE:HA	2.01	0.41
1:B:218:ASP:OD1	1:B:218:ASP:N	2.53	0.41
1:D:3:THR:H	1:D:6:THR:HG22	1.85	0.41
1:A:92:ASN:HB2	1:A:188:LEU:CD1	2.51	0.41
1:B:134:PRO:CG	1:B:176:CYS:SG	3.09	0.41
1:F:139:ARG:NH2	1:F:149:GLN:OE1	2.53	0.41
1:A:58:THR:HG22	1:A:197:MET:SD	2.60	0.41
1:D:36:LYS:HB2	1:D:72:LEU:HD23	2.02	0.41
1:E:3:THR:HG22	1:F:70:GLU:OE1	2.21	0.41
1:E:167:LEU:O	1:E:170:TRP:HZ3	2.02	0.41
1:D:30:ASP:HB3	1:D:123:GLY:O	2.21	0.40
1:C:29:ILE:HD13	1:C:170:TRP:CE2	2.56	0.40
1:D:200:GLU:HG2	1:D:213:VAL:HG23	2.03	0.40
1:D:32:THR:HG23	1:D:72:LEU:HD21	2.03	0.40
1:E:36:LYS:HG3	1:E:165:LEU:HD23	2.04	0.40
1:B:30:ASP:HB3	1:B:123:GLY:O	2.21	0.40
1:B:212:ARG:HB2	1:B:223:GLU:HB2	2.02	0.40
1:D:83:TYR:HB3	1:D:89:ILE:HG21	2.04	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:B:55:GLU:CD	1:B:55:GLU:OE2[8_555]	1.26	0.94
1:B:55:GLU:OE1	1:B:55:GLU:OE2[8_555]	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	265/286 (93%)	258 (97%)	7 (3%)	0	100	100
1	B	257/286 (90%)	248 (96%)	9 (4%)	0	100	100
1	C	247/286 (86%)	242 (98%)	5 (2%)	0	100	100
1	D	234/286 (82%)	229 (98%)	5 (2%)	0	100	100
1	E	257/286 (90%)	252 (98%)	5 (2%)	0	100	100
1	F	244/286 (85%)	238 (98%)	6 (2%)	0	100	100
All	All	1504/1716 (88%)	1467 (98%)	37 (2%)	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	205/236 (87%)	205 (100%)	0	100	100
1	B	204/236 (86%)	204 (100%)	0	100	100
1	C	203/236 (86%)	203 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	183/236 (78%)	178 (97%)	5 (3%)	44 68
1	E	206/236 (87%)	204 (99%)	2 (1%)	76 89
1	F	197/236 (84%)	195 (99%)	2 (1%)	76 89
All	All	1198/1416 (85%)	1189 (99%)	9 (1%)	81 92

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	101	LYS
1	D	110	ASP
1	D	145	ARG
1	D	155	LYS
1	D	190	HIS
1	E	71	GLU
1	E	165	LEU
1	F	77	GLN
1	F	195	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

6 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	A	301	-	4,4,4	0.94	0	6,6,6	0.44	0
2	PO4	E	301	-	4,4,4	0.89	0	6,6,6	0.55	0
2	PO4	D	301	-	4,4,4	0.86	0	6,6,6	0.46	0
2	PO4	C	301	-	4,4,4	0.95	0	6,6,6	0.46	0
2	PO4	F	301	-	4,4,4	0.85	0	6,6,6	0.57	0
2	PO4	B	301	-	4,4,4	0.89	0	6,6,6	0.47	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, 95^{th} 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	269/286 (94%)	0.06	7 (2%) 56 52	24, 53, 89, 104	0
1	B	258/286 (90%)	-0.05	5 (1%) 66 64	25, 46, 86, 113	0
1	C	251/286 (87%)	-0.12	0 100 100	23, 36, 69, 92	0
1	D	238/286 (83%)	0.04	2 (0%) 86 85	29, 53, 80, 97	0
1	E	261/286 (91%)	0.15	9 (3%) 45 41	24, 53, 88, 105	0
1	F	248/286 (86%)	-0.11	4 (1%) 72 69	24, 42, 68, 102	0
All	All	1525/1716 (88%)	-0.00	27 (1%) 68 66	23, 46, 82, 113	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	113	ALA	3.8
1	B	133	ARG	3.5
1	A	134	PRO	3.4
1	F	140	SER	3.1
1	F	138	ALA	3.1
1	F	142	ALA	3.1
1	A	279	TRP	3.0
1	E	105	TYR	2.9
1	A	136	LEU	2.7
1	E	18	LEU	2.7
1	E	118	ALA	2.6
1	A	140	SER	2.5
1	A	151	ALA	2.4
1	F	139	ARG	2.4
1	B	130	ASN	2.3
1	B	127	ASN	2.3
1	E	112	ALA	2.2
1	E	119	ALA	2.2
1	E	21	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	118	ALA	2.2
1	A	135	GLY	2.1
1	B	134	PRO	2.1
1	B	128	ASP	2.0
1	A	97	TRP	2.0
1	E	13	ALA	2.0
1	D	125	ILE	2.0
1	E	42	LEU	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, 95^{th} 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	D	301	5/5	0.89	0.23	61,74,83,84	5
2	PO4	B	301	5/5	0.90	0.28	49,61,67,83	5
2	PO4	F	301	5/5	0.92	0.20	30,45,54,62	5
2	PO4	E	301	5/5	0.93	0.18	32,52,65,67	5
2	PO4	A	301	5/5	0.93	0.23	30,41,50,65	5
2	PO4	C	301	5/5	0.95	0.22	51,53,57,58	5

6.5 Other polymers (i)

There are no such residues in this entry.