



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 15, 2017 – 06:12 AM EDT

PDB ID : 2RHS
Title : PheRS from Staphylococcus haemolyticus- rational protein engineering and inhibitor studies
Authors : Evdokimov, A.G.; Mekel, M.
Deposited on : unknown
Resolution : 2.20 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

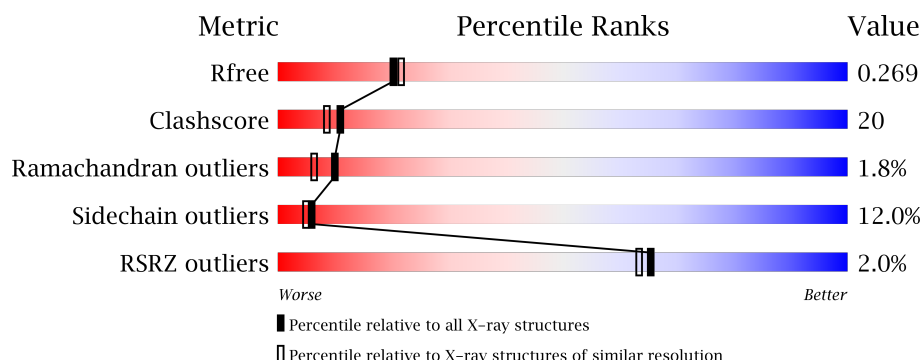
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	100719	4002 (2.20-2.20)
Clashscore	112137	4730 (2.20-2.20)
Ramachandran outliers	110173	4656 (2.20-2.20)
Sidechain outliers	110143	4657 (2.20-2.20)
RSRZ outliers	101464	4033 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	294	<div> <div>54%</div> <div>28%</div> <div>15%</div> </div>
1	C	294	<div> <div>59%</div> <div>28%</div> <div>5%</div> <div>8%</div> </div>
2	B	800	<div> <div>68%</div> <div>26%</div> <div>5%</div> </div>
2	D	800	<div> <div>4%</div> <div>55%</div> <div>33%</div> <div>10%</div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 17461 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 Phenylalanyl-tRNA synthetase alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	249	Total	C	N	O	S	0	3	0
			2006	1270	337	389	10			
1	C	271	Total	C	N	O	S	0	4	0
			2181	1381	367	418	15			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	58	MET	-	EXPRESSION TAG	UNP Q4L5E3
A	59	GLY	-	EXPRESSION TAG	UNP Q4L5E3
A	60	SER	-	EXPRESSION TAG	UNP Q4L5E3
A	61	SER	-	EXPRESSION TAG	UNP Q4L5E3
A	62	HIS	-	EXPRESSION TAG	UNP Q4L5E3
A	63	HIS	-	EXPRESSION TAG	UNP Q4L5E3
A	64	HIS	-	EXPRESSION TAG	UNP Q4L5E3
A	65	HIS	-	EXPRESSION TAG	UNP Q4L5E3
A	66	HIS	-	EXPRESSION TAG	UNP Q4L5E3
A	67	HIS	-	EXPRESSION TAG	UNP Q4L5E3
A	68	SER	-	EXPRESSION TAG	UNP Q4L5E3
A	69	SER	-	EXPRESSION TAG	UNP Q4L5E3
A	70	GLY	-	EXPRESSION TAG	UNP Q4L5E3
A	71	LEU	-	EXPRESSION TAG	UNP Q4L5E3
A	72	VAL	-	EXPRESSION TAG	UNP Q4L5E3
A	73	PRO	-	EXPRESSION TAG	UNP Q4L5E3
A	74	ARG	-	EXPRESSION TAG	UNP Q4L5E3
A	75	GLY	-	EXPRESSION TAG	UNP Q4L5E3
A	76	SER	-	EXPRESSION TAG	UNP Q4L5E3
A	77	HIS	-	EXPRESSION TAG	UNP Q4L5E3
A	78	MET	-	EXPRESSION TAG	UNP Q4L5E3
A	79	GLY	-	EXPRESSION TAG	UNP Q4L5E3
A	80	THR	-	EXPRESSION TAG	UNP Q4L5E3
A	81	GLU	-	EXPRESSION TAG	UNP Q4L5E3
A	82	LEU	-	EXPRESSION TAG	UNP Q4L5E3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	83	MET	-	EXPRESSION TAG	UNP Q4L5E3
C	58	MET	-	EXPRESSION TAG	UNP Q4L5E3
C	59	GLY	-	EXPRESSION TAG	UNP Q4L5E3
C	60	SER	-	EXPRESSION TAG	UNP Q4L5E3
C	61	SER	-	EXPRESSION TAG	UNP Q4L5E3
C	62	HIS	-	EXPRESSION TAG	UNP Q4L5E3
C	63	HIS	-	EXPRESSION TAG	UNP Q4L5E3
C	64	HIS	-	EXPRESSION TAG	UNP Q4L5E3
C	65	HIS	-	EXPRESSION TAG	UNP Q4L5E3
C	66	HIS	-	EXPRESSION TAG	UNP Q4L5E3
C	67	HIS	-	EXPRESSION TAG	UNP Q4L5E3
C	68	SER	-	EXPRESSION TAG	UNP Q4L5E3
C	69	SER	-	EXPRESSION TAG	UNP Q4L5E3
C	70	GLY	-	EXPRESSION TAG	UNP Q4L5E3
C	71	LEU	-	EXPRESSION TAG	UNP Q4L5E3
C	72	VAL	-	EXPRESSION TAG	UNP Q4L5E3
C	73	PRO	-	EXPRESSION TAG	UNP Q4L5E3
C	74	ARG	-	EXPRESSION TAG	UNP Q4L5E3
C	75	GLY	-	EXPRESSION TAG	UNP Q4L5E3
C	76	SER	-	EXPRESSION TAG	UNP Q4L5E3
C	77	HIS	-	EXPRESSION TAG	UNP Q4L5E3
C	78	MET	-	EXPRESSION TAG	UNP Q4L5E3
C	79	GLY	-	EXPRESSION TAG	UNP Q4L5E3
C	80	THR	-	EXPRESSION TAG	UNP Q4L5E3
C	81	GLU	-	EXPRESSION TAG	UNP Q4L5E3
C	82	LEU	-	EXPRESSION TAG	UNP Q4L5E3
C	83	MET	-	EXPRESSION TAG	UNP Q4L5E3

- Molecule 2 is a protein called Phenylalanyl-tRNA synthetase beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	786	Total	C	N	O	S	0	3	0
			6141	3864	1037	1223	17			
2	D	785	Total	C	N	O	S	0	2	0
			6116	3846	1031	1222	17			

There are 10 discrepancies between the modelled and reference sequences:

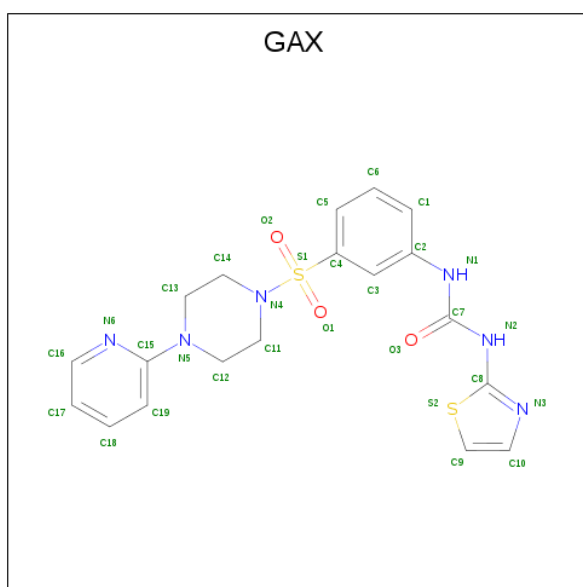
Chain	Residue	Modelled	Actual	Comment	Reference
B	34	ASN	ASP	ENGINEERED	UNP Q4L5E4
B	144	PRO	GLN	ENGINEERED	UNP Q4L5E4
B	661	GLY	GLU	ENGINEERED	UNP Q4L5E4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	663	ALA	GLN	ENGINEERED	UNP Q4L5E4
B	664	GLY	ASP	ENGINEERED	UNP Q4L5E4
D	34	ASN	ASP	ENGINEERED	UNP Q4L5E4
D	144	PRO	GLN	ENGINEERED	UNP Q4L5E4
D	661	GLY	GLU	ENGINEERED	UNP Q4L5E4
D	663	ALA	GLN	ENGINEERED	UNP Q4L5E4
D	664	GLY	ASP	ENGINEERED	UNP Q4L5E4

- Molecule 3 is 1-{3-[(4-pyridin-2-ylpiperazin-1-yl)sulfonyl]phenyl}-3-(1,3-thiazol-2-yl)urea (three-letter code: GAX) (formula: C₁₉H₂₀N₆O₃S₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			30	19	6	3	2		
3	C	1	Total	C	N	O	S	0	0
			30	19	6	3	2		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	1	Total	Zn	0	0
			1	1		

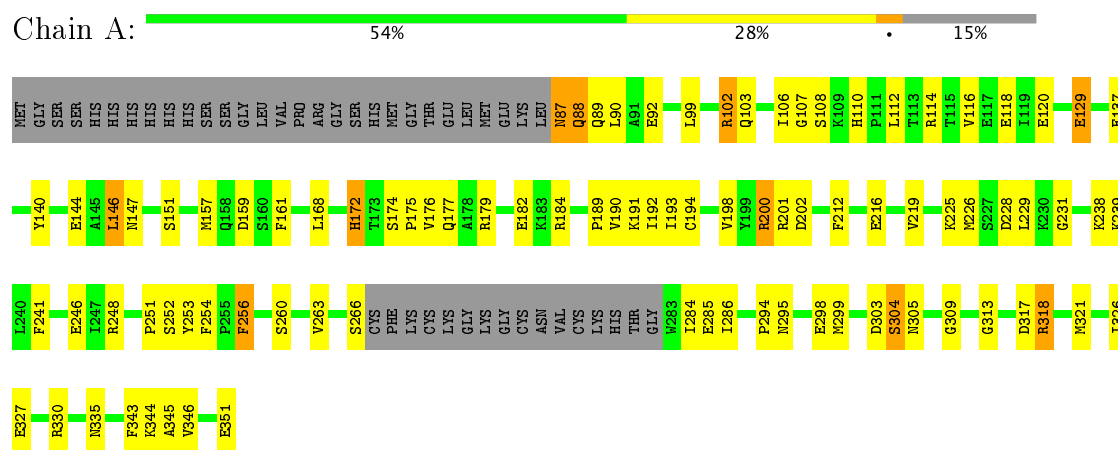
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	110	Total	O	0	0
			110	110		
6	B	403	Total	O	0	0
			403	403		
6	C	119	Total	O	0	0
			119	119		
6	D	314	Total	O	0	0
			314	314		

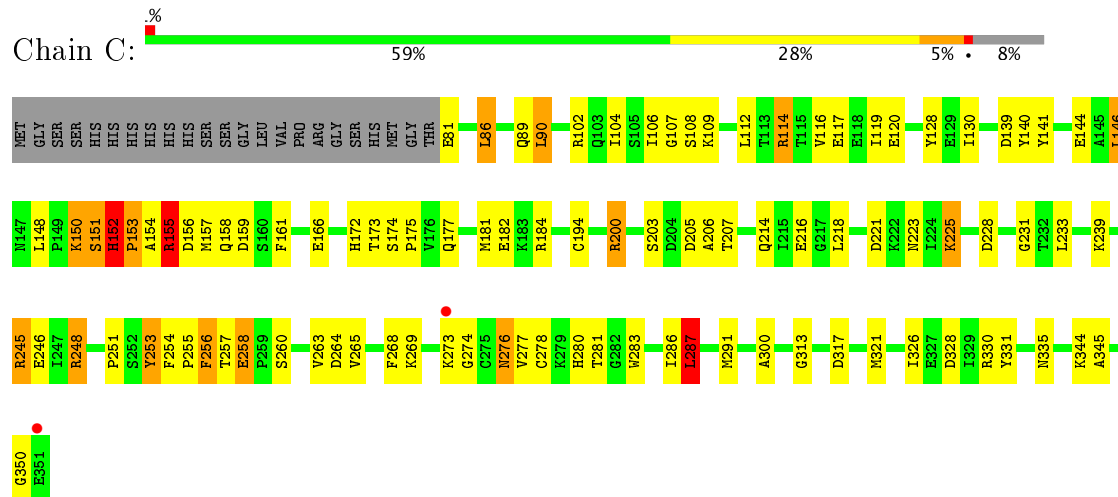
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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 ($\text{RSRZ} > 2$). 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.

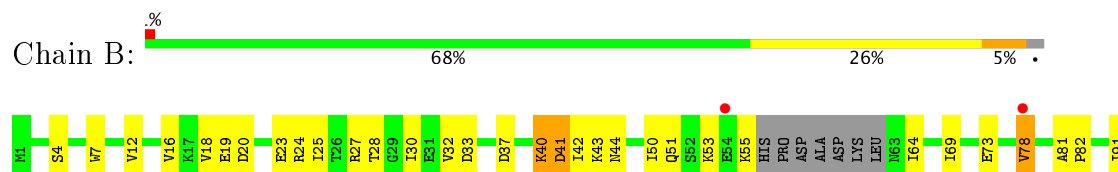
• Molecule 1: Phenylalanyl-tRNA synthetase alpha chain

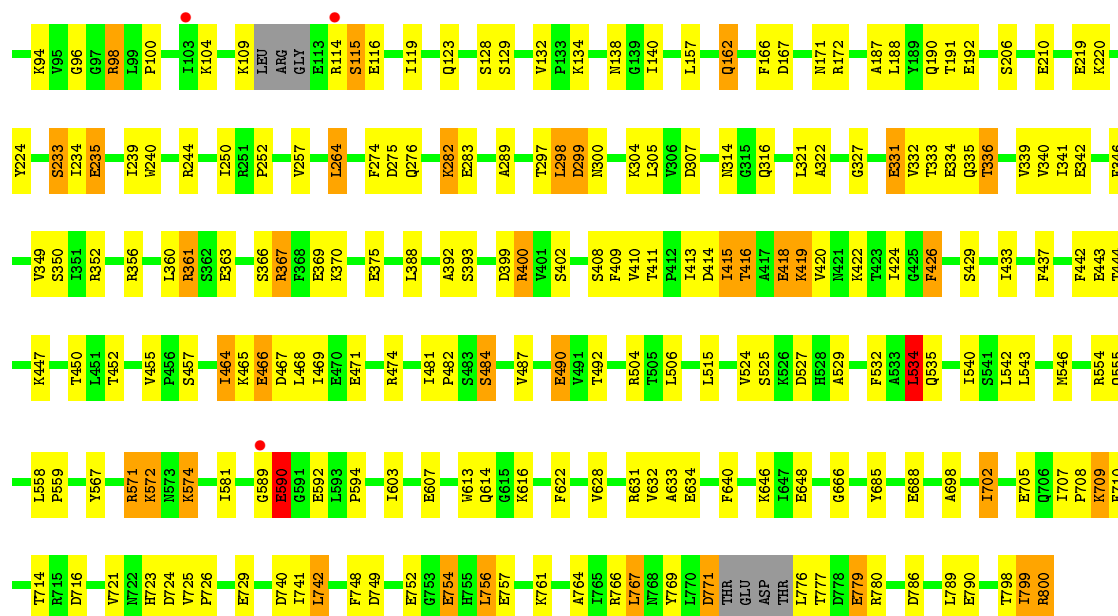


• Molecule 1: Phenylalanyl-tRNA synthetase alpha chain

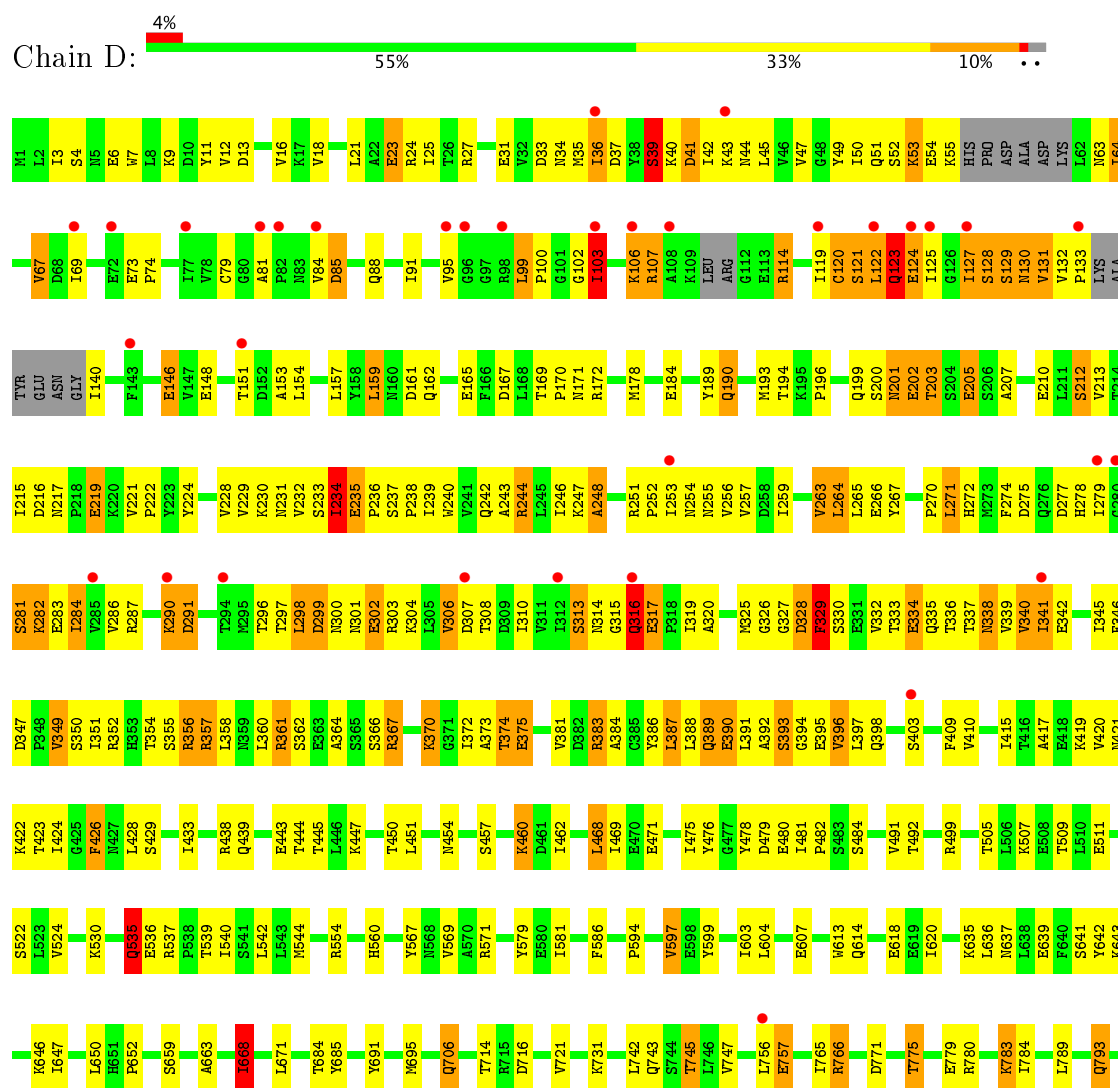


• Molecule 2: Phenylalanyl-tRNA synthetase beta chain





• Molecule 2: Phenylalanyl-tRNA synthetase beta chain



1799
ARG

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	60.71Å 87.86Å 234.04Å 90.00° 90.59° 90.00°	Depositor
Resolution (Å)	57.30 – 2.20 49.95 – 2.20	Depositor EDS
% Data completeness (in resolution range)	89.3 (57.30-2.20) 89.3 (49.95-2.20)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.02 (at 2.20Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.193 , 0.271 0.192 , 0.269	Depositor DCC
R_{free} test set	5602 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	32.8	Xtriage
Anisotropy	0.127	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 47.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.047 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	17461	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.14% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, SO4, GAX

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	0.46	0/2051	0.94	1/2771 (0.0%)
1	C	0.43	0/2233	0.88	2/3012 (0.1%)
2	B	0.43	0/6241	0.89	6/8452 (0.1%)
2	D	0.39	0/6212	0.81	3/8415 (0.0%)
All	All	0.42	0/16737	0.87	12/22650 (0.1%)

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	C	0	3
2	B	0	4
2	D	0	7
All	All	0	14

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	330	ARG	NE-CZ-NH1	-6.27	117.16	120.30
2	B	504	ARG	NE-CZ-NH2	-6.08	117.26	120.30
2	D	742	LEU	CA-CB-CG	-6.04	101.40	115.30
2	B	400	ARG	NE-CZ-NH2	-5.97	117.32	120.30
2	B	504	ARG	NE-CZ-NH1	5.85	123.23	120.30

There are no chirality outliers.

5 of 14 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	298	LEU	Peptide
2	B	534	LEU	Peptide
2	B	740	ASP	Peptide
2	B	752	GLU	Peptide
1	C	273	LYS	Peptide

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	2006	0	1949	66	0
1	C	2181	0	2130	96	0
2	B	6141	0	6121	188	0
2	D	6116	0	6088	349	0
3	A	30	0	20	2	0
3	C	30	0	20	3	0
4	B	5	0	0	0	0
4	D	5	0	0	1	0
5	C	1	0	0	0	0
6	A	110	0	0	2	0
6	B	403	0	0	17	0
6	C	119	0	0	5	0
6	D	314	0	0	9	0
All	All	17461	0	16328	663	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 20.

The worst 5 of 663 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)
2:D:91:ILE:CD1	2:D:153:ALA:HB1	1.74	1.17
2:B:424:ILE:HD11	2:B:469:ILE:HG23	1.26	1.15
1:A:87:ASN:HD22	1:A:87:ASN:N	1.44	1.14
2:D:53:LYS:HB3	2:D:53:LYS:NZ	1.65	1.11
2:B:464:ILE:HG13	2:B:466:GLU:HG2	1.22	1.10

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	246/294 (84%)	226 (92%)	20 (8%)	0	100	100
1	C	271/294 (92%)	252 (93%)	13 (5%)	6 (2%)	8	4
2	B	780/800 (98%)	726 (93%)	47 (6%)	7 (1%)	20	18
2	D	778/800 (97%)	674 (87%)	79 (10%)	25 (3%)	5	2
All	All	2075/2188 (95%)	1878 (90%)	159 (8%)	38 (2%)	10	6

5 of 38 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	151	SER
1	C	152	HIS
1	C	155	ARG
2	D	39	SER
2	D	114	ARG

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	220/257 (86%)	199 (90%)	21 (10%)	10	9
1	C	240/257 (93%)	216 (90%)	24 (10%)	9	8
2	B	678/688 (98%)	608 (90%)	70 (10%)	8	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	D	676/688 (98%)	571 (84%)	105 (16%)	3 2
All	All	1814/1890 (96%)	1594 (88%)	220 (12%)	6 5

5 of 220 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	151	SER
2	D	53	LYS
2	D	607	GLU
1	C	158	GLN
1	C	253[B]	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	276	ASN
2	D	44	ASN
2	D	338	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 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	$\# Z > 2$
3	GAX	A	1	-	31,33,33	2.14	4 (12%)	38,46,46	2.45	17 (44%)
4	SO4	B	801	-	4,4,4	0.16	0	6,6,6	0.30	0
3	GAX	C	2	-	31,33,33	2.25	4 (12%)	38,46,46	3.06	19 (50%)
4	SO4	D	801	-	4,4,4	0.18	0	6,6,6	0.17	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
3	GAX	A	1	-	-	0/22/34/34	0/4/4/4
4	SO4	B	801	-	-	0/0/0/0	0/0/0/0
3	GAX	C	2	-	-	0/22/34/34	0/4/4/4
4	SO4	D	801	-	-	0/0/0/0	0/0/0/0

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2	GAX	C4-S1	-11.37	1.60	1.76
3	A	1	GAX	C4-S1	-10.20	1.61	1.76
3	A	1	GAX	C2-N1	-3.88	1.34	1.41
3	C	2	GAX	C2-N1	-2.82	1.36	1.41
3	A	1	GAX	C7-N1	-2.55	1.32	1.37

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2	GAX	O1-S1-O2	-5.88	109.57	119.46
3	A	1	GAX	O1-S1-O2	-5.56	110.11	119.46
3	C	2	GAX	C13-N5-C15	-5.34	107.75	120.33
3	C	2	GAX	C4-S1-N4	-4.88	101.36	107.31
3	C	2	GAX	C11-N4-C14	-4.31	107.22	112.11

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1	GAX	2	0
3	C	2	GAX	3	0
4	D	801	SO4	1	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 ⓘ

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, 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	249/294 (84%)	-0.47	0 100 100	16, 29, 51, 83	0
1	C	271/294 (92%)	-0.40	2 (0%) 87 86	13, 31, 59, 83	0
2	B	786/800 (98%)	-0.42	5 (0%) 89 88	17, 34, 56, 83	1 (0%)
2	D	785/800 (98%)	0.02	34 (4%) 36 34	16, 46, 85, 105	1 (0%)
All	All	2091/2188 (95%)	-0.26	41 (1%) 65 63	13, 35, 75, 105	2 (0%)

The worst 5 of 41 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	43	LYS	5.1
2	D	103	ILE	4.7
2	D	151	THR	4.5
2	D	316	GLN	4.2
2	B	78	VAL	4.0

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	GAX	A	1	30/30	0.94	0.13	1.86	21,39,63,65	0
3	GAX	C	2	30/30	0.96	0.10	-0.51	22,40,56,57	0
5	ZN	C	3	1/1	0.97	0.10	-0.52	47,47,47,47	0
4	SO4	B	801	5/5	0.99	0.07	-	44,44,52,53	0
4	SO4	D	801	5/5	0.98	0.10	-	37,41,44,47	0

6.5 Other polymers [i](#)

There are no such residues in this entry.