Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 07:14 am BST

PDB ID	:	5LK6
Title	:	Crystal structure of a lipase carboxylesterase from Sulfolobus islandicus
Authors	:	Schwarz-Linnet, T.; Teilum, K.; Olsen, J.G.
Deposited on	:	2016-07-21
Resolution	:	2.60 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:

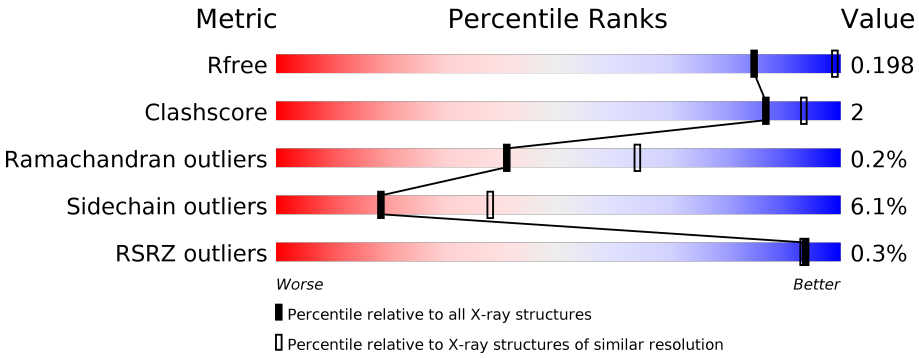
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 <=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	314	86% 9%
1	B	314	84% 10%
1	C	314	% 84% 10%
1	D	314	84% 11%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9846 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 Alpha/beta hydrolase fold-3 domain protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	302	Total	C	N	O	S	0	0	0
			2342	1514	391	432	5			
1	B	302	Total	C	N	O	S	0	0	0
			2342	1514	391	432	5			
1	C	302	Total	C	N	O	S	0	0	0
			2342	1514	391	432	5			
1	D	302	Total	C	N	O	S	0	0	0
			2342	1514	391	432	5			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	306	ALA	-	expression tag	UNP F0NDQ1
A	307	ALA	-	expression tag	UNP F0NDQ1
A	308	ALA	-	expression tag	UNP F0NDQ1
A	309	HIS	-	expression tag	UNP F0NDQ1
A	310	HIS	-	expression tag	UNP F0NDQ1
A	311	HIS	-	expression tag	UNP F0NDQ1
A	312	HIS	-	expression tag	UNP F0NDQ1
A	313	HIS	-	expression tag	UNP F0NDQ1
A	314	HIS	-	expression tag	UNP F0NDQ1
B	306	ALA	-	expression tag	UNP F0NDQ1
B	307	ALA	-	expression tag	UNP F0NDQ1
B	308	ALA	-	expression tag	UNP F0NDQ1
B	309	HIS	-	expression tag	UNP F0NDQ1
B	310	HIS	-	expression tag	UNP F0NDQ1
B	311	HIS	-	expression tag	UNP F0NDQ1
B	312	HIS	-	expression tag	UNP F0NDQ1
B	313	HIS	-	expression tag	UNP F0NDQ1
B	314	HIS	-	expression tag	UNP F0NDQ1
C	306	ALA	-	expression tag	UNP F0NDQ1
C	307	ALA	-	expression tag	UNP F0NDQ1
C	308	ALA	-	expression tag	UNP F0NDQ1

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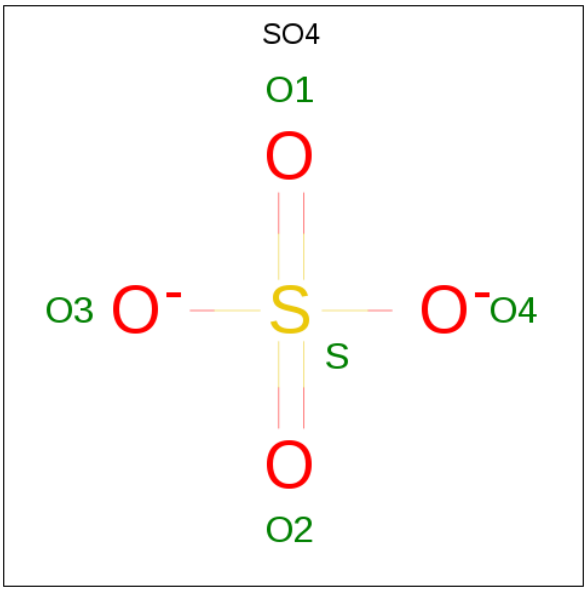
Chain	Residue	Modelled	Actual	Comment	Reference
C	309	HIS	-	expression tag	UNP F0NDQ1
C	310	HIS	-	expression tag	UNP F0NDQ1
C	311	HIS	-	expression tag	UNP F0NDQ1
C	312	HIS	-	expression tag	UNP F0NDQ1
C	313	HIS	-	expression tag	UNP F0NDQ1
C	314	HIS	-	expression tag	UNP F0NDQ1
D	306	ALA	-	expression tag	UNP F0NDQ1
D	307	ALA	-	expression tag	UNP F0NDQ1
D	308	ALA	-	expression tag	UNP F0NDQ1
D	309	HIS	-	expression tag	UNP F0NDQ1
D	310	HIS	-	expression tag	UNP F0NDQ1
D	311	HIS	-	expression tag	UNP F0NDQ1
D	312	HIS	-	expression tag	UNP F0NDQ1
D	313	HIS	-	expression tag	UNP F0NDQ1
D	314	HIS	-	expression tag	UNP F0NDQ1

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0

- Molecule 3 is water.

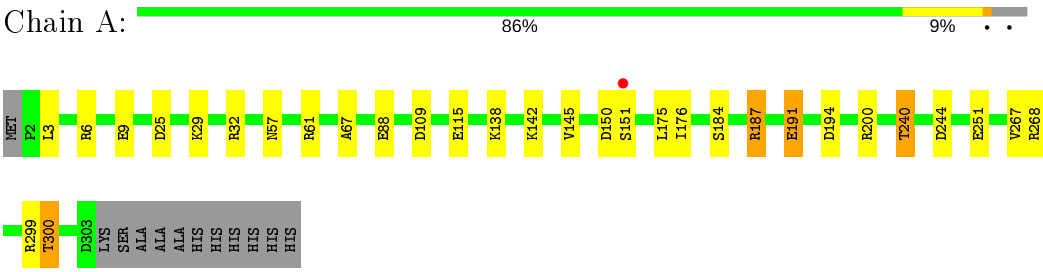
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	104	Total O 104 104	0	0
3	B	118	Total O 118 118	0	0
3	C	109	Total O 109 109	0	0
3	D	107	Total O 107 107	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

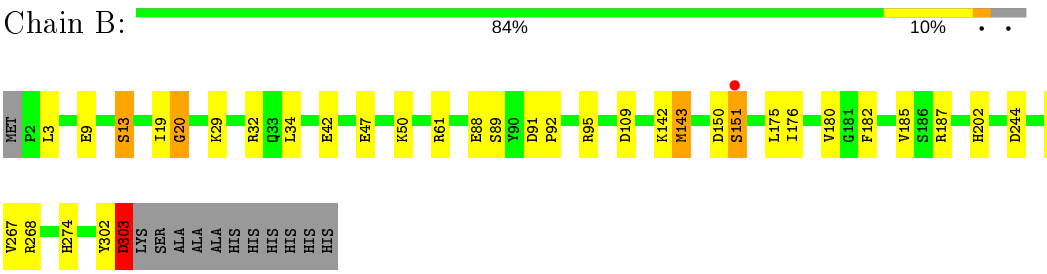
- Molecule 1: Alpha/beta hydrolase fold-3 domain protein

Chain A:



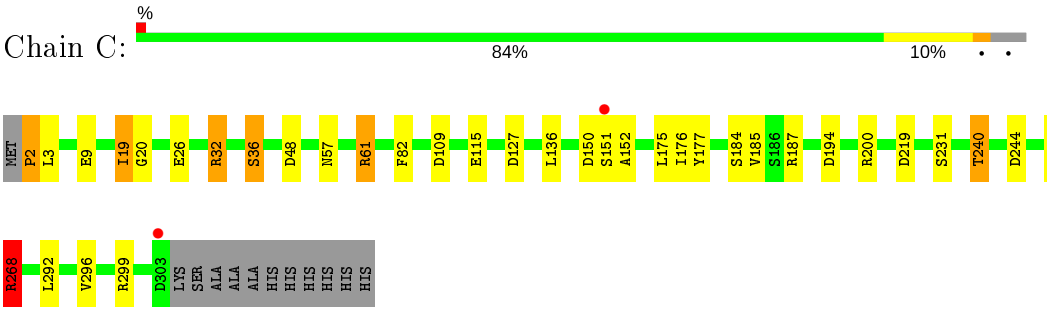
- Molecule 1: Alpha/beta hydrolase fold-3 domain protein

Chain B:



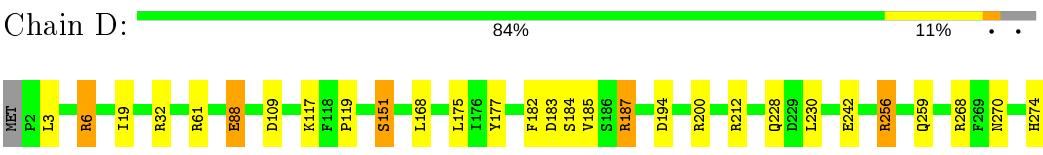
- Molecule 1: Alpha/beta hydrolase fold-3 domain protein

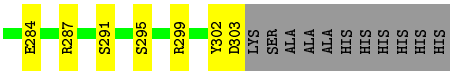
Chain C:



- Molecule 1: Alpha/beta hydrolase fold-3 domain protein

Chain D:




E284
R287
S291
S295
R299
Y302
D303
LYS
SER
ALA
ALA
HIS
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	166.41Å 166.41Å 185.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.42 – 2.60 29.42 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.3 (29.42-2.60) 98.4 (29.42-2.60)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	0.14	Depositor
$< I/\sigma(I) >$ [1]	4.59 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.157 , 0.194 0.165 , 0.198	Depositor DCC
R_{free} test set	3952 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	27.0	Xtriage
Anisotropy	0.098	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 30.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9846	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.55% 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: SO4

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	1.02	6/2397 (0.3%)	1.03	12/3257 (0.4%)
1	B	0.98	6/2397 (0.3%)	1.03	14/3257 (0.4%)
1	C	1.05	11/2397 (0.5%)	1.05	12/3257 (0.4%)
1	D	1.04	7/2397 (0.3%)	1.06	17/3257 (0.5%)
All	All	1.02	30/9588 (0.3%)	1.04	55/13028 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	D	0	1
All	All	0	2

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	151	SER	CB-OG	12.56	1.58	1.42
1	C	151	SER	CB-OG	11.50	1.57	1.42
1	A	151	SER	CB-OG	11.39	1.57	1.42
1	C	151	SER	CA-CB	11.14	1.69	1.52
1	A	151	SER	CA-CB	10.98	1.69	1.52
1	D	151	SER	CB-OG	10.57	1.55	1.42
1	D	151	SER	CA-CB	9.75	1.67	1.52
1	D	88	GLU	CG-CD	8.99	1.65	1.51
1	B	151	SER	CA-CB	7.98	1.65	1.52
1	C	115	GLU	CG-CD	7.43	1.63	1.51
1	C	151	SER	N-CA	7.23	1.60	1.46
1	A	151	SER	N-CA	7.05	1.60	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	88	GLU	CB-CG	6.61	1.64	1.52
1	C	115	GLU	CD-OE2	6.49	1.32	1.25
1	D	151	SER	N-CA	6.46	1.59	1.46
1	B	151	SER	N-CA	6.34	1.59	1.46
1	A	88	GLU	CG-CD	6.13	1.61	1.51
1	C	231	SER	CB-OG	-6.09	1.34	1.42
1	C	9	GLU	CD-OE2	5.82	1.32	1.25
1	B	9	GLU	CG-CD	5.72	1.60	1.51
1	B	88	GLU	CG-CD	5.68	1.60	1.51
1	B	88	GLU	CD-OE1	5.67	1.31	1.25
1	C	26	GLU	CG-CD	5.56	1.60	1.51
1	D	279	PHE	CG-CD1	5.43	1.47	1.38
1	A	88	GLU	CD-OE1	5.40	1.31	1.25
1	C	115	GLU	CD-OE1	5.36	1.31	1.25
1	D	284	GLU	CG-CD	5.35	1.59	1.51
1	A	191	GLU	CD-OE1	5.32	1.31	1.25
1	C	26	GLU	CD-OE1	5.24	1.31	1.25
1	C	32	ARG	CZ-NH1	5.03	1.39	1.33

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	268	ARG	NE-CZ-NH2	-11.96	114.32	120.30
1	C	268	ARG	NE-CZ-NH1	9.04	124.82	120.30
1	A	194	ASP	CB-CG-OD1	-7.65	111.41	118.30
1	D	88	GLU	OE1-CD-OE2	-7.21	114.65	123.30
1	A	200	ARG	NE-CZ-NH2	-7.13	116.73	120.30
1	B	303	ASP	CB-CG-OD1	-6.98	112.02	118.30
1	C	194	ASP	CB-CG-OD1	-6.81	112.17	118.30
1	A	151	SER	N-CA-CB	6.78	120.67	110.50
1	D	88	GLU	CB-CA-C	6.73	123.86	110.40
1	A	299	ARG	NE-CZ-NH2	-6.72	116.94	120.30
1	D	200	ARG	NE-CZ-NH2	-6.61	116.99	120.30
1	D	194	ASP	CB-CG-OD1	-6.50	112.45	118.30
1	D	268	ARG	NE-CZ-NH2	-6.42	117.09	120.30
1	C	244	ASP	CB-CG-OD1	6.42	124.08	118.30
1	A	200	ARG	NE-CZ-NH1	6.41	123.50	120.30
1	D	200	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	D	151	SER	CA-CB-OG	6.21	127.97	111.20
1	B	32	ARG	NE-CZ-NH1	6.21	123.40	120.30
1	D	268	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	D	151	SER	CB-CA-C	5.90	121.31	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	95	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	C	151	SER	N-CA-CB	5.83	119.25	110.50
1	D	187	ARG	NE-CZ-NH1	5.81	123.20	120.30
1	A	151	SER	CA-CB-OG	5.67	126.52	111.20
1	B	151	SER	N-CA-CB	5.67	119.01	110.50
1	A	151	SER	N-CA-C	-5.62	95.82	111.00
1	B	256	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	D	19	ILE	C-N-CA	-5.62	110.50	122.30
1	B	244	ASP	CB-CG-OD1	5.60	123.34	118.30
1	B	143	MET	CG-SD-CE	5.59	109.14	100.20
1	D	259	GLN	CA-CB-CG	5.57	125.65	113.40
1	D	256	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	C	231	SER	CB-CA-C	-5.52	99.60	110.10
1	A	32	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	D	32	ARG	NE-CZ-NH2	-5.39	117.60	120.30
1	A	244	ASP	CB-CG-OD1	5.37	123.14	118.30
1	B	61	ARG	NE-CZ-NH2	-5.37	117.61	120.30
1	C	200	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	B	151	SER	CA-CB-OG	5.29	125.47	111.20
1	C	219	ASP	CB-CG-OD2	-5.29	113.54	118.30
1	B	256	ARG	CB-CA-C	5.26	120.92	110.40
1	A	61	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	B	268	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	C	3	LEU	CB-CG-CD2	-5.22	102.12	111.00
1	B	61	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	C	151	SER	CA-CB-OG	5.21	125.26	111.20
1	A	187	ARG	CG-CD-NE	-5.20	100.88	111.80
1	B	32	ARG	NE-CZ-NH2	-5.19	117.71	120.30
1	A	151	SER	CB-CA-C	5.17	119.93	110.10
1	B	151	SER	CB-CA-C	5.15	119.89	110.10
1	C	187	ARG	NE-CZ-NH2	-5.15	117.72	120.30
1	D	212	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	D	183	ASP	CB-CG-OD1	5.09	122.88	118.30
1	C	127	ASP	CB-CG-OD1	5.03	122.83	118.30
1	D	268	ARG	CB-CG-CD	-5.01	98.59	111.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	20	GLY	Peptide
1	D	184	SER	Peptide

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	2342	0	2342	6	0
1	B	2342	0	2342	9	0
1	C	2342	0	2342	17	0
1	D	2342	0	2342	11	0
2	A	10	0	0	0	0
2	B	10	0	0	0	0
2	C	15	0	0	0	0
2	D	5	0	0	0	0
3	A	104	0	0	0	0
3	B	118	0	0	0	0
3	C	109	0	0	7	0
3	D	107	0	0	5	0
All	All	9846	0	9368	40	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 (40) 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:20:GLY:N	3:C:501:HOH:O	1.74	1.14
1:C:36:SER:HB2	3:C:532:HOH:O	1.69	0.91
1:C:19:ILE:O	3:C:502:HOH:O	1.89	0.88
1:C:240:THR:HG21	1:C:251:GLU:OE2	1.82	0.80
1:B:302:TYR:O	1:B:303:ASP:HB2	1.87	0.72
1:D:88:GLU:HG3	3:D:517:HOH:O	1.91	0.68
1:C:19:ILE:CA	3:C:501:HOH:O	2.44	0.66
1:C:48:ASP:OD1	1:C:61:ARG:HG2	1.97	0.65
1:B:302:TYR:O	1:B:303:ASP:CB	2.47	0.62
1:D:256:ARG:HD2	3:D:568:HOH:O	2.00	0.61
1:C:2:PRO:HB3	3:C:590:HOH:O	2.02	0.60
1:A:240:THR:HG21	1:A:251:GLU:OE2	2.01	0.59
1:D:117:LYS:HE3	3:D:558:HOH:O	2.06	0.55
1:C:292:LEU:O	1:C:296:VAL:HG13	2.09	0.52
1:D:117:LYS:CE	3:D:558:HOH:O	2.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:240:THR:HG22	1:C:268:ARG:HA	1.91	0.50
1:C:32:ARG:HD3	3:C:602:HOH:O	2.13	0.48
1:B:150:ASP:HA	1:B:176:ILE:O	2.13	0.48
1:D:151:SER:HB2	1:D:274:HIS:NE2	2.28	0.48
1:D:302:TYR:O	1:D:303:ASP:CG	2.52	0.48
1:A:191:GLU:OE2	1:C:2:PRO:HB2	2.14	0.48
1:B:151:SER:HB2	1:B:274:HIS:NE2	2.29	0.47
1:D:230:LEU:CD1	1:D:256:ARG:HG2	2.45	0.47
1:C:251:GLU:OE2	1:C:268:ARG:HD3	2.14	0.46
1:A:267:VAL:HG13	1:B:267:VAL:HG13	1.98	0.45
1:A:150:ASP:HA	1:A:176:ILE:O	2.16	0.45
1:D:242:GLU:HB2	1:D:270:ASN:HA	1.98	0.45
1:A:240:THR:HG22	1:A:268:ARG:HA	1.98	0.45
1:C:299:ARG:NH1	1:D:287:ARG:O	2.50	0.45
1:C:150:ASP:HA	1:C:176:ILE:O	2.17	0.44
1:D:6:ARG:NH2	3:D:502:HOH:O	2.39	0.43
1:B:19:ILE:HB	1:B:202:HIS:ND1	2.33	0.43
1:C:82:PHE:CE1	1:C:152:ALA:HB1	2.54	0.42
1:B:91:ASP:HB3	1:B:92:PRO:HD3	2.00	0.42
1:C:32:ARG:NH2	3:C:510:HOH:O	2.53	0.42
1:D:280:PHE:N	1:D:281:PRO:CD	2.83	0.41
1:B:180:VAL:HG22	1:B:249:GLN:HG3	2.03	0.41
1:C:247:ARG:HD2	1:C:268:ARG:HD2	2.01	0.41
1:A:296:VAL:O	1:A:300:THR:HG23	2.20	0.41
1:B:19:ILE:O	1:B:20:GLY:C	2.59	0.41

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	300/314 (96%)	284 (95%)	15 (5%)	1 (0%)	41 64

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	300/314 (96%)	283 (94%)	16 (5%)	1 (0%)	41 64
1	C	300/314 (96%)	282 (94%)	17 (6%)	1 (0%)	41 64
1	D	300/314 (96%)	287 (96%)	13 (4%)	0	100 100
All	All	1200/1256 (96%)	1136 (95%)	61 (5%)	3 (0%)	41 64

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	67	ALA
1	B	13	SER
1	C	19	ILE

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	250/259 (96%)	233 (93%)	17 (7%)	16 32
1	B	250/259 (96%)	233 (93%)	17 (7%)	16 32
1	C	250/259 (96%)	238 (95%)	12 (5%)	25 49
1	D	250/259 (96%)	235 (94%)	15 (6%)	19 39
All	All	1000/1036 (96%)	939 (94%)	61 (6%)	18 38

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
1	A	6	ARG
1	A	9	GLU
1	A	25	ASP
1	A	29	LYS
1	A	57	ASN
1	A	109	ASP
1	A	115	GLU

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Mol	Chain	Res	Type
1	A	138	LYS
1	A	142	LYS
1	A	145	VAL
1	A	175	LEU
1	A	184	SER
1	A	187	ARG
1	A	240	THR
1	A	282	LEU
1	A	300	THR
1	B	3	LEU
1	B	13	SER
1	B	29	LYS
1	B	34	LEU
1	B	42	GLU
1	B	47	GLU
1	B	50	LYS
1	B	89	SER
1	B	109	ASP
1	B	142	LYS
1	B	143	MET
1	B	175	LEU
1	B	182	PHE
1	B	185	VAL
1	B	187	ARG
1	B	256	ARG
1	B	303	ASP
1	C	2	PRO
1	C	36	SER
1	C	57	ASN
1	C	61	ARG
1	C	109	ASP
1	C	136	LEU
1	C	175	LEU
1	C	177	TYR
1	C	184	SER
1	C	185	VAL
1	C	240	THR
1	C	268	ARG
1	D	3	LEU
1	D	6	ARG
1	D	61	ARG
1	D	109	ASP

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Mol	Chain	Res	Type
1	D	119	PRO
1	D	168	LEU
1	D	175	LEU
1	D	177	TYR
1	D	182	PHE
1	D	185	VAL
1	D	187	ARG
1	D	228	GLN
1	D	291	SER
1	D	295	SER
1	D	299	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	259	GLN
1	C	57	ASN
1	D	57	ASN
1	D	228	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)

8 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	SO4	D	401	-	4,4,4	0.15	0	6,6,6	0.81	0
2	SO4	B	401	-	4,4,4	0.54	0	6,6,6	1.77	2 (33%)
2	SO4	C	401	-	4,4,4	0.45	0	6,6,6	0.84	0
2	SO4	A	402	-	4,4,4	0.76	0	6,6,6	1.10	1 (16%)
2	SO4	C	402	-	4,4,4	0.34	0	6,6,6	0.82	0
2	SO4	C	403	-	4,4,4	0.43	0	6,6,6	0.91	0
2	SO4	B	402	-	4,4,4	0.50	0	6,6,6	1.11	0
2	SO4	A	401	-	4,4,4	0.71	0	6,6,6	1.37	2 (33%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	401	SO4	O4-S-O2	2.59	122.81	109.31
2	A	401	SO4	O4-S-O3	-2.28	99.33	109.06
2	B	401	SO4	O4-S-O3	-2.27	99.36	109.06
2	A	401	SO4	O3-S-O2	2.11	120.32	109.31
2	A	402	SO4	O4-S-O3	-2.05	100.29	109.06

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

There are no such residues in this entry.

5.8 Polymer linkage issues

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	302/314 (96%)	-0.76	1 (0%)	94	93	15, 26, 49, 65	0
1	B	302/314 (96%)	-0.80	1 (0%)	94	93	16, 24, 50, 72	0
1	C	302/314 (96%)	-0.73	2 (0%)	87	86	16, 26, 46, 73	0
1	D	302/314 (96%)	-0.88	0	100	100	15, 23, 45, 69	0
All	All	1208/1256 (96%)	-0.79	4 (0%)	94	93	15, 24, 47, 73	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	151	SER	2.5
1	C	151	SER	2.2
1	A	151	SER	2.1
1	C	303	ASP	2.1

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

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

6.3 Carbohydrates

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, 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	SO4	C	401	5/5	0.97	0.17	42,45,54,57	0
2	SO4	B	402	5/5	0.97	0.14	55,56,60,65	0
2	SO4	C	403	5/5	0.98	0.19	42,49,52,57	0
2	SO4	A	402	5/5	0.98	0.23	53,53,55,60	0
2	SO4	C	402	5/5	0.99	0.14	31,31,34,35	0
2	SO4	D	401	5/5	0.99	0.13	28,29,31,32	0
2	SO4	B	401	5/5	0.99	0.15	34,34,36,36	0
2	SO4	A	401	5/5	0.99	0.16	31,32,33,37	0

6.5 Other polymers (i)

There are no such residues in this entry.