Full wwPDB X-ray Structure Validation Report (i)

Sep 2, 2023 – 08:53 PM EDT

PDB ID	:	3QFH
Title	:	2.05 Angstrom Resolution Crystal Structure of Epidermin Leader Peptide Processing Serine Protease (EpiP) from Staphylococcus aureus.
Authors	:	Minasov, G.; Halavaty, A.; Shuvalova, L.; Dubrovska, I.; Winsor, J.; Bagnoli, F.; Falugi, F.; Bottomley, M.; Grandi, G.; Anderson, W.F.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on	:	2011-01-21
Resolution	:	2.05 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 (i) 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 (i)) were used in the production of this report:

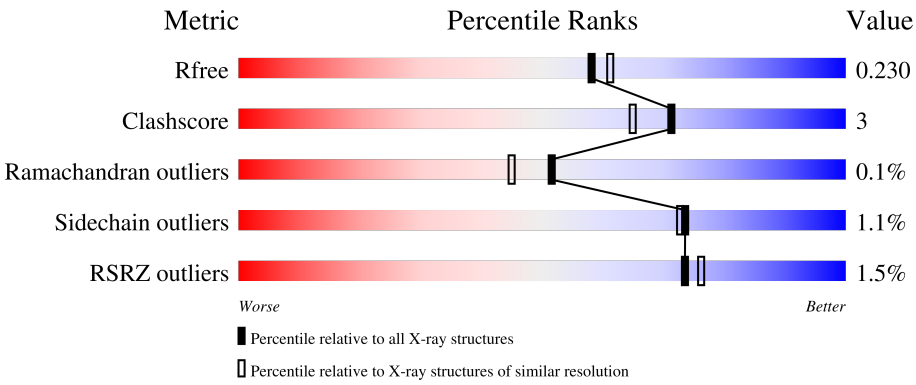
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 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 2.05 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	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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	447	.% 87% 8% 5%
1	B	447	.% 87% 8% • 5%
1	C	447	2% 85% 10% 6%
1	D	447	2% 87% 8% 5%

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Mol	Chain	Length	Quality of chain
1	E	447	2% 90% 5% 5%
1	F	447	% 87% 9% 5%
1	G	447	% 86% 8% 6%
1	H	447	% 87% 8% 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
5	SO4	B	458	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 28510 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 Epidermin leader peptide processing serine protease EpiP.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	424	3344	2092	584	655	13	0	3	0
1	B	425	3370	2110	589	659	12	0	5	0
1	C	421	3344	2091	586	656	11	0	5	0
1	D	426	3351	2098	584	656	13	0	2	0
1	E	426	3343	2093	583	655	12	0	1	0
1	F	426	3350	2097	584	657	12	0	2	0
1	G	421	3309	2073	578	647	11	0	1	0
1	H	426	3352	2098	585	657	12	0	2	0

There are 136 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-16	MET	-	expression tag	UNP Q5HEV5
A	-15	GLY	-	expression tag	UNP Q5HEV5
A	-14	SER	-	expression tag	UNP Q5HEV5
A	-13	SER	-	expression tag	UNP Q5HEV5
A	-12	HIS	-	expression tag	UNP Q5HEV5
A	-11	HIS	-	expression tag	UNP Q5HEV5
A	-10	HIS	-	expression tag	UNP Q5HEV5
A	-9	TYR	-	expression tag	UNP Q5HEV5
A	-8	HIS	-	expression tag	UNP Q5HEV5
A	-7	HIS	-	expression tag	UNP Q5HEV5
A	-6	GLU	-	expression tag	UNP Q5HEV5
A	-5	ASN	-	expression tag	UNP Q5HEV5
A	-4	LEU	-	expression tag	UNP Q5HEV5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	TYR	-	expression tag	UNP Q5HEV5
A	-2	PHE	-	expression tag	UNP Q5HEV5
A	-1	GLN	-	expression tag	UNP Q5HEV5
A	0	GLY	-	expression tag	UNP Q5HEV5
B	-16	MET	-	expression tag	UNP Q5HEV5
B	-15	GLY	-	expression tag	UNP Q5HEV5
B	-14	SER	-	expression tag	UNP Q5HEV5
B	-13	SER	-	expression tag	UNP Q5HEV5
B	-12	HIS	-	expression tag	UNP Q5HEV5
B	-11	HIS	-	expression tag	UNP Q5HEV5
B	-10	HIS	-	expression tag	UNP Q5HEV5
B	-9	TYR	-	expression tag	UNP Q5HEV5
B	-8	HIS	-	expression tag	UNP Q5HEV5
B	-7	HIS	-	expression tag	UNP Q5HEV5
B	-6	GLU	-	expression tag	UNP Q5HEV5
B	-5	ASN	-	expression tag	UNP Q5HEV5
B	-4	LEU	-	expression tag	UNP Q5HEV5
B	-3	TYR	-	expression tag	UNP Q5HEV5
B	-2	PHE	-	expression tag	UNP Q5HEV5
B	-1	GLN	-	expression tag	UNP Q5HEV5
B	0	GLY	-	expression tag	UNP Q5HEV5
C	-16	MET	-	expression tag	UNP Q5HEV5
C	-15	GLY	-	expression tag	UNP Q5HEV5
C	-14	SER	-	expression tag	UNP Q5HEV5
C	-13	SER	-	expression tag	UNP Q5HEV5
C	-12	HIS	-	expression tag	UNP Q5HEV5
C	-11	HIS	-	expression tag	UNP Q5HEV5
C	-10	HIS	-	expression tag	UNP Q5HEV5
C	-9	TYR	-	expression tag	UNP Q5HEV5
C	-8	HIS	-	expression tag	UNP Q5HEV5
C	-7	HIS	-	expression tag	UNP Q5HEV5
C	-6	GLU	-	expression tag	UNP Q5HEV5
C	-5	ASN	-	expression tag	UNP Q5HEV5
C	-4	LEU	-	expression tag	UNP Q5HEV5
C	-3	TYR	-	expression tag	UNP Q5HEV5
C	-2	PHE	-	expression tag	UNP Q5HEV5
C	-1	GLN	-	expression tag	UNP Q5HEV5
C	0	GLY	-	expression tag	UNP Q5HEV5
D	-16	MET	-	expression tag	UNP Q5HEV5
D	-15	GLY	-	expression tag	UNP Q5HEV5
D	-14	SER	-	expression tag	UNP Q5HEV5
D	-13	SER	-	expression tag	UNP Q5HEV5

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-12	HIS	-	expression tag	UNP Q5HEV5
D	-11	HIS	-	expression tag	UNP Q5HEV5
D	-10	HIS	-	expression tag	UNP Q5HEV5
D	-9	TYR	-	expression tag	UNP Q5HEV5
D	-8	HIS	-	expression tag	UNP Q5HEV5
D	-7	HIS	-	expression tag	UNP Q5HEV5
D	-6	GLU	-	expression tag	UNP Q5HEV5
D	-5	ASN	-	expression tag	UNP Q5HEV5
D	-4	LEU	-	expression tag	UNP Q5HEV5
D	-3	TYR	-	expression tag	UNP Q5HEV5
D	-2	PHE	-	expression tag	UNP Q5HEV5
D	-1	GLN	-	expression tag	UNP Q5HEV5
D	0	GLY	-	expression tag	UNP Q5HEV5
E	-16	MET	-	expression tag	UNP Q5HEV5
E	-15	GLY	-	expression tag	UNP Q5HEV5
E	-14	SER	-	expression tag	UNP Q5HEV5
E	-13	SER	-	expression tag	UNP Q5HEV5
E	-12	HIS	-	expression tag	UNP Q5HEV5
E	-11	HIS	-	expression tag	UNP Q5HEV5
E	-10	HIS	-	expression tag	UNP Q5HEV5
E	-9	TYR	-	expression tag	UNP Q5HEV5
E	-8	HIS	-	expression tag	UNP Q5HEV5
E	-7	HIS	-	expression tag	UNP Q5HEV5
E	-6	GLU	-	expression tag	UNP Q5HEV5
E	-5	ASN	-	expression tag	UNP Q5HEV5
E	-4	LEU	-	expression tag	UNP Q5HEV5
E	-3	TYR	-	expression tag	UNP Q5HEV5
E	-2	PHE	-	expression tag	UNP Q5HEV5
E	-1	GLN	-	expression tag	UNP Q5HEV5
E	0	GLY	-	expression tag	UNP Q5HEV5
F	-16	MET	-	expression tag	UNP Q5HEV5
F	-15	GLY	-	expression tag	UNP Q5HEV5
F	-14	SER	-	expression tag	UNP Q5HEV5
F	-13	SER	-	expression tag	UNP Q5HEV5
F	-12	HIS	-	expression tag	UNP Q5HEV5
F	-11	HIS	-	expression tag	UNP Q5HEV5
F	-10	HIS	-	expression tag	UNP Q5HEV5
F	-9	TYR	-	expression tag	UNP Q5HEV5
F	-8	HIS	-	expression tag	UNP Q5HEV5
F	-7	HIS	-	expression tag	UNP Q5HEV5
F	-6	GLU	-	expression tag	UNP Q5HEV5
F	-5	ASN	-	expression tag	UNP Q5HEV5

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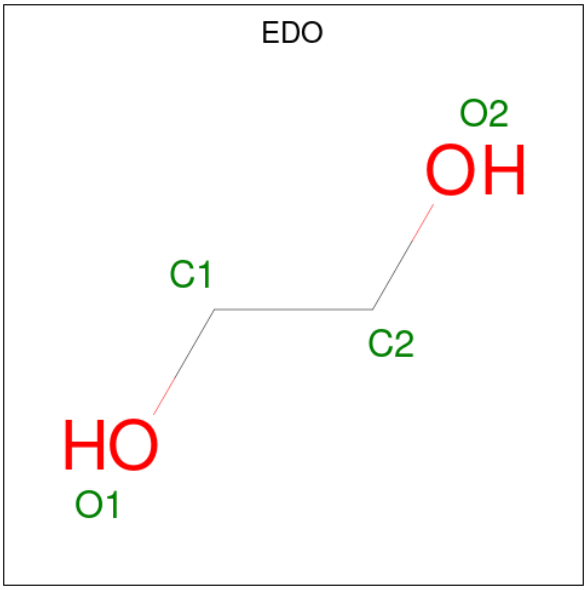
Chain	Residue	Modelled	Actual	Comment	Reference
F	-4	LEU	-	expression tag	UNP Q5HEV5
F	-3	TYR	-	expression tag	UNP Q5HEV5
F	-2	PHE	-	expression tag	UNP Q5HEV5
F	-1	GLN	-	expression tag	UNP Q5HEV5
F	0	GLY	-	expression tag	UNP Q5HEV5
G	-16	MET	-	expression tag	UNP Q5HEV5
G	-15	GLY	-	expression tag	UNP Q5HEV5
G	-14	SER	-	expression tag	UNP Q5HEV5
G	-13	SER	-	expression tag	UNP Q5HEV5
G	-12	HIS	-	expression tag	UNP Q5HEV5
G	-11	HIS	-	expression tag	UNP Q5HEV5
G	-10	HIS	-	expression tag	UNP Q5HEV5
G	-9	TYR	-	expression tag	UNP Q5HEV5
G	-8	HIS	-	expression tag	UNP Q5HEV5
G	-7	HIS	-	expression tag	UNP Q5HEV5
G	-6	GLU	-	expression tag	UNP Q5HEV5
G	-5	ASN	-	expression tag	UNP Q5HEV5
G	-4	LEU	-	expression tag	UNP Q5HEV5
G	-3	TYR	-	expression tag	UNP Q5HEV5
G	-2	PHE	-	expression tag	UNP Q5HEV5
G	-1	GLN	-	expression tag	UNP Q5HEV5
G	0	GLY	-	expression tag	UNP Q5HEV5
H	-16	MET	-	expression tag	UNP Q5HEV5
H	-15	GLY	-	expression tag	UNP Q5HEV5
H	-14	SER	-	expression tag	UNP Q5HEV5
H	-13	SER	-	expression tag	UNP Q5HEV5
H	-12	HIS	-	expression tag	UNP Q5HEV5
H	-11	HIS	-	expression tag	UNP Q5HEV5
H	-10	HIS	-	expression tag	UNP Q5HEV5
H	-9	TYR	-	expression tag	UNP Q5HEV5
H	-8	HIS	-	expression tag	UNP Q5HEV5
H	-7	HIS	-	expression tag	UNP Q5HEV5
H	-6	GLU	-	expression tag	UNP Q5HEV5
H	-5	ASN	-	expression tag	UNP Q5HEV5
H	-4	LEU	-	expression tag	UNP Q5HEV5
H	-3	TYR	-	expression tag	UNP Q5HEV5
H	-2	PHE	-	expression tag	UNP Q5HEV5
H	-1	GLN	-	expression tag	UNP Q5HEV5
H	0	GLY	-	expression tag	UNP Q5HEV5

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

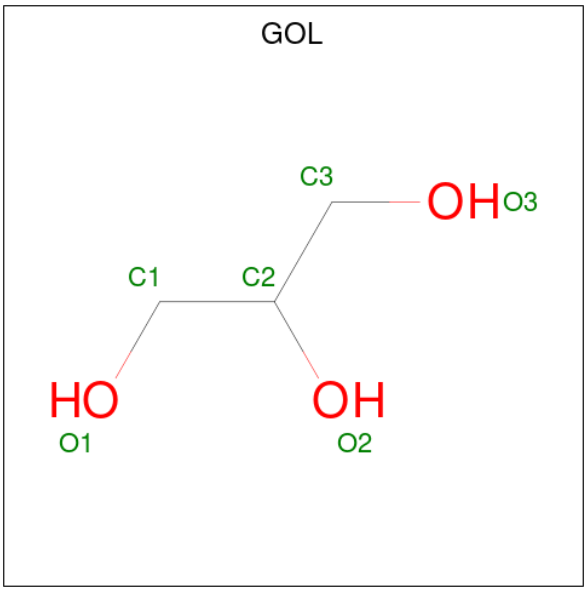
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
2	A	1	1	1	0	0
			Total	Na		
2	D	1	1	1	0	0
			Total	Na		
2	H	1	1	1	0	0

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



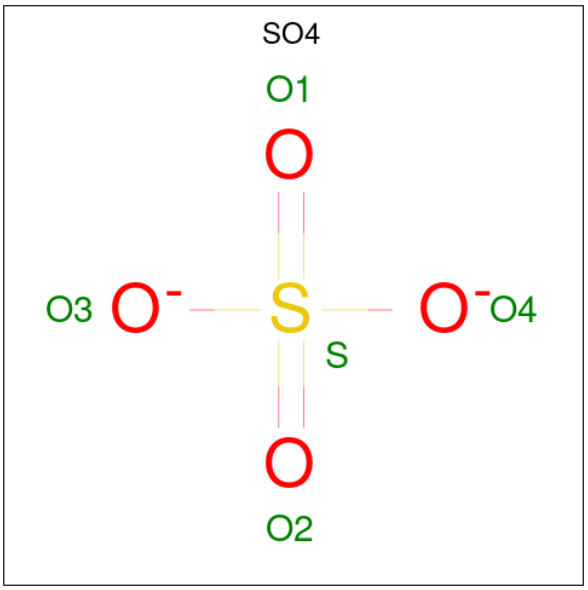
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	4	2	2	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	6	3	3	0	0
			Total	C	O		
4	B	1	6	3	3	0	0
			Total	C	O		
4	B	1	6	3	3	0	0
			Total	C	O		
4	E	1	6	3	3	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	E	1	Total O S 5 4 1	0	0
5	E	1	Total O S 5 4 1	0	0
5	F	1	Total O S 5 4 1	0	0
5	F	1	Total O S 5 4 1	0	0
5	F	1	Total O S 5 4 1	0	0
5	F	1	Total O S 5 4 1	0	0
5	G	1	Total O S 5 4 1	0	0
5	G	1	Total O S 5 4 1	0	0
5	G	1	Total O S 5 4 1	0	0
5	G	1	Total O S 5 4 1	0	0
5	H	1	Total O S 5 4 1	0	0
5	H	1	Total O S 5 4 1	0	0
5	H	1	Total O S 5 4 1	0	0
5	H	1	Total O S 5 4 1	0	0
5	H	1	Total O S 5 4 1	0	0
5	H	1	Total O S 5 4 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	208	Total O 210 210	0	3
6	B	208	Total O 209 209	0	2
6	C	165	Total O 167 167	0	2

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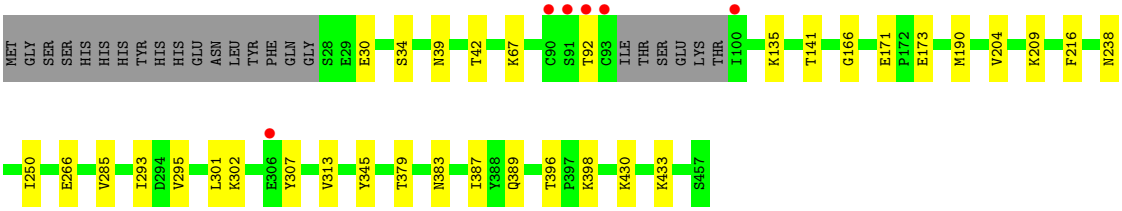
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	D	219	221	221	0	2
			Total	O		
6	E	185	186	186	0	1
			Total	O		
6	F	168	171	171	0	3
			Total	O		
6	G	139	141	141	0	2
			Total	O		
6	H	219	221	221	0	2

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.

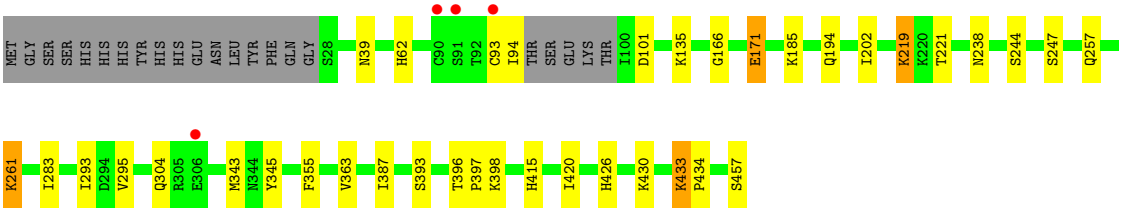
• Molecule 1: Epidermin leader peptide processing serine protease EpiP

Chain A:



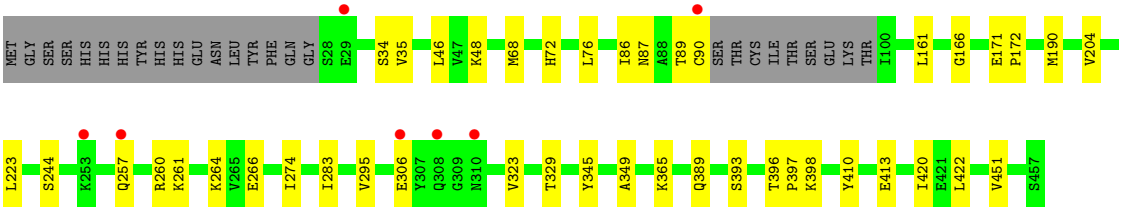
• Molecule 1: Epidermin leader peptide processing serine protease EpiP

Chain B:



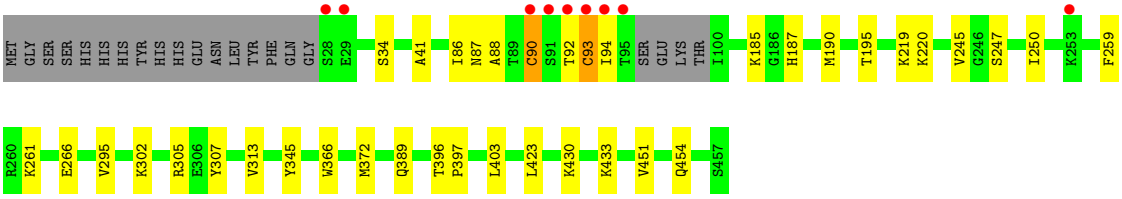
• Molecule 1: Epidermin leader peptide processing serine protease EpiP

Chain C:



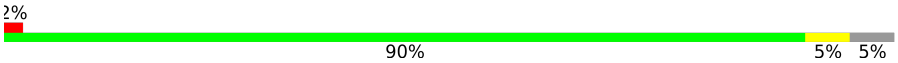
• Molecule 1: Epidermin leader peptide processing serine protease EpiP

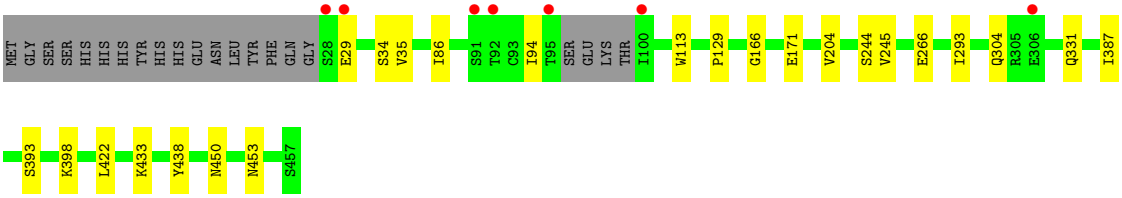
Chain D:



• Molecule 1: Epidermin leader peptide processing serine protease EpiP

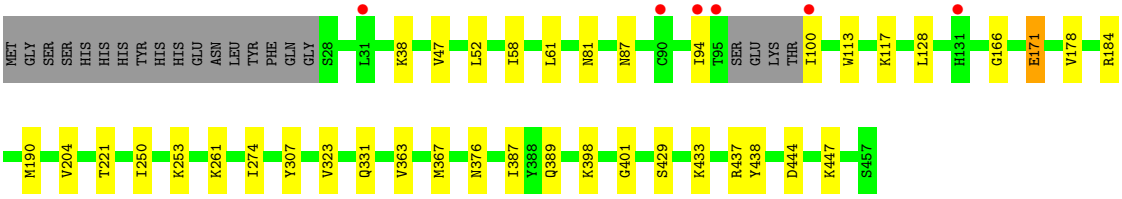
Chain E:





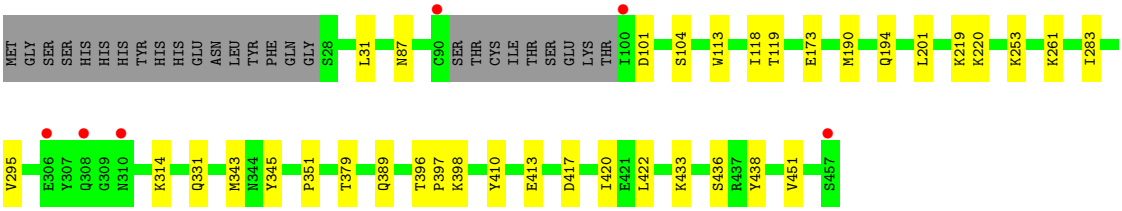
• Molecule 1: Epidermin leader peptide processing serine protease EpiP

Chain F:



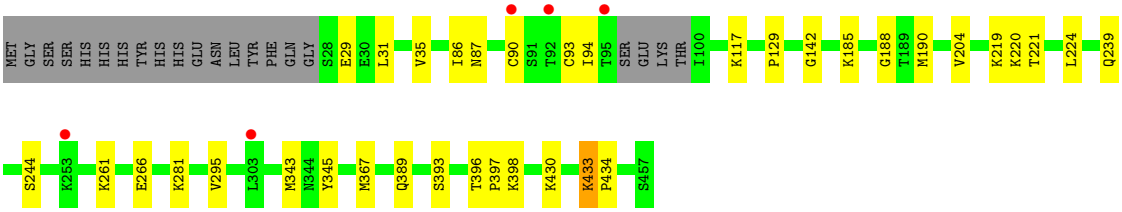
• Molecule 1: Epidermin leader peptide processing serine protease EpiP

Chain G:



• Molecule 1: Epidermin leader peptide processing serine protease EpiP

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	85.50Å 94.70Å 123.00Å 89.98° 90.37° 116.79°	Depositor
Resolution (Å)	29.69 – 2.05 29.25 – 2.05	Depositor EDS
% Data completeness (in resolution range)	97.8 (29.69-2.05) 95.8 (29.25-2.05)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.56 (at 2.04Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.170 , 0.216 0.182 , 0.230	Depositor DCC
R_{free} test set	10599 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	31.2	Xtriage
Anisotropy	0.340	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 24.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.007 for h,-h-k,-l 0.427 for -h,-k,l 0.004 for -h,h+k,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	28510	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.01% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, GOL, NA, EDO

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	0.55	0/3403	0.65	0/4591
1	B	0.54	0/3429	0.66	0/4626
1	C	0.49	0/3403	0.63	0/4590
1	D	0.55	0/3410	0.65	0/4601
1	E	0.53	0/3402	0.65	0/4591
1	F	0.51	0/3409	0.65	0/4601
1	G	0.49	0/3368	0.64	0/4544
1	H	0.57	0/3411	0.67	0/4603
All	All	0.53	0/27235	0.65	0/36747

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	3344	0	3293	21	0
1	B	3370	0	3325	34	0
1	C	3344	0	3287	23	0
1	D	3351	0	3306	26	0
1	E	3343	0	3296	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3350	0	3302	20	0
1	G	3309	0	3263	21	0
1	H	3352	0	3305	24	0
2	A	1	0	0	0	0
2	D	1	0	0	0	0
2	H	1	0	0	0	0
3	A	4	0	6	0	0
4	A	6	0	8	0	0
4	B	12	0	16	4	0
4	E	6	0	8	2	0
5	A	25	0	0	0	0
5	B	30	0	0	2	0
5	C	20	0	0	0	0
5	D	20	0	0	0	0
5	E	25	0	0	0	0
5	F	20	0	0	1	0
5	G	20	0	0	0	0
5	H	30	0	0	1	0
6	A	210	0	0	1	0
6	B	209	0	0	1	0
6	C	167	0	0	1	0
6	D	221	0	0	1	0
6	E	186	0	0	2	0
6	F	171	0	0	1	0
6	G	141	0	0	0	0
6	H	221	0	0	4	0
All	All	28510	0	26415	185	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 3.

All (185) 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:D:94:ILE:HD13	1:D:247:SER:HB2	1.48	0.94
1:E:35:VAL:HG22	1:E:86:ILE:HD12	1.54	0.90
1:D:41:ALA:HB3	6:D:1380:HOH:O	1.84	0.77
1:E:35:VAL:HG13	1:E:86:ILE:CD1	2.18	0.74
1:E:35:VAL:HG22	1:E:86:ILE:CD1	2.18	0.73
1:B:194:GLN:OE1	1:B:398:LYS:NZ	2.23	0.70
1:E:245:VAL:HG12	6:E:497:HOH:O	1.90	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:ILE:H	1:B:94:ILE:HD12	1.58	0.68
1:B:101:ASP:O	1:B:202[A]:ILE:HD11	1.94	0.68
1:F:204[B]:VAL:HG21	1:F:398:LYS:HA	1.75	0.67
1:H:90:CYS:HG	1:H:93:CYS:HG	1.41	0.66
1:F:94:ILE:HD13	1:F:221:THR:HG23	1.79	0.65
1:B:185:LYS:NZ	1:B:219:LYS:O	2.24	0.65
1:B:343:MET:HE1	4:B:7:GOL:H12	1.79	0.64
1:E:35:VAL:HG13	1:E:86:ILE:HD11	1.80	0.63
1:E:166:GLY:HA3	1:E:171:GLU:HG3	1.79	0.63
1:C:295:VAL:HG21	1:C:345:TYR:CD1	2.35	0.62
1:B:415:HIS:HA	4:B:6:GOL:H12	1.82	0.62
1:B:293:ILE:HD11	1:B:304:GLN:NE2	2.15	0.61
1:D:94:ILE:CD1	1:D:247:SER:HB2	2.28	0.61
1:B:430:LYS:HD2	1:E:387:ILE:HD12	1.81	0.61
1:H:185:LYS:NZ	1:H:219:LYS:O	2.30	0.60
1:C:413:GLU:H	1:C:413:GLU:CD	2.05	0.60
1:B:426:HIS:ND1	6:B:803:HOH:O	2.32	0.59
1:H:94:ILE:HD13	1:H:221:THR:HG22	1.85	0.58
1:E:94:ILE:H	1:E:94:ILE:HD12	1.67	0.58
1:A:173:GLU:OE2	1:A:173:GLU:N	2.26	0.58
1:C:244:SER:HB3	1:C:393:SER:HB2	1.85	0.57
1:B:355:PHE:CE1	1:D:454:GLN:HG2	2.39	0.57
1:B:457:SER:OXT	1:E:393:SER:OG	2.21	0.57
1:D:92:THR:HG21	1:D:220:LYS:NZ	2.18	0.57
1:F:166:GLY:HA3	1:F:171:GLU:HG3	1.87	0.56
1:G:433:LYS:HB3	1:G:438:TYR:CD2	2.40	0.56
1:G:410:TYR:OH	1:G:451:VAL:HG22	2.05	0.56
1:F:444:ASP:OD1	1:F:447:LYS:NZ	2.30	0.56
1:B:166:GLY:HA3	1:B:171:GLU:HG3	1.88	0.55
1:C:190:MET:SD	1:C:389:GLN:HG3	2.48	0.54
1:D:190:MET:SD	1:D:389:GLN:HG3	2.47	0.54
1:F:204[A]:VAL:HG23	1:F:401:GLY:HA3	1.89	0.54
1:E:34:SER:OG	1:E:266:GLU:OE2	2.22	0.53
1:F:178:VAL:HG22	6:F:1500:HOH:O	2.09	0.52
1:D:92:THR:CB	1:D:220:LYS:HZ3	2.22	0.52
1:E:94:ILE:HD12	1:E:94:ILE:N	2.23	0.52
1:H:90:CYS:SG	1:H:93:CYS:SG	3.01	0.52
1:G:351:PRO:O	1:G:398:LYS:HE2	2.09	0.52
1:A:293:ILE:HD11	1:A:301:LEU:HD23	1.92	0.52
1:E:293:ILE:HD11	1:E:304:GLN:HE21	1.75	0.52
1:D:403:LEU:HD21	1:D:423:LEU:HD22	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:244:SER:HB3	1:E:393:SER:HB2	1.93	0.51
1:F:204[A]:VAL:CG2	1:F:401:GLY:HA3	2.40	0.51
1:G:295:VAL:HG21	1:G:345:TYR:CD1	2.46	0.51
1:B:94:ILE:HD12	1:B:94:ILE:N	2.24	0.51
1:B:219:LYS:HA	1:B:219:LYS:CE	2.41	0.51
1:A:204:VAL:HG21	1:A:398:LYS:HA	1.92	0.51
1:F:433:LYS:HB3	1:F:438:TYR:CD2	2.45	0.51
1:H:94:ILE:HD11	1:H:220:LYS:HB3	1.93	0.51
1:A:250:ILE:HD13	1:A:307:TYR:CD1	2.46	0.51
1:C:34:SER:OG	1:C:266:GLU:OE2	2.22	0.51
1:F:250:ILE:HD13	1:F:307:TYR:CD1	2.45	0.51
1:A:383:ASN:HA	1:H:433:LYS:HD2	1.93	0.50
1:C:410:TYR:OH	1:C:451:VAL:HG22	2.11	0.50
1:C:89:THR:O	1:C:90:CYS:C	2.49	0.50
1:C:166:GLY:HA3	1:C:171:GLU:HG3	1.92	0.50
1:E:35:VAL:HG13	1:E:86:ILE:HD13	1.91	0.50
1:F:47:VAL:HA	1:F:52:LEU:HD12	1.93	0.50
1:A:387:ILE:HD12	1:H:430:LYS:HD2	1.94	0.50
1:B:257[A]:GLN:HE22	1:B:261:LYS:HE2	1.77	0.50
1:G:101:ASP:OD2	1:G:104:SER:OG	2.23	0.50
1:G:173:GLU:OE2	1:G:173:GLU:N	2.37	0.50
1:E:129:PRO:HA	4:E:8:GOL:H31	1.94	0.50
1:E:450:ASN:OD1	1:E:453:ASN:ND2	2.43	0.50
1:D:92:THR:HG21	1:D:220:LYS:HZ2	1.76	0.49
1:G:194:GLN:OE1	1:G:398:LYS:NZ	2.46	0.49
1:B:135:LYS:HB3	1:B:238:ASN:OD1	2.12	0.49
1:E:293:ILE:HD11	1:E:304:GLN:NE2	2.28	0.49
1:B:387:ILE:HD12	1:D:430:LYS:HD2	1.95	0.49
1:A:285:VAL:HG12	1:A:396:THR:HG23	1.95	0.49
1:A:430:LYS:HD2	1:F:387:ILE:HD12	1.93	0.48
1:D:88:ALA:HB3	1:D:90:CYS:HB2	1.93	0.48
1:C:396:THR:N	1:C:397:PRO:HD2	2.28	0.48
1:G:253:LYS:HE3	1:G:314:LYS:HZ3	1.79	0.48
1:A:293:ILE:CD1	1:A:301:LEU:HD23	2.43	0.48
1:D:88:ALA:CB	1:D:90:CYS:HB2	2.43	0.48
1:A:190:MET:SD	1:A:389:GLN:HG3	2.53	0.48
1:E:433:LYS:HB3	1:E:438:TYR:CD2	2.49	0.48
1:A:173:GLU:H	1:A:173:GLU:CD	2.16	0.47
1:B:219:LYS:HA	1:B:219:LYS:HE2	1.95	0.47
1:D:185:LYS:NZ	1:D:219:LYS:O	2.36	0.47
1:E:166:GLY:HA3	1:E:171:GLU:CG	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:295:VAL:HG21	1:H:345:TYR:CD1	2.49	0.46
1:G:118:ILE:HG13	1:G:119:THR:HG23	1.97	0.46
1:D:187:HIS:HA	1:D:190:MET:CE	2.45	0.46
1:G:413:GLU:H	1:G:413:GLU:CD	2.18	0.46
1:A:34:SER:OG	1:A:266:GLU:OE2	2.25	0.46
1:B:94:ILE:HG21	1:B:221:THR:HG22	1.98	0.46
1:C:329:THR:HG23	1:C:349:ALA:HB1	1.98	0.46
1:A:209:LYS:NZ	6:A:1297:HOH:O	2.20	0.45
1:C:274:ILE:HD13	1:C:323:VAL:CG2	2.46	0.45
1:A:166:GLY:HA3	1:A:171:GLU:HG3	1.98	0.45
1:G:253:LYS:NZ	1:G:314:LYS:NZ	2.64	0.45
1:H:94:ILE:CD1	1:H:221:THR:HG22	2.47	0.45
1:F:100:ILE:CD1	1:F:128:LEU:HD12	2.46	0.45
1:A:141:THR:HG22	1:A:216:PHE:CD2	2.52	0.45
1:B:355:PHE:CZ	1:D:454:GLN:HG2	2.51	0.45
1:C:223:LEU:HD23	1:C:223:LEU:HA	1.87	0.45
1:E:129:PRO:HA	4:E:8:GOL:C3	2.46	0.45
1:D:250:ILE:HD13	1:D:307:TYR:CD1	2.52	0.45
1:B:94:ILE:HA	1:B:247:SER:CB	2.46	0.45
1:B:433:LYS:HB2	1:B:434:PRO:HA	1.99	0.45
1:G:219:LYS:HB3	1:G:220:LYS:H	1.59	0.45
1:C:257:GLN:HE22	1:C:261:LYS:HE2	1.81	0.44
1:E:204:VAL:HG21	1:E:398:LYS:HA	1.99	0.44
1:F:190:MET:SD	1:F:389:GLN:HG3	2.57	0.44
1:H:239:GLN:HG3	1:H:281:LYS:O	2.16	0.44
1:B:219:LYS:HE2	1:B:219:LYS:CA	2.47	0.44
1:B:396:THR:N	1:B:397:PRO:HD2	2.32	0.44
1:G:422:LEU:HD23	1:G:422:LEU:O	2.17	0.44
1:A:135:LYS:HB3	1:A:238:ASN:OD1	2.17	0.44
1:B:62:HIS:NE2	5:B:458:SO4:O3	2.44	0.44
1:C:283:ILE:HG23	1:C:420:ILE:HD11	1.99	0.44
1:G:190:MET:SD	1:G:389:GLN:HG3	2.58	0.44
1:D:302:LYS:HA	1:D:313:VAL:HG21	1.99	0.44
1:H:433:LYS:HB2	1:H:434:PRO:HA	2.00	0.44
1:D:396:THR:N	1:D:397:PRO:HD2	2.32	0.44
1:B:94:ILE:HA	1:B:247:SER:HB2	2.00	0.43
1:F:58:ILE:HG21	1:F:61:LEU:HD12	1.99	0.43
1:H:190:MET:SD	1:H:389:GLN:HG3	2.58	0.43
1:H:35:VAL:HG22	1:H:86[A]:ILE:HG12	2.01	0.43
1:H:35:VAL:HG22	1:H:86[B]:ILE:HG13	2.01	0.43
1:H:396:THR:N	1:H:397:PRO:HD2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:VAL:HG21	1:A:345:TYR:CD1	2.53	0.43
1:B:244:SER:HB3	1:B:393:SER:HB2	1.99	0.43
1:H:224:LEU:HD13	6:H:512:HOH:O	2.17	0.43
1:D:93:CYS:HB3	1:D:305:ARG:NH2	2.33	0.43
1:H:117:LYS:NZ	6:H:529:HOH:O	2.52	0.43
1:A:302:LYS:HA	1:A:313:VAL:HG21	2.01	0.43
1:B:39:ASN:ND2	5:B:458:SO4:O2	2.52	0.43
1:F:113:TRP:CZ3	1:F:331:GLN:HA	2.54	0.43
1:G:31:LEU:HD12	1:G:31:LEU:N	2.34	0.43
1:H:29:GLU:OE2	1:H:31:LEU:HD21	2.19	0.43
1:C:35:VAL:HG22	1:C:86:ILE:HG13	2.00	0.42
1:C:68:MET:HE2	1:C:72:HIS:CB	2.49	0.42
1:C:257:GLN:HB3	6:C:1043:HOH:O	2.19	0.42
1:H:244:SER:HB3	1:H:393:SER:HB2	2.01	0.42
1:C:422:LEU:HD23	1:C:422:LEU:C	2.40	0.42
1:B:261:LYS:N	1:B:261:LYS:HD3	2.34	0.42
1:B:415:HIS:HA	4:B:6:GOL:C1	2.49	0.42
1:F:363:VAL:O	1:F:367:MET:HG2	2.20	0.42
1:G:113:TRP:CZ3	1:G:331:GLN:HA	2.54	0.42
1:G:396:THR:N	1:G:397:PRO:HD2	2.34	0.42
1:H:343:MET:HE3	6:H:1257:HOH:O	2.19	0.42
1:G:283:ILE:HG23	1:G:420:ILE:HD11	2.01	0.42
1:C:171:GLU:HA	1:C:172:PRO:HD2	1.94	0.42
1:D:295:VAL:HG21	1:D:345:TYR:CD1	2.55	0.42
1:A:39:ASN:OD1	1:A:42:THR:HG23	2.20	0.42
1:G:422:LEU:HD23	1:G:422:LEU:C	2.39	0.42
1:B:93:CYS:SG	1:B:94:ILE:HD12	2.60	0.41
1:B:363:VAL:HG22	1:D:451:VAL:HG12	2.02	0.41
4:B:7:GOL:H31	6:E:1105:HOH:O	2.20	0.41
1:E:113:TRP:CZ3	1:E:331:GLN:HA	2.55	0.41
1:G:201:LEU:HD21	1:G:379:THR:HA	2.02	0.41
1:H:204:VAL:HG21	1:H:398:LYS:HA	2.00	0.41
1:C:204:VAL:HG21	1:C:398:LYS:HA	2.02	0.41
1:H:94:ILE:HD13	1:H:221:THR:H	1.85	0.41
1:D:34:SER:OG	1:D:266:GLU:OE2	2.23	0.41
1:F:429:SER:HA	5:F:459:SO4:O4	2.20	0.41
1:A:190:MET:HB3	1:A:379:THR:HG21	2.02	0.41
1:F:94:ILE:HD13	1:F:221:THR:CG2	2.49	0.41
1:F:274:ILE:HD13	1:F:323:VAL:CG2	2.49	0.41
1:D:86:ILE:HG23	1:D:259:PHE:HA	2.03	0.41
1:D:187:HIS:HA	1:D:190:MET:HE2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:161:LEU:HD22	1:C:161:LEU:N	2.34	0.41
1:C:260:ARG:HD3	1:C:264:LYS:HB3	2.03	0.41
1:H:142:GLY:O	1:H:188:GLY:HA3	2.20	0.41
1:A:30:GLU:HG2	1:A:67:LYS:HG2	2.01	0.41
1:C:46:LEU:HD21	1:C:76:LEU:HD11	2.02	0.41
1:B:295:VAL:HG21	1:B:345:TYR:CD1	2.56	0.41
5:H:460:SO4:O2	6:H:1373:HOH:O	2.22	0.41
1:D:366:TRP:CZ2	1:D:372[B]:MET:HG2	2.56	0.40
1:B:283:ILE:HG23	1:B:420:ILE:HD11	2.02	0.40
1:F:38:LYS:HD2	1:F:81:ASN:O	2.21	0.40
1:G:343:MET:HG2	1:G:436:SER:HB3	2.02	0.40
1:H:90:CYS:SG	1:H:266:GLU:HG2	2.62	0.40
1:D:195:THR:HG23	1:D:397:PRO:CB	2.51	0.40
1:E:422:LEU:C	1:E:422:LEU:HD23	2.42	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	423/447 (95%)	408 (96%)	15 (4%)	0	100	100
1	B	426/447 (95%)	413 (97%)	13 (3%)	0	100	100
1	C	422/447 (94%)	409 (97%)	12 (3%)	1 (0%)	47	39
1	D	424/447 (95%)	407 (96%)	16 (4%)	1 (0%)	47	39
1	E	423/447 (95%)	409 (97%)	14 (3%)	0	100	100
1	F	424/447 (95%)	409 (96%)	15 (4%)	0	100	100
1	G	418/447 (94%)	406 (97%)	12 (3%)	0	100	100
1	H	424/447 (95%)	413 (97%)	11 (3%)	0	100	100
All	All	3384/3576 (95%)	3274 (97%)	108 (3%)	2 (0%)	51	45

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	306	GLU
1	D	90	CYS

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	365/383 (95%)	363 (100%)	2 (0%)	88	89
1	B	368/383 (96%)	364 (99%)	4 (1%)	73	73
1	C	364/383 (95%)	360 (99%)	4 (1%)	73	73
1	D	366/383 (96%)	361 (99%)	5 (1%)	67	65
1	E	365/383 (95%)	364 (100%)	1 (0%)	92	93
1	F	366/383 (96%)	358 (98%)	8 (2%)	52	46
1	G	360/383 (94%)	357 (99%)	3 (1%)	81	82
1	H	366/383 (96%)	361 (99%)	5 (1%)	67	65
All	All	2920/3064 (95%)	2888 (99%)	32 (1%)	73	73

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	92	THR
1	A	433	LYS
1	B	171	GLU
1	B	219	LYS
1	B	261	LYS
1	B	433	LYS
1	C	48	LYS
1	C	87	ASN
1	C	365[A]	LYS
1	C	365[B]	LYS
1	D	87	ASN
1	D	93	CYS

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Mol	Chain	Res	Type
1	D	245	VAL
1	D	261	LYS
1	D	433	LYS
1	E	29	GLU
1	F	87	ASN
1	F	117	LYS
1	F	171	GLU
1	F	184	ARG
1	F	253	LYS
1	F	261	LYS
1	F	376	ASN
1	F	437	ARG
1	G	87	ASN
1	G	261	LYS
1	G	417	ASP
1	H	87	ASN
1	H	129	PRO
1	H	261	LYS
1	H	367	MET
1	H	433	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	304	GLN
1	C	74	ASN
1	C	257	GLN
1	D	254	ASN
1	E	57	ASN
1	E	304	GLN
1	E	376	ASN
1	F	376	ASN
1	G	376	ASN
1	H	373	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 46 ligands modelled in this entry, 3 are monoatomic - leaving 43 for Mogul analysis.

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	$\#\|Z\| > 2$
5	SO4	H	463	-	4,4,4	0.18	0	6,6,6	0.31	0
5	SO4	C	459	-	4,4,4	0.15	0	6,6,6	0.12	0
5	SO4	B	460	-	4,4,4	0.14	0	6,6,6	0.17	0
5	SO4	F	458	-	4,4,4	0.13	0	6,6,6	0.14	0
5	SO4	B	461	-	4,4,4	0.16	0	6,6,6	0.06	0
5	SO4	H	458	-	4,4,4	0.17	0	6,6,6	0.23	0
5	SO4	H	459	-	4,4,4	0.19	0	6,6,6	0.29	0
5	SO4	H	462	-	4,4,4	0.14	0	6,6,6	0.08	0
4	GOL	B	7	-	5,5,5	0.30	0	5,5,5	0.31	0
5	SO4	C	460	-	4,4,4	0.18	0	6,6,6	0.17	0
5	SO4	E	460	-	4,4,4	0.19	0	6,6,6	0.25	0
5	SO4	B	462	-	4,4,4	0.12	0	6,6,6	0.13	0
5	SO4	E	461	-	4,4,4	0.11	0	6,6,6	0.29	0
5	SO4	A	459	-	4,4,4	0.15	0	6,6,6	0.21	0
5	SO4	C	461	-	4,4,4	0.14	0	6,6,6	0.09	0
5	SO4	E	458	-	4,4,4	0.14	0	6,6,6	0.18	0
5	SO4	F	459	-	4,4,4	0.17	0	6,6,6	0.21	0
5	SO4	H	460	-	4,4,4	0.14	0	6,6,6	0.23	0
5	SO4	E	462	-	4,4,4	0.12	0	6,6,6	0.34	0
5	SO4	A	460	2	4,4,4	0.20	0	6,6,6	0.14	0
5	SO4	G	459	-	4,4,4	0.14	0	6,6,6	0.12	0
5	SO4	G	458	-	4,4,4	0.16	0	6,6,6	0.18	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	SO4	E	459	-	4,4,4	0.15	0	6,6,6	0.11	0
5	SO4	A	461	-	4,4,4	0.13	0	6,6,6	0.08	0
5	SO4	D	10	-	4,4,4	0.21	0	6,6,6	0.30	0
3	EDO	A	4	-	3,3,3	0.54	0	2,2,2	0.14	0
5	SO4	H	461	2	4,4,4	0.18	0	6,6,6	0.17	0
5	SO4	G	461	-	4,4,4	0.12	0	6,6,6	0.15	0
5	SO4	D	458	-	4,4,4	0.19	0	6,6,6	0.19	0
5	SO4	B	463	-	4,4,4	0.15	0	6,6,6	0.12	0
5	SO4	B	459	-	4,4,4	0.17	0	6,6,6	0.34	0
5	SO4	B	458	-	4,4,4	0.15	0	6,6,6	0.13	0
5	SO4	D	459	2	4,4,4	0.19	0	6,6,6	0.11	0
4	GOL	E	8	-	5,5,5	0.42	0	5,5,5	0.39	0
5	SO4	C	458	-	4,4,4	0.15	0	6,6,6	0.17	0
5	SO4	F	460	-	4,4,4	0.11	0	6,6,6	0.23	0
5	SO4	F	461	-	4,4,4	0.15	0	6,6,6	0.22	0
5	SO4	D	9	-	4,4,4	0.19	0	6,6,6	0.33	0
5	SO4	G	460	-	4,4,4	0.15	0	6,6,6	0.15	0
5	SO4	A	458	-	4,4,4	0.15	0	6,6,6	0.09	0
4	GOL	A	5	-	5,5,5	0.43	0	5,5,5	0.30	0
5	SO4	A	462	-	4,4,4	0.17	0	6,6,6	0.09	0
4	GOL	B	6	-	5,5,5	0.42	0	5,5,5	0.46	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
4	GOL	B	7	-	-	2/4/4/4	-
4	GOL	E	8	-	-	4/4/4/4	-
4	GOL	A	5	-	-	2/4/4/4	-
3	EDO	A	4	-	-	1/1/1/1	-
4	GOL	B	6	-	-	1/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	5	GOL	O1-C1-C2-C3
4	E	8	GOL	O1-C1-C2-C3
4	E	8	GOL	O1-C1-C2-O2
4	B	6	GOL	O1-C1-C2-C3
4	B	7	GOL	O1-C1-C2-C3
4	E	8	GOL	C1-C2-C3-O3
4	A	5	GOL	O1-C1-C2-O2
4	B	7	GOL	O1-C1-C2-O2
4	E	8	GOL	O2-C2-C3-O3
3	A	4	EDO	O1-C1-C2-O2

There are no ring outliers.

6 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	7	GOL	2	0
5	F	459	SO4	1	0
5	H	460	SO4	1	0
5	B	458	SO4	2	0
4	E	8	GOL	2	0
4	B	6	GOL	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	424/447 (94%)	-0.20	6 (1%)	75	78	21, 33, 57, 77	0
1	B	425/447 (95%)	-0.21	4 (0%)	84	86	21, 32, 55, 79	0
1	C	421/447 (94%)	-0.17	7 (1%)	70	73	24, 40, 62, 81	0
1	D	426/447 (95%)	-0.22	9 (2%)	63	67	20, 33, 56, 91	0
1	E	426/447 (95%)	-0.10	7 (1%)	72	74	23, 36, 63, 86	0
1	F	426/447 (95%)	-0.09	6 (1%)	75	78	24, 37, 64, 89	0
1	G	421/447 (94%)	-0.13	6 (1%)	75	78	26, 41, 63, 81	0
1	H	426/447 (95%)	-0.24	5 (1%)	79	81	19, 33, 56, 84	0
All	All	3395/3576 (94%)	-0.17	50 (1%)	73	76	19, 36, 61, 91	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	95	THR	5.4
1	D	93	CYS	5.1
1	B	91	SER	4.9
1	D	91	SER	4.8
1	D	92	THR	4.5
1	D	95	THR	4.2
1	D	94	ILE	4.0
1	G	90	CYS	4.0
1	E	95	THR	3.9
1	E	28	SER	3.9
1	H	92	THR	3.7
1	D	90	CYS	3.6
1	G	308	GLN	3.5
1	F	94	ILE	3.5
1	G	306	GLU	3.5
1	C	253	LYS	3.4

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Mol	Chain	Res	Type	RSRZ
1	E	91	SER	3.4
1	A	91	SER	3.3
1	D	29	GLU	3.2
1	G	457	SER	3.2
1	C	306	GLU	3.0
1	C	29	GLU	2.9
1	B	93	CYS	2.8
1	E	306	GLU	2.8
1	C	308	GLN	2.8
1	C	310	ASN	2.7
1	H	90	CYS	2.6
1	E	29	GLU	2.6
1	F	131	HIS	2.5
1	B	90	CYS	2.5
1	A	92	THR	2.4
1	A	90	CYS	2.4
1	A	93	CYS	2.4
1	H	303	LEU	2.4
1	H	253	LYS	2.4
1	A	100	ILE	2.4
1	E	100	ILE	2.3
1	D	28	SER	2.3
1	G	310	ASN	2.3
1	B	306	GLU	2.2
1	F	90	CYS	2.2
1	F	100	ILE	2.2
1	E	92	THR	2.2
1	D	253	LYS	2.2
1	G	100	ILE	2.1
1	C	90	CYS	2.1
1	F	31	LEU	2.1
1	A	306	GLU	2.0
1	F	95	THR	2.0
1	C	257	GLN	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	GOL	E	8	6/6	0.32	0.26	68,70,71,76	0
5	SO4	E	462	5/5	0.72	0.20	62,63,65,66	5
5	SO4	E	459	5/5	0.73	0.23	54,54,55,55	5
4	GOL	B	7	6/6	0.77	0.16	50,58,58,61	0
4	GOL	B	6	6/6	0.77	0.13	51,53,55,58	0
5	SO4	B	460	5/5	0.81	0.28	47,49,50,52	5
5	SO4	F	458	5/5	0.81	0.16	60,62,64,66	5
5	SO4	B	463	5/5	0.82	0.23	46,46,50,50	5
5	SO4	F	461	5/5	0.84	0.14	61,64,65,66	5
5	SO4	B	462	5/5	0.87	0.18	49,50,51,53	5
2	NA	A	1	1/1	0.87	0.15	65,65,65,65	0
5	SO4	B	461	5/5	0.87	0.16	56,56,57,57	5
5	SO4	A	461	5/5	0.88	0.18	55,56,57,58	5
5	SO4	C	461	5/5	0.88	0.19	50,50,51,52	5
5	SO4	G	458	5/5	0.88	0.14	55,58,59,61	5
5	SO4	G	459	5/5	0.88	0.13	58,59,61,62	5
2	NA	H	3	1/1	0.89	0.32	59,59,59,59	0
2	NA	D	2	1/1	0.89	0.31	60,60,60,60	0
5	SO4	H	463	5/5	0.89	0.24	35,40,42,43	5
4	GOL	A	5	6/6	0.90	0.10	53,58,58,59	0
5	SO4	C	459	5/5	0.90	0.17	39,41,42,43	5
5	SO4	H	462	5/5	0.91	0.17	50,51,53,54	5
3	EDO	A	4	4/4	0.91	0.12	53,54,55,56	0
5	SO4	G	460	5/5	0.92	0.14	43,45,46,47	5
5	SO4	G	461	5/5	0.92	0.12	57,59,60,61	5
5	SO4	F	460	5/5	0.92	0.10	65,65,67,69	0
5	SO4	A	460	5/5	0.92	0.14	57,63,63,65	5
5	SO4	D	459	5/5	0.93	0.13	54,54,56,59	5
5	SO4	H	459	5/5	0.93	0.18	59,62,65,67	0
5	SO4	A	458	5/5	0.93	0.09	54,56,57,58	5
5	SO4	D	10	5/5	0.93	0.13	58,59,62,64	0
5	SO4	C	460	5/5	0.94	0.14	51,56,56,57	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	SO4	A	462	5/5	0.94	0.12	52,52,53,55	5
5	SO4	E	458	5/5	0.95	0.11	50,55,57,59	5
5	SO4	B	458	5/5	0.95	0.10	57,58,60,60	5
5	SO4	E	460	5/5	0.95	0.09	60,60,61,67	0
5	SO4	H	461	5/5	0.95	0.13	56,59,60,60	5
5	SO4	E	461	5/5	0.95	0.09	59,62,63,64	0
5	SO4	A	459	5/5	0.95	0.13	47,50,54,60	0
5	SO4	F	459	5/5	0.96	0.11	61,62,66,67	0
5	SO4	D	458	5/5	0.96	0.10	54,55,56,57	5
5	SO4	H	460	5/5	0.96	0.09	51,52,53,55	5
5	SO4	C	458	5/5	0.97	0.16	47,48,48,50	5
5	SO4	B	459	5/5	0.97	0.09	41,50,53,55	0
5	SO4	D	9	5/5	0.97	0.07	51,54,55,56	0
5	SO4	H	458	5/5	0.98	0.09	50,52,53,53	0

6.5 Other polymers (i)

There are no such residues in this entry.