



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:43 PM UTC

PDB ID : 2RJT / pdb_00002rjt
Title : Crystal Structure Analysis of a Surface Entropy Reduction Mutant of *S. pneumoniae* FabF
Authors : Soisson, S.M.; Parthasarathy, G.; Becker, J.
Deposited on : 2007-10-15
Resolution : 1.75 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

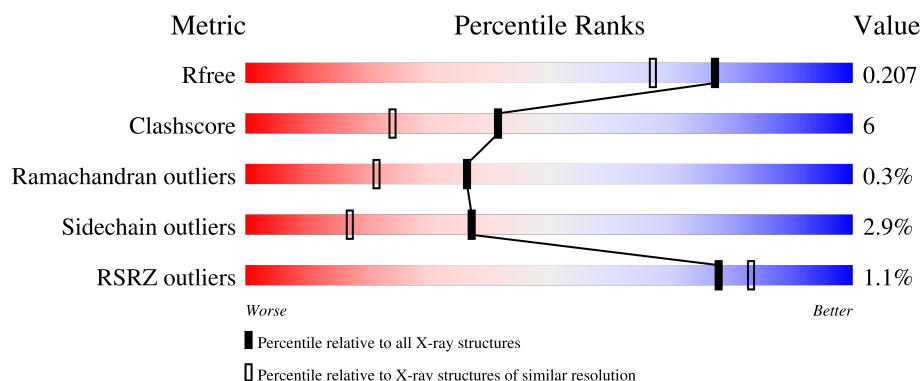
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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}	180053	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (1.76-1.76)

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 $\leq 5\%$. 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	428	
1	B	428	
1	C	428	
1	D	428	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14001 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 Beta-ketoacyl-ACP synthase II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	408	Total	C	N	O	S	0	1	0
			3047	1927	523	585	12			
1	D	408	Total	C	N	O	S	0	2	0
			3053	1930	524	587	12			
1	C	408	Total	C	N	O	S	0	2	0
			3057	1933	525	586	13			
1	B	408	Total	C	N	O	S	0	2	0
			3053	1930	524	587	12			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	GLY	-	expression tag	UNP Q9FBC2
A	-17	SER	-	expression tag	UNP Q9FBC2
A	-16	SER	-	expression tag	UNP Q9FBC2
A	-15	HIS	-	expression tag	UNP Q9FBC2
A	-14	HIS	-	expression tag	UNP Q9FBC2
A	-13	HIS	-	expression tag	UNP Q9FBC2
A	-12	HIS	-	expression tag	UNP Q9FBC2
A	-11	HIS	-	expression tag	UNP Q9FBC2
A	-10	HIS	-	expression tag	UNP Q9FBC2
A	-9	SER	-	expression tag	UNP Q9FBC2
A	-8	SER	-	expression tag	UNP Q9FBC2
A	-7	GLY	-	expression tag	UNP Q9FBC2
A	-6	LEU	-	expression tag	UNP Q9FBC2
A	-5	VAL	-	expression tag	UNP Q9FBC2
A	-4	PRO	-	expression tag	UNP Q9FBC2
A	-3	ARG	-	expression tag	UNP Q9FBC2
A	-2	GLY	-	expression tag	UNP Q9FBC2
A	-1	SER	-	expression tag	UNP Q9FBC2
A	0	HIS	-	expression tag	UNP Q9FBC2
A	22	ALA	GLU	engineered mutation	UNP Q9FBC2
A	94	ALA	GLU	engineered mutation	UNP Q9FBC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	325	ALA	GLU	engineered mutation	UNP Q9FBC2
A	383	ALA	GLU	engineered mutation	UNP Q9FBC2
A	409	ALA	GLU	engineered mutation	UNP Q9FBC2
D	-18	GLY	-	expression tag	UNP Q9FBC2
D	-17	SER	-	expression tag	UNP Q9FBC2
D	-16	SER	-	expression tag	UNP Q9FBC2
D	-15	HIS	-	expression tag	UNP Q9FBC2
D	-14	HIS	-	expression tag	UNP Q9FBC2
D	-13	HIS	-	expression tag	UNP Q9FBC2
D	-12	HIS	-	expression tag	UNP Q9FBC2
D	-11	HIS	-	expression tag	UNP Q9FBC2
D	-10	HIS	-	expression tag	UNP Q9FBC2
D	-9	SER	-	expression tag	UNP Q9FBC2
D	-8	SER	-	expression tag	UNP Q9FBC2
D	-7	GLY	-	expression tag	UNP Q9FBC2
D	-6	LEU	-	expression tag	UNP Q9FBC2
D	-5	VAL	-	expression tag	UNP Q9FBC2
D	-4	PRO	-	expression tag	UNP Q9FBC2
D	-3	ARG	-	expression tag	UNP Q9FBC2
D	-2	GLY	-	expression tag	UNP Q9FBC2
D	-1	SER	-	expression tag	UNP Q9FBC2
D	0	HIS	-	expression tag	UNP Q9FBC2
D	22	ALA	GLU	engineered mutation	UNP Q9FBC2
D	94	ALA	GLU	engineered mutation	UNP Q9FBC2
D	325	ALA	GLU	engineered mutation	UNP Q9FBC2
D	383	ALA	GLU	engineered mutation	UNP Q9FBC2
D	409	ALA	GLU	engineered mutation	UNP Q9FBC2
C	-18	GLY	-	expression tag	UNP Q9FBC2
C	-17	SER	-	expression tag	UNP Q9FBC2
C	-16	SER	-	expression tag	UNP Q9FBC2
C	-15	HIS	-	expression tag	UNP Q9FBC2
C	-14	HIS	-	expression tag	UNP Q9FBC2
C	-13	HIS	-	expression tag	UNP Q9FBC2
C	-12	HIS	-	expression tag	UNP Q9FBC2
C	-11	HIS	-	expression tag	UNP Q9FBC2
C	-10	HIS	-	expression tag	UNP Q9FBC2
C	-9	SER	-	expression tag	UNP Q9FBC2
C	-8	SER	-	expression tag	UNP Q9FBC2
C	-7	GLY	-	expression tag	UNP Q9FBC2
C	-6	LEU	-	expression tag	UNP Q9FBC2
C	-5	VAL	-	expression tag	UNP Q9FBC2
C	-4	PRO	-	expression tag	UNP Q9FBC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	ARG	-	expression tag	UNP Q9FBC2
C	-2	GLY	-	expression tag	UNP Q9FBC2
C	-1	SER	-	expression tag	UNP Q9FBC2
C	0	HIS	-	expression tag	UNP Q9FBC2
C	22	ALA	GLU	engineered mutation	UNP Q9FBC2
C	94	ALA	GLU	engineered mutation	UNP Q9FBC2
C	325	ALA	GLU	engineered mutation	UNP Q9FBC2
C	383	ALA	GLU	engineered mutation	UNP Q9FBC2
C	409	ALA	GLU	engineered mutation	UNP Q9FBC2
B	-18	GLY	-	expression tag	UNP Q9FBC2
B	-17	SER	-	expression tag	UNP Q9FBC2
B	-16	SER	-	expression tag	UNP Q9FBC2
B	-15	HIS	-	expression tag	UNP Q9FBC2
B	-14	HIS	-	expression tag	UNP Q9FBC2
B	-13	HIS	-	expression tag	UNP Q9FBC2
B	-12	HIS	-	expression tag	UNP Q9FBC2
B	-11	HIS	-	expression tag	UNP Q9FBC2
B	-10	HIS	-	expression tag	UNP Q9FBC2
B	-9	SER	-	expression tag	UNP Q9FBC2
B	-8	SER	-	expression tag	UNP Q9FBC2
B	-7	GLY	-	expression tag	UNP Q9FBC2
B	-6	LEU	-	expression tag	UNP Q9FBC2
B	-5	VAL	-	expression tag	UNP Q9FBC2
B	-4	PRO	-	expression tag	UNP Q9FBC2
B	-3	ARG	-	expression tag	UNP Q9FBC2
B	-2	GLY	-	expression tag	UNP Q9FBC2
B	-1	SER	-	expression tag	UNP Q9FBC2
B	0	HIS	-	expression tag	UNP Q9FBC2
B	22	ALA	GLU	engineered mutation	UNP Q9FBC2
B	94	ALA	GLU	engineered mutation	UNP Q9FBC2
B	325	ALA	GLU	engineered mutation	UNP Q9FBC2
B	383	ALA	GLU	engineered mutation	UNP Q9FBC2
B	409	ALA	GLU	engineered mutation	UNP Q9FBC2

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	507	Total O 507 507	0	0
2	D	472	Total O 472 472	0	0
2	C	408	Total O 408 408	0	0

Continued on next page...

Continued from previous page...

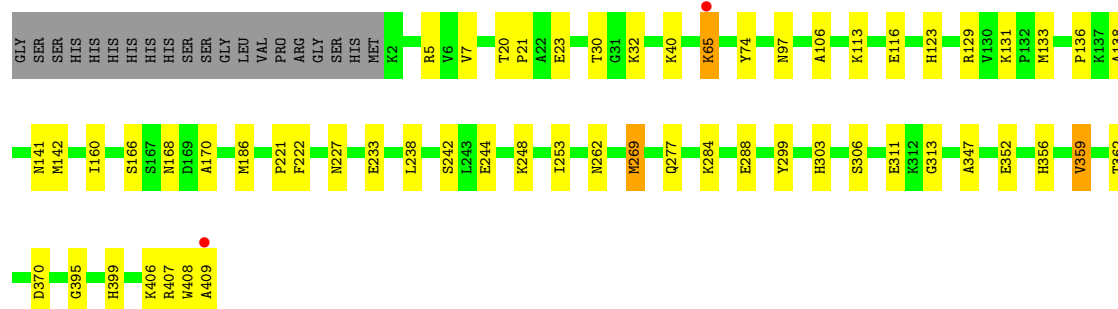
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	404	Total 404	O 404	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

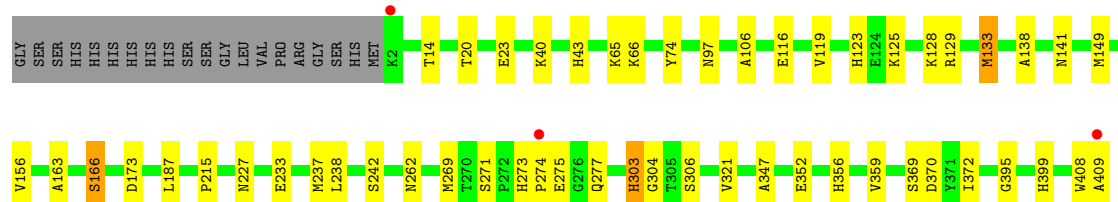
• Molecule 1: Beta-ketoacyl-ACP synthase II

Chain A: 



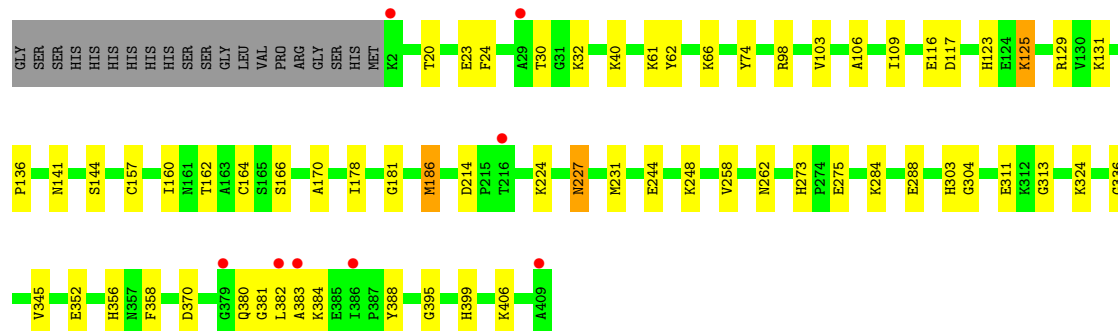
• Molecule 1: Beta-ketoacyl-ACP synthase II

Chain D: 



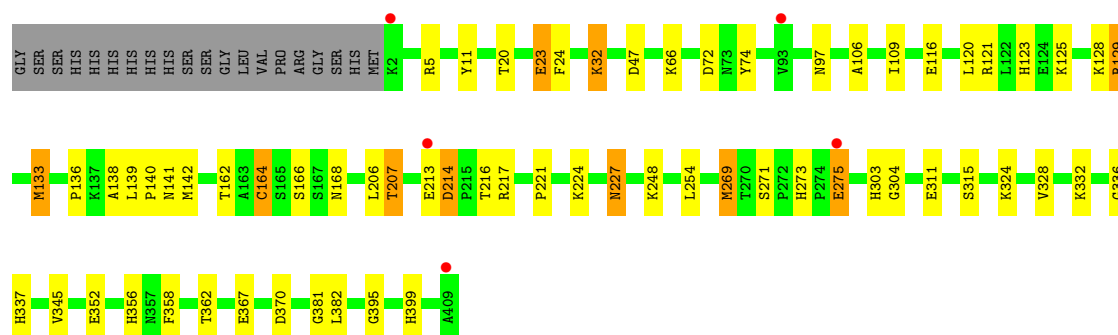
• Molecule 1: Beta-ketoacyl-ACP synthase II

Chain C: 



● Molecule 1: Beta-ketoacyl-ACP synthase II

Chain B:  %



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	112.42Å 115.87Å 278.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.90 – 1.75 45.90 – 1.75	Depositor EDS
% Data completeness (in resolution range)	99.3 (45.90-1.75) 99.5 (45.90-1.75)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.99 (at 1.75Å)	Xtriage
Refinement program	TNT, BUSTER-TNT 2.1.1	Depositor
R, R_{free}	0.167 , 0.207 (Not available) , 0.207	Depositor DCC
R_{free} test set	9058 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	24.2	Xtriage
Anisotropy	0.331	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 47.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.036 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	14001	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% 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

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	0.88	2/3110 (0.1%)	1.05	11/4218 (0.3%)
1	B	0.79	3/3116 (0.1%)	1.09	18/4226 (0.4%)
1	C	0.77	1/3120 (0.0%)	1.05	10/4230 (0.2%)
1	D	0.88	3/3116 (0.1%)	1.07	14/4226 (0.3%)
All	All	0.83	9/12462 (0.1%)	1.06	53/16900 (0.3%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	149	MET	SD-CE	-8.18	1.59	1.79
1	B	133	MET	SD-CE	-6.37	1.63	1.79
1	A	269	MET	SD-CE	-6.25	1.64	1.79
1	B	269	MET	SD-CE	-5.96	1.64	1.79
1	A	186	MET	CG-SD	-5.77	1.66	1.80
1	D	133	MET	SD-CE	5.56	1.93	1.79
1	C	231	MET	SD-CE	5.19	1.92	1.79
1	D	359	VAL	CA-CB	5.09	1.58	1.53
1	B	328	VAL	CA-CB	5.08	1.61	1.54

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	303	HIS	N-CA-C	-9.75	100.61	111.14
1	A	303	HIS	N-CA-C	-8.82	101.61	111.14
1	B	303	HIS	N-CA-C	-8.12	102.50	111.36
1	B	214	ASP	CA-C-N	8.05	127.78	119.56
1	B	214	ASP	C-N-CA	8.05	127.78	119.56
1	D	138	ALA	N-CA-C	8.02	121.19	111.40
1	D	303	HIS	N-CA-C	-7.48	103.06	111.14
1	B	47	ASP	N-CA-C	-6.74	105.21	113.50
1	B	271	SER	CA-C-N	-6.73	113.71	120.31
1	B	271	SER	C-N-CA	-6.73	113.71	120.31
1	A	138	ALA	N-CA-C	6.67	121.72	112.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	72	ASP	N-CA-C	-6.66	101.56	110.55
1	B	395	GLY	N-CA-C	6.42	121.67	112.82
1	B	97	ASN	N-CA-C	-6.33	98.22	108.41
1	D	271	SER	CA-C-N	-6.18	114.25	120.31
1	D	271	SER	C-N-CA	-6.18	114.25	120.31
1	A	395	GLY	N-CA-C	6.18	122.65	112.89
1	C	324	LYS	N-CA-C	6.09	120.72	113.16
1	D	119	VAL	N-CA-C	-6.06	104.61	110.42
1	C	395	GLY	N-CA-C	6.03	121.14	112.82
1	B	142	MET	N-CA-C	5.95	117.77	111.28
1	C	336	GLY	N-CA-C	-5.95	101.88	112.58
1	C	181	GLY	N-CA-C	5.92	124.20	115.08
1	A	97	ASN	N-CA-C	-5.90	98.08	108.23
1	B	168	ASN	N-CA-C	-5.85	104.98	111.36
1	D	166	SER	N-CA-C	5.85	118.13	111.11
1	A	142	MET	N-CA-C	5.78	117.58	111.28
1	B	336	GLY	N-CA-C	-5.78	102.18	112.58
1	D	347	ALA	N-CA-C	-5.76	105.09	111.36
1	A	5	ARG	N-CA-C	-5.74	101.99	110.48
1	D	242	SER	N-CA-C	-5.69	103.02	110.53
1	B	332	LYS	N-CA-C	-5.68	106.20	113.01
1	B	138	ALA	N-CA-C	5.61	120.24	112.45
1	C	258	VAL	N-CA-C	5.60	119.13	113.47
1	C	20	THR	CA-C-N	-5.58	113.14	119.28
1	C	20	THR	C-N-CA	-5.58	113.14	119.28
1	B	5	ARG	N-CA-C	-5.58	102.23	110.48
1	D	97	ASN	N-CA-C	-5.55	98.68	108.23
1	A	168	ASN	N-CA-C	-5.51	105.35	111.36
1	D	163	ALA	CB-CA-C	-5.39	110.34	116.54
1	D	395	GLY	N-CA-C	5.38	121.39	112.89
1	C	131	LYS	N-CA-C	5.32	116.39	109.64
1	B	315	SER	N-CA-C	-5.31	105.39	111.07
1	D	187	LEU	N-CA-C	-5.23	100.21	108.73
1	D	321	VAL	N-CA-C	5.18	116.27	111.45
1	B	162	THR	N-CA-C	-5.16	104.28	110.88
1	A	362	THR	N-CA-C	-5.13	100.14	108.41
1	A	359	VAL	CA-C-O	5.13	121.99	119.12
1	C	162	THR	N-CA-C	-5.12	104.22	110.61
1	A	242	SER	N-CA-C	-5.09	103.82	110.53
1	D	14	THR	N-CA-C	-5.05	100.22	108.76
1	A	347	ALA	N-CA-C	-5.05	105.86	111.36
1	B	324	LYS	N-CA-C	5.01	119.40	113.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3047	0	2993	42	0
1	B	3053	0	2997	55	0
1	C	3057	0	3008	47	0
1	D	3053	0	2997	37	0
2	A	507	0	0	10	0
2	B	404	0	0	13	0
2	C	408	0	0	13	0
2	D	472	0	0	9	0
All	All	14001	0	11995	156	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 6.

All (156) 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:141:ASN:HD22	1:C:399:HIS:HE1	1.10	0.93
1:D:273:HIS:CD2	1:D:274:PRO:HD2	2.06	0.91
1:A:399:HIS:HE1	1:B:141:ASN:HD22	1.23	0.87
1:D:269:MET:HE2	1:C:136:PRO:HB3	1.60	0.83
1:A:407:ARG:O	1:A:409:ALA:HB3	1.78	0.82
1:D:141:ASN:HD22	1:C:399:HIS:CE1	1.96	0.81
1:C:244:GLU:HG3	1:C:248:LYS:HE3	1.61	0.81
1:D:399:HIS:HE1	1:C:141:ASN:HD22	1.28	0.81
1:A:244:GLU:HG2	1:A:248:LYS:HE2	1.61	0.80
1:B:129:ARG:HH11	1:B:129:ARG:HG3	1.46	0.79
1:A:20:THR:OG1	1:A:23:GLU:HG3	1.83	0.79
1:B:273:HIS:CE1	1:B:275:GLU:HG3	2.19	0.78
1:A:399:HIS:CE1	1:B:141:ASN:HD22	2.03	0.77
1:D:40:LYS:HE2	2:D:581:HOH:O	1.85	0.77
1:A:141:ASN:HD22	1:B:399:HIS:HE1	1.28	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:MET:HE3	1:B:136:PRO:HB3	1.68	0.76
1:A:123:HIS:HE1	1:B:116:GLU:OE1	1.67	0.76
1:D:399:HIS:CE1	1:C:141:ASN:HD22	2.05	0.74
1:D:43:HIS:NE2	1:B:207:THR:HG21	2.02	0.74
1:A:244:GLU:CG	1:A:248:LYS:HE2	2.17	0.73
1:D:116:GLU:OE1	1:C:123:HIS:HE1	1.70	0.73
1:A:262:ASN:HB2	2:B:503:HOH:O	1.88	0.72
1:C:406:LYS:HD3	2:C:797:HOH:O	1.88	0.72
1:C:178:ILE:HD11	1:C:186[A]:MET:HG3	1.71	0.72
1:A:141:ASN:HD22	1:B:399:HIS:CE1	2.07	0.71
1:B:129:ARG:HG3	1:B:129:ARG:NH1	2.04	0.70
1:B:129:ARG:HD2	1:B:129:ARG:N	2.07	0.70
1:C:244:GLU:O	1:C:248:LYS:HG3	1.92	0.68
1:B:275:GLU:HG2	2:B:794:HOH:O	1.93	0.68
1:D:65:LYS:HB2	2:D:799:HOH:O	1.92	0.68
1:A:269:MET:CE	1:B:136:PRO:HB3	2.25	0.67
1:D:123:HIS:HE1	1:C:116:GLU:OE1	1.78	0.67
1:D:125:LYS:HB3	1:D:129:ARG:HG3	1.77	0.66
1:B:20:THR:OG1	1:B:23:GLU:HG3	1.97	0.65
1:A:116:GLU:OE1	1:B:123:HIS:HE1	1.79	0.65
1:B:129:ARG:NH1	2:B:675:HOH:O	2.27	0.62
1:B:227:ASN:HD22	1:B:227:ASN:N	1.97	0.62
1:B:227:ASN:HD22	1:B:227:ASN:H	1.46	0.62
1:A:106:ALA:HB1	1:A:166:SER:HB3	1.81	0.61
1:D:262:ASN:HB2	2:C:549:HOH:O	1.99	0.61
1:B:125:LYS:HB3	1:B:129:ARG:HG2	1.83	0.60
1:C:178:ILE:CD1	1:C:186[A]:MET:HG3	2.31	0.59
1:D:133:MET:HE1	2:C:806:HOH:O	2.01	0.59
1:C:358:PHE:CZ	1:C:381:GLY:HA3	2.38	0.59
1:A:30:THR:OG1	1:A:32:LYS:HD2	2.03	0.59
1:C:178:ILE:HD11	1:C:186[A]:MET:CG	2.32	0.59
2:D:482:HOH:O	1:C:262:ASN:HB2	2.03	0.58
1:D:269:MET:HE2	1:C:136:PRO:CB	2.32	0.58
1:D:275:GLU:N	1:D:275:GLU:OE1	2.36	0.58
1:B:106:ALA:HB1	1:B:166:SER:HB3	1.85	0.58
1:A:136:PRO:HB3	1:B:269:MET:HE3	1.86	0.57
1:A:313:GLY:HA3	2:A:629:HOH:O	2.04	0.57
1:B:273:HIS:HE1	1:B:275:GLU:CG	2.17	0.57
1:D:106:ALA:HB1	1:D:166:SER:HB3	1.86	0.57
1:B:207:THR:HG23	2:B:532:HOH:O	2.05	0.56
1:A:65:LYS:HE2	2:A:823:HOH:O	2.05	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:30:THR:OG1	1:C:32:LYS:HG3	2.06	0.56
1:A:133:MET:HE1	2:B:751:HOH:O	2.06	0.55
1:B:273:HIS:CE1	1:B:275:GLU:CG	2.88	0.55
1:D:273:HIS:HD2	1:D:275:GLU:H	1.53	0.55
1:A:352:GLU:O	1:A:356:HIS:HD2	1.90	0.54
1:B:217:ARG:HD3	2:B:600:HOH:O	2.07	0.54
1:A:40:LYS:HE3	1:A:233:GLU:OE2	2.07	0.53
1:C:352:GLU:HA	1:C:352:GLU:OE1	2.08	0.53
1:D:125:LYS:CB	1:D:129:ARG:HG3	2.37	0.53
1:D:273:HIS:HD2	1:D:274:PRO:HD2	1.65	0.53
1:B:224:LYS:HE3	2:B:721:HOH:O	2.07	0.53
1:C:106:ALA:HB1	1:C:166:SER:HB3	1.90	0.53
1:B:125:LYS:CB	1:B:129:ARG:HG2	2.39	0.52
1:D:273:HIS:CE1	1:D:277:GLN:HB3	2.44	0.52
1:B:121:ARG:HD2	2:B:810:HOH:O	2.10	0.52
1:C:160:ILE:HD12	1:C:170:ALA:HA	1.92	0.52
1:A:113:LYS:NZ	2:A:832:HOH:O	2.43	0.51
1:C:129:ARG:HG3	1:C:129:ARG:NH1	2.26	0.51
1:D:408:TRP:O	1:D:409:ALA:HB2	2.11	0.51
1:C:129:ARG:HG3	1:C:129:ARG:HH11	1.76	0.51
1:D:352:GLU:O	1:D:356:HIS:HD2	1.93	0.51
1:B:121:ARG:HB2	2:B:810:HOH:O	2.11	0.51
1:C:273:HIS:CD2	1:C:275:GLU:H	2.29	0.50
1:C:383:ALA:O	1:C:384:LYS:HB3	2.10	0.50
1:C:352:GLU:O	1:C:356:HIS:HD2	1.95	0.50
1:D:116:GLU:OE1	1:C:123:HIS:CE1	2.59	0.50
1:D:274:PRO:HG2	1:D:275:GLU:OE1	2.12	0.50
1:C:40:LYS:HD3	2:C:782:HOH:O	2.12	0.49
1:C:388:TYR:CE2	1:C:406:LYS:HG3	2.47	0.49
1:B:125:LYS:HB3	1:B:129:ARG:CG	2.41	0.49
1:A:160:ILE:HD12	1:A:170:ALA:HA	1.95	0.49
1:A:7:VAL:HB	1:A:253:ILE:HG23	1.95	0.49
1:C:214:ASP:HB2	2:C:734:HOH:O	2.12	0.49
1:D:128:LYS:NZ	2:D:768:HOH:O	2.46	0.49
1:C:313:GLY:HA3	2:C:706:HOH:O	2.13	0.49
1:C:23:GLU:HG2	2:C:700:HOH:O	2.12	0.48
1:A:409:ALA:HB2	2:A:682:HOH:O	2.12	0.48
1:C:227:ASN:H	1:C:227:ASN:HD22	1.61	0.48
1:B:128:LYS:C	1:B:129:ARG:HD2	2.39	0.48
1:D:20:THR:OG1	1:D:23:GLU:HG3	2.14	0.48
1:D:237:MET:C	1:D:238:LEU:HD12	2.39	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:224:LYS:HD2	2:C:781:HOH:O	2.14	0.47
1:B:133:MET:HA	1:B:133:MET:HE2	1.95	0.47
1:B:269:MET:HE2	2:B:672:HOH:O	2.13	0.47
1:D:262:ASN:OD1	2:D:668:HOH:O	2.20	0.47
1:D:123:HIS:CE1	1:C:116:GLU:OE1	2.63	0.47
1:B:206:LEU:O	1:B:207:THR:HB	2.13	0.47
1:D:369:SER:HB2	1:D:372:ILE:HG13	1.97	0.46
1:A:65:LYS:HG3	2:A:823:HOH:O	2.16	0.46
1:B:273:HIS:ND1	1:B:275:GLU:HG3	2.30	0.46
1:D:40:LYS:HE3	1:D:233:GLU:OE2	2.14	0.46
1:B:214:ASP:OD1	1:B:216:THR:OG1	2.32	0.46
1:C:98:ARG:NH2	2:C:496:HOH:O	2.49	0.46
1:D:215:PRO:HG3	2:D:789:HOH:O	2.15	0.46
1:A:123:HIS:CE1	1:B:120:LEU:HD11	2.52	0.45
1:A:133:MET:HE3	2:D:732:HOH:O	2.16	0.45
1:A:406:LYS:HE3	2:A:889:HOH:O	2.15	0.45
1:B:352:GLU:O	1:B:356:HIS:HD2	2.00	0.45
1:A:277:GLN:NE2	2:A:905:HOH:O	2.49	0.45
1:C:227:ASN:HD22	1:C:227:ASN:N	2.15	0.44
1:B:352:GLU:HA	1:B:352:GLU:OE1	2.17	0.44
1:C:125:LYS:HB3	1:C:129:ARG:HG3	2.00	0.44
1:B:164:CYS:HB3	1:B:337:HIS:CE1	2.53	0.44
1:A:370:ASP:CB	2:A:779:HOH:O	2.66	0.43
1:B:125:LYS:CB	1:B:129:ARG:CG	2.96	0.43
1:C:117:ASP:OD2	2:C:687:HOH:O	2.21	0.43
1:C:388:TYR:OH	1:C:406:LYS:HE2	2.18	0.43
1:B:24:PHE:CZ	1:B:345[A]:VAL:HG13	2.53	0.43
1:A:116:GLU:OE1	1:B:123:HIS:CE1	2.67	0.43
1:A:221:PRO:O	1:A:222:PHE:HB2	2.19	0.43
1:C:103:VAL:O	1:C:157:CYS:HA	2.19	0.43
1:C:284:LYS:NZ	2:C:749:HOH:O	2.52	0.43
1:A:408:TRP:HA	1:A:409:ALA:C	2.44	0.43
1:D:303:HIS:CE1	2:D:819:HOH:O	2.71	0.43
1:C:370:ASP:CB	2:C:526:HOH:O	2.66	0.42
1:B:227:ASN:N	1:B:227:ASN:ND2	2.67	0.42
1:A:32:LYS:HB3	2:A:916:HOH:O	2.18	0.42
1:D:156:VAL:HG22	1:C:262:ASN:ND2	2.34	0.42
1:B:358:PHE:CZ	1:B:381:GLY:HA3	2.54	0.42
1:A:123:HIS:CE1	1:B:116:GLU:OE1	2.59	0.42
1:A:284:LYS:O	1:A:288:GLU:HG3	2.18	0.42
1:A:299:TYR:CE1	1:A:359:VAL:HG13	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:139:LEU:HA	1:B:140:PRO:HD3	1.94	0.42
1:A:269:MET:CE	1:B:136:PRO:CB	2.94	0.42
1:B:224:LYS:HE3	1:B:367:GLU:OE2	2.20	0.42
1:C:380:GLN:NE2	1:C:381:GLY:O	2.53	0.41
1:A:40:LYS:CE	1:A:233:GLU:OE2	2.68	0.41
1:D:273:HIS:HA	1:D:274:PRO:HD3	1.79	0.41
1:B:11:TYR:CE2	1:B:254:LEU:HD12	2.55	0.41
1:B:206:LEU:O	1:B:207:THR:HG22	2.21	0.41
1:A:370:ASP:CB	2:A:581:HOH:O	2.69	0.41
1:A:238:LEU:HD12	1:A:238:LEU:N	2.36	0.41
1:B:370:ASP:CB	2:B:554:HOH:O	2.69	0.41
1:C:24:PHE:CZ	1:C:345[A]:VAL:HG13	2.56	0.41
1:C:61:LYS:HE2	1:C:62:TYR:OH	2.21	0.40
1:C:370:ASP:CB	2:C:594:HOH:O	2.70	0.40
1:D:370:ASP:CB	2:D:838:HOH:O	2.69	0.40
1:B:23:GLU:HB3	2:B:754:HOH:O	2.21	0.40
1:B:221:PRO:HD2	1:B:362:THR:CG2	2.51	0.40
1:B:32:LYS:HD2	2:B:455:HOH:O	2.21	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	407/428 (95%)	397 (98%)	9 (2%)	1 (0%)	43	27
1	B	408/428 (95%)	399 (98%)	8 (2%)	1 (0%)	43	27
1	C	408/428 (95%)	399 (98%)	8 (2%)	1 (0%)	43	27
1	D	408/428 (95%)	397 (97%)	9 (2%)	2 (0%)	24	11
All	All	1631/1712 (95%)	1592 (98%)	34 (2%)	5 (0%)	36	21

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	304	GLY
1	C	304	GLY
1	D	306	SER
1	A	306	SER
1	D	304	GLY

5.3.2 Protein sidechains ⓘ

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	314/332 (95%)	307 (98%)	7 (2%)	45	26
1	B	315/332 (95%)	301 (96%)	14 (4%)	25	7
1	C	316/332 (95%)	304 (96%)	12 (4%)	29	10
1	D	315/332 (95%)	311 (99%)	4 (1%)	61	46
All	All	1260/1328 (95%)	1223 (97%)	37 (3%)	37	17

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	PRO
1	A	65	LYS
1	A	74	TYR
1	A	129	ARG
1	A	131	LYS
1	A	227	ASN
1	A	311	GLU
1	D	66	LYS
1	D	74	TYR
1	D	173	ASP
1	D	227	ASN
1	C	66	LYS
1	C	74	TYR
1	C	109	ILE
1	C	125	LYS
1	C	144	SER
1	C	164	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	186[A]	MET
1	C	186[B]	MET
1	C	227	ASN
1	C	288	GLU
1	C	311	GLU
1	C	382	LEU
1	B	23	GLU
1	B	32	LYS
1	B	66	LYS
1	B	74	TYR
1	B	109	ILE
1	B	129	ARG
1	B	164	CYS
1	B	207	THR
1	B	213	GLU
1	B	227	ASN
1	B	248	LYS
1	B	275	GLU
1	B	311	GLU
1	B	382	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	123	HIS
1	A	154	ASN
1	A	227	ASN
1	A	273	HIS
1	A	356	HIS
1	A	392	ASN
1	A	399	HIS
1	D	123	HIS
1	D	154	ASN
1	D	227	ASN
1	D	273	HIS
1	D	356	HIS
1	D	392	ASN
1	D	399	HIS
1	C	123	HIS
1	C	227	ASN
1	C	273	HIS
1	C	356	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	399	HIS
1	B	123	HIS
1	B	227	ASN
1	B	273	HIS
1	B	301	ASN
1	B	356	HIS
1	B	392	ASN
1	B	399	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, 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	408/428 (95%)	-0.40	2 (0%) 87 90	8, 22, 35, 74	1 (0%)
1	B	408/428 (95%)	0.08	5 (1%) 76 82	11, 29, 46, 82	2 (0%)
1	C	408/428 (95%)	0.10	8 (1%) 65 71	12, 29, 46, 84	2 (0%)
1	D	408/428 (95%)	-0.27	3 (0%) 84 88	9, 23, 40, 78	2 (0%)
All	All	1632/1712 (95%)	-0.12	18 (1%) 78 83	8, 26, 42, 84	7 (0%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	409	ALA	7.1
1	D	409	ALA	6.3
1	C	409	ALA	5.4
1	A	409	ALA	5.2
1	D	274	PRO	3.2
1	C	2	LYS	2.8
1	B	275	GLU	2.6
1	D	2	LYS	2.4
1	B	2	LYS	2.3
1	C	216	THR	2.2
1	C	379	GLY	2.2
1	C	386	ILE	2.2
1	C	382	LEU	2.1
1	C	383	ALA	2.1
1	A	65	LYS	2.1
1	B	213	GLU	2.1
1	C	29	ALA	2.0
1	B	93	VAL	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.