wwPDB X-ray Structure Validation Summary Report (i)

Apr 28, 2025 – 07:47 PM EDT

PDB ID	:	3G17 / pdb_00003g17
Title	:	Structure of putative 2-dehydropantoate 2-reductase from staphylococcus aureus
Authors	:	Ramagopal, U.A.; Toro, R.; Burley, S.K.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on	:	2009-01-29
Resolution	:	2.30 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
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 (1)) were used in the production of this report:

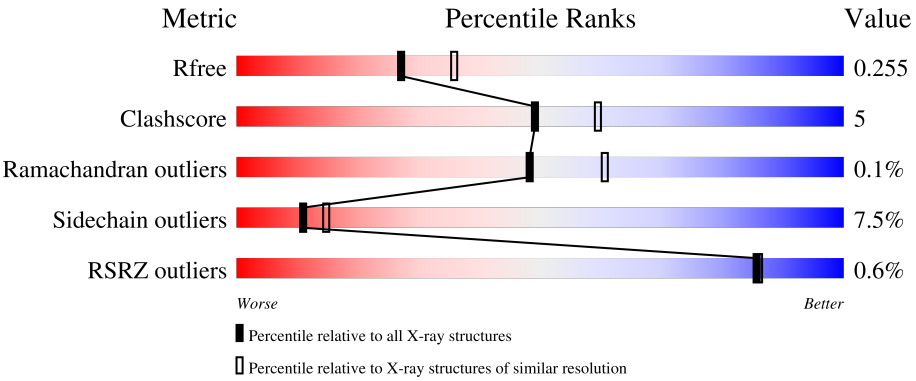
MolProbity	:	4-5-2 with Phenix2.0rc1
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

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 2.30 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.



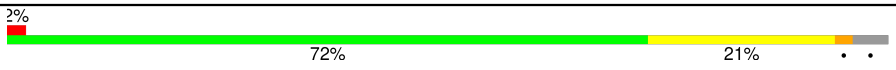
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	5963 (2.30-2.30)
Clashscore	180529	6698 (2.30-2.30)
Ramachandran outliers	177936	6640 (2.30-2.30)
Sidechain outliers	177891	6640 (2.30-2.30)
RSRZ outliers	164620	5963 (2.30-2.30)

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	294	% 85% 11%
1	B	294	82% 13%
1	C	294	76% 19%
1	D	294	81% 15%
1	E	294	83% 13%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	294	
1	G	294	
1	H	294	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 18687 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 Similar to 2-dehydropantoate 2-reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	286	Total	C	N	O	S	0	0	0
			2268	1449	389	423	7			
1	B	286	Total	C	N	O	S	0	0	0
			2278	1453	390	428	7			
1	C	285	Total	C	N	O	S	0	1	0
			2273	1452	388	426	7			
1	D	287	Total	C	N	O	S	0	0	0
			2291	1460	395	429	7			
1	E	288	Total	C	N	O	S	0	1	0
			2303	1467	399	430	7			
1	F	282	Total	C	N	O	S	0	0	0
			2245	1430	390	418	7			
1	G	290	Total	C	N	O	S	0	0	0
			2318	1477	403	431	7			
1	H	290	Total	C	N	O	S	0	0	0
			2315	1476	402	430	7			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP Q99R37
A	2	SER	-	expression tag	UNP Q99R37
A	287	GLU	-	expression tag	UNP Q99R37
A	288	GLY	-	expression tag	UNP Q99R37
A	289	HIS	-	expression tag	UNP Q99R37
A	290	HIS	-	expression tag	UNP Q99R37
A	291	HIS	-	expression tag	UNP Q99R37
A	292	HIS	-	expression tag	UNP Q99R37
A	293	HIS	-	expression tag	UNP Q99R37
A	294	HIS	-	expression tag	UNP Q99R37
B	1	MET	-	expression tag	UNP Q99R37
B	2	SER	-	expression tag	UNP Q99R37
B	287	GLU	-	expression tag	UNP Q99R37

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	288	GLY	-	expression tag	UNP Q99R37
B	289	HIS	-	expression tag	UNP Q99R37
B	290	HIS	-	expression tag	UNP Q99R37
B	291	HIS	-	expression tag	UNP Q99R37
B	292	HIS	-	expression tag	UNP Q99R37
B	293	HIS	-	expression tag	UNP Q99R37
B	294	HIS	-	expression tag	UNP Q99R37
C	1	MET	-	expression tag	UNP Q99R37
C	2	SER	-	expression tag	UNP Q99R37
C	287	GLU	-	expression tag	UNP Q99R37
C	288	GLY	-	expression tag	UNP Q99R37
C	289	HIS	-	expression tag	UNP Q99R37
C	290	HIS	-	expression tag	UNP Q99R37
C	291	HIS	-	expression tag	UNP Q99R37
C	292	HIS	-	expression tag	UNP Q99R37
C	293	HIS	-	expression tag	UNP Q99R37
C	294	HIS	-	expression tag	UNP Q99R37
D	1	MET	-	expression tag	UNP Q99R37
D	2	SER	-	expression tag	UNP Q99R37
D	287	GLU	-	expression tag	UNP Q99R37
D	288	GLY	-	expression tag	UNP Q99R37
D	289	HIS	-	expression tag	UNP Q99R37
D	290	HIS	-	expression tag	UNP Q99R37
D	291	HIS	-	expression tag	UNP Q99R37
D	292	HIS	-	expression tag	UNP Q99R37
D	293	HIS	-	expression tag	UNP Q99R37
D	294	HIS	-	expression tag	UNP Q99R37
E	1	MET	-	expression tag	UNP Q99R37
E	2	SER	-	expression tag	UNP Q99R37
E	287	GLU	-	expression tag	UNP Q99R37
E	288	GLY	-	expression tag	UNP Q99R37
E	289	HIS	-	expression tag	UNP Q99R37
E	290	HIS	-	expression tag	UNP Q99R37
E	291	HIS	-	expression tag	UNP Q99R37
E	292	HIS	-	expression tag	UNP Q99R37
E	293	HIS	-	expression tag	UNP Q99R37
E	294	HIS	-	expression tag	UNP Q99R37
F	1	MET	-	expression tag	UNP Q99R37
F	2	SER	-	expression tag	UNP Q99R37
F	287	GLU	-	expression tag	UNP Q99R37
F	288	GLY	-	expression tag	UNP Q99R37
F	289	HIS	-	expression tag	UNP Q99R37

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	290	HIS	-	expression tag	UNP Q99R37
F	291	HIS	-	expression tag	UNP Q99R37
F	292	HIS	-	expression tag	UNP Q99R37
F	293	HIS	-	expression tag	UNP Q99R37
F	294	HIS	-	expression tag	UNP Q99R37
G	1	MET	-	expression tag	UNP Q99R37
G	2	SER	-	expression tag	UNP Q99R37
G	287	GLU	-	expression tag	UNP Q99R37
G	288	GLY	-	expression tag	UNP Q99R37
G	289	HIS	-	expression tag	UNP Q99R37
G	290	HIS	-	expression tag	UNP Q99R37
G	291	HIS	-	expression tag	UNP Q99R37
G	292	HIS	-	expression tag	UNP Q99R37
G	293	HIS	-	expression tag	UNP Q99R37
G	294	HIS	-	expression tag	UNP Q99R37
H	1	MET	-	expression tag	UNP Q99R37
H	2	SER	-	expression tag	UNP Q99R37
H	287	GLU	-	expression tag	UNP Q99R37
H	288	GLY	-	expression tag	UNP Q99R37
H	289	HIS	-	expression tag	UNP Q99R37
H	290	HIS	-	expression tag	UNP Q99R37
H	291	HIS	-	expression tag	UNP Q99R37
H	292	HIS	-	expression tag	UNP Q99R37
H	293	HIS	-	expression tag	UNP Q99R37
H	294	HIS	-	expression tag	UNP Q99R37

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	74	Total O 74 74	0	0
2	B	60	Total O 60 60	0	0
2	C	51	Total O 51 51	0	0
2	D	38	Total O 38 38	0	0
2	E	31	Total O 31 31	0	0
2	F	29	Total O 29 29	0	0
2	G	60	Total O 60 60	0	0

Continued on next page...

Continued from previous page...

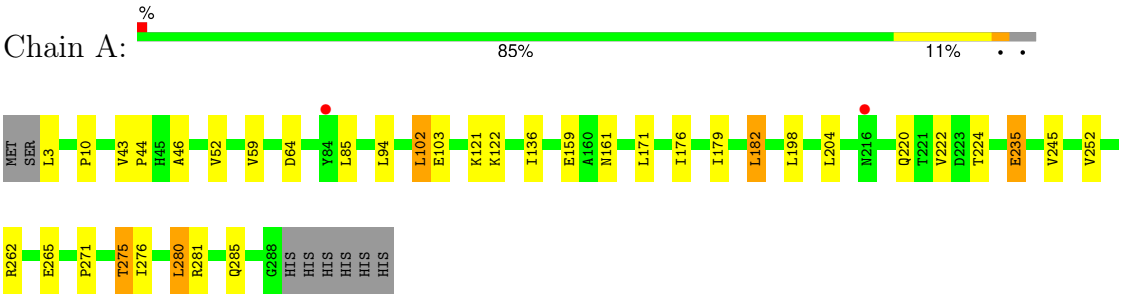
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	H	53	Total	O	0	0
			53	53		

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.

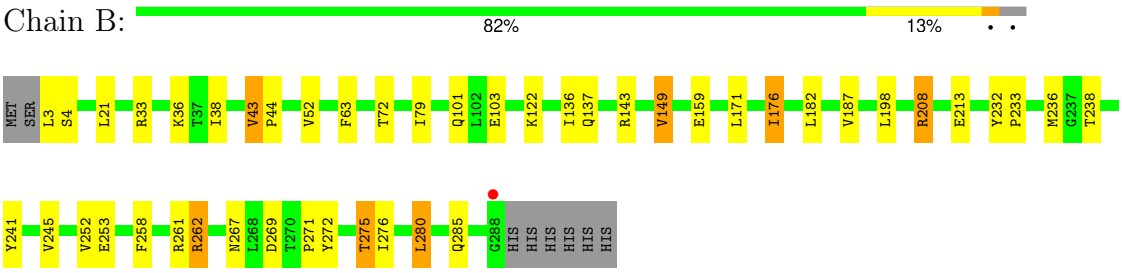
• Molecule 1: Similar to 2-dehydropantoate 2-reductase

Chain A:



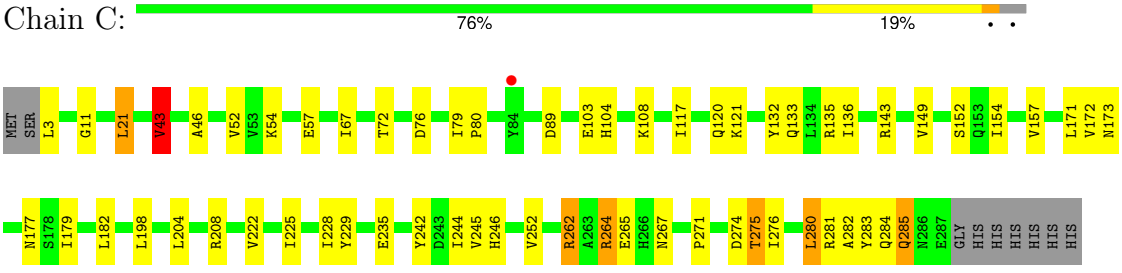
• Molecule 1: Similar to 2-dehydropantoate 2-reductase

Chain B:



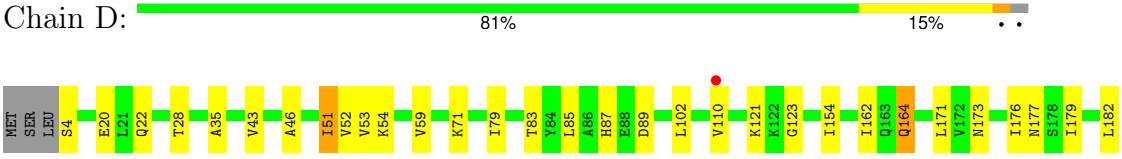
• Molecule 1: Similar to 2-dehydropantoate 2-reductase

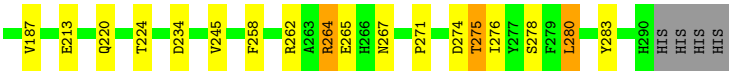
Chain C:



• Molecule 1: Similar to 2-dehydropantoate 2-reductase

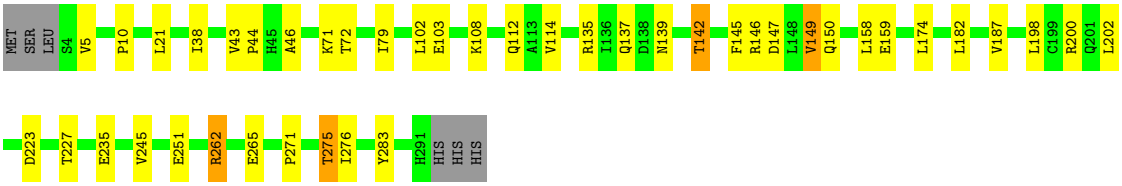
Chain D:





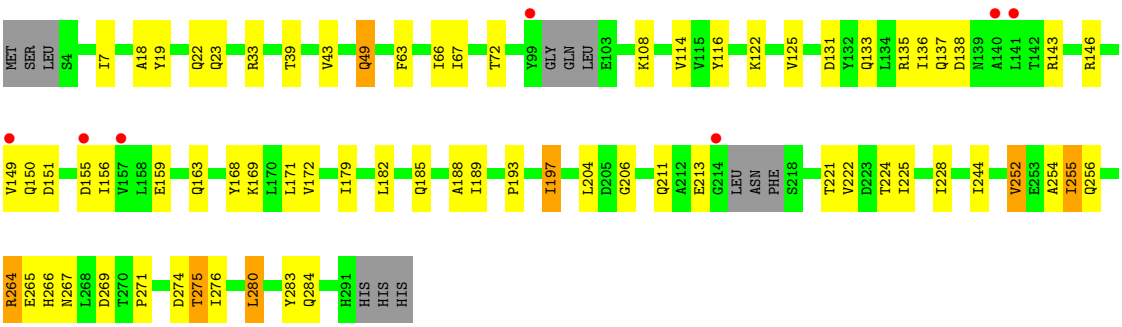
• Molecule 1: Similar to 2-dehydropantoate 2-reductase

Chain E:



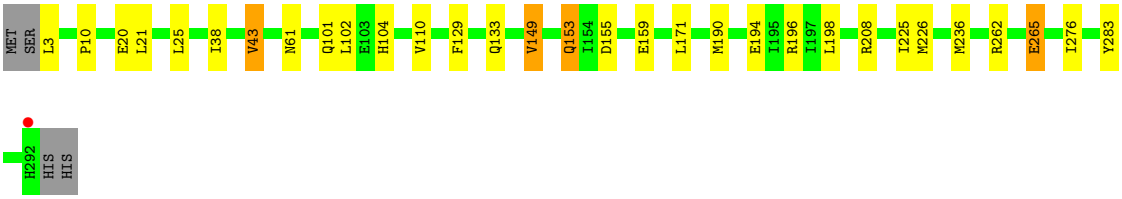
• Molecule 1: Similar to 2-dehydropantoate 2-reductase

Chain F:



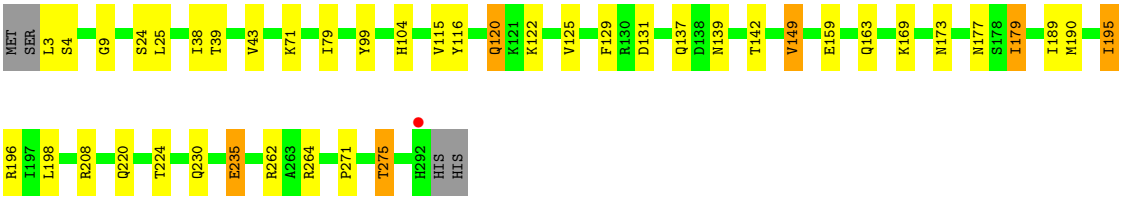
• Molecule 1: Similar to 2-dehydropantoate 2-reductase

Chain G:



• Molecule 1: Similar to 2-dehydropantoate 2-reductase

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	75.24Å 99.64Å 100.26Å 103.66° 105.23° 102.26°	Depositor
Resolution (Å)	50.00 – 2.30 50.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.2 (50.00-2.30) 98.2 (50.00-2.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.34 (at 2.29Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.200 , 0.260 0.198 , 0.255	Depositor DCC
R_{free} test set	5744 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	36.0	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 25.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.007 for -h,-l,-k	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	18687	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.21% 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

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	0.78	0/2314	0.93	1/3155 (0.0%)
1	B	0.79	1/2324 (0.0%)	0.92	2/3168 (0.1%)
1	C	0.71	0/2322	0.92	2/3166 (0.1%)
1	D	0.80	1/2339 (0.0%)	0.96	2/3188 (0.1%)
1	E	0.80	1/2355 (0.0%)	0.92	1/3210 (0.0%)
1	F	0.69	0/2291	0.96	1/3121 (0.0%)
1	G	0.80	1/2368 (0.0%)	0.91	0/3228
1	H	0.76	1/2365 (0.0%)	0.94	2/3224 (0.1%)
All	All	0.77	5/18678 (0.0%)	0.93	11/25460 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	79	ILE	CA-CB	9.57	1.58	1.54
1	D	79	ILE	CA-CB	7.99	1.58	1.54
1	B	79	ILE	CA-CB	7.19	1.57	1.54
1	H	79	ILE	CA-CB	6.41	1.57	1.54
1	G	43	VAL	CA-CB	5.35	1.61	1.54

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	9	GLY	CA-C-N	-7.61	113.97	121.65
1	H	9	GLY	C-N-CA	-7.61	113.97	121.65
1	B	252	VAL	N-CA-C	5.58	116.31	110.62
1	B	176	ILE	N-CA-C	5.52	116.25	110.62
1	F	252	VAL	N-CA-C	5.35	116.72	110.62

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	2268	0	2254	23	0
1	B	2278	0	2264	22	0
1	C	2273	0	2259	36	0
1	D	2291	0	2269	23	0
1	E	2303	0	2281	21	0
1	F	2245	0	2218	40	0
1	G	2318	0	2294	15	0
1	H	2315	0	2290	27	0
2	A	74	0	0	2	0
2	B	60	0	0	0	0
2	C	51	0	0	0	0
2	D	38	0	0	0	0
2	E	31	0	0	0	0
2	F	29	0	0	1	0
2	G	60	0	0	0	0
2	H	53	0	0	0	0
All	All	18687	0	18129	192	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 5.

The worst 5 of 192 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:262:ARG:HH11	1:B:262:ARG:HG3	1.19	1.01
1:H:137:GLN:O	1:H:142:THR:HG21	1.68	0.91
1:F:137:GLN:HE21	1:F:138:ASP:H	1.16	0.89
1:B:262:ARG:HG3	1:B:262:ARG:NH1	1.85	0.88
1:F:171:LEU:HD11	1:F:206:GLY:HA3	1.56	0.86

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	284/294 (97%)	273 (96%)	11 (4%)	0	100 100
1	B	284/294 (97%)	269 (95%)	15 (5%)	0	100 100
1	C	284/294 (97%)	270 (95%)	14 (5%)	0	100 100
1	D	285/294 (97%)	275 (96%)	10 (4%)	0	100 100
1	E	287/294 (98%)	276 (96%)	11 (4%)	0	100 100
1	F	276/294 (94%)	255 (92%)	19 (7%)	2 (1%)	19 23
1	G	288/294 (98%)	278 (96%)	10 (4%)	0	100 100
1	H	288/294 (98%)	276 (96%)	12 (4%)	0	100 100
All	All	2276/2352 (97%)	2172 (95%)	102 (4%)	2 (0%)	48 60

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	188	ALA
1	F	255	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	244/256 (95%)	231 (95%)	13 (5%)	19 28
1	B	247/256 (96%)	224 (91%)	23 (9%)	7 9
1	C	246/256 (96%)	220 (89%)	26 (11%)	5 6

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	248/256 (97%)	230 (93%)	18 (7%)	11 16
1	E	250/256 (98%)	234 (94%)	16 (6%)	14 20
1	F	242/256 (94%)	218 (90%)	24 (10%)	6 8
1	G	251/256 (98%)	240 (96%)	11 (4%)	24 35
1	H	250/256 (98%)	231 (92%)	19 (8%)	11 14
All	All	1978/2048 (97%)	1828 (92%)	150 (8%)	11 14

5 of 150 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	267	ASN
1	H	179	ILE
1	F	280	LEU
1	G	276	ILE
1	C	143	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 48 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	289	HIS
1	G	22	GLN
1	F	112	GLN
1	F	144	GLN
1	G	104	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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	286/294 (97%)	-0.34	2 (0%)	84	84	22, 32, 47, 53	0
1	B	286/294 (97%)	-0.09	1 (0%)	90	90	22, 36, 59, 64	0
1	C	285/294 (96%)	-0.04	1 (0%)	89	89	25, 39, 54, 61	1 (0%)
1	D	287/294 (97%)	-0.22	1 (0%)	90	90	20, 33, 51, 60	0
1	E	288/294 (97%)	-0.29	0	100	100	14, 33, 48, 62	1 (0%)
1	F	282/294 (95%)	0.41	7 (2%)	58	59	27, 44, 63, 66	0
1	G	290/294 (98%)	-0.36	1 (0%)	90	90	20, 31, 45, 59	0
1	H	290/294 (98%)	-0.25	1 (0%)	90	90	23, 35, 48, 57	0
All	All	2294/2352 (97%)	-0.15	14 (0%)	85	86	14, 35, 56, 66	2 (0%)

The worst 5 of 14 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	214	GLY	4.4
1	F	155	ASP	3.4
1	A	84	TYR	3.2
1	F	99	TYR	2.6
1	F	157	VAL	2.3

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 monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.