Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 12:00 PM GMT

PDB ID	:	3QP9
Title	:	The Structure of a C2-type Ketoreductase from a Modular Polyketide Synthase
Authors	:	Zheng, J.; Keatinge-Clay, A.T.
Deposited on	:	2011-02-11
Resolution	:	1.88 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

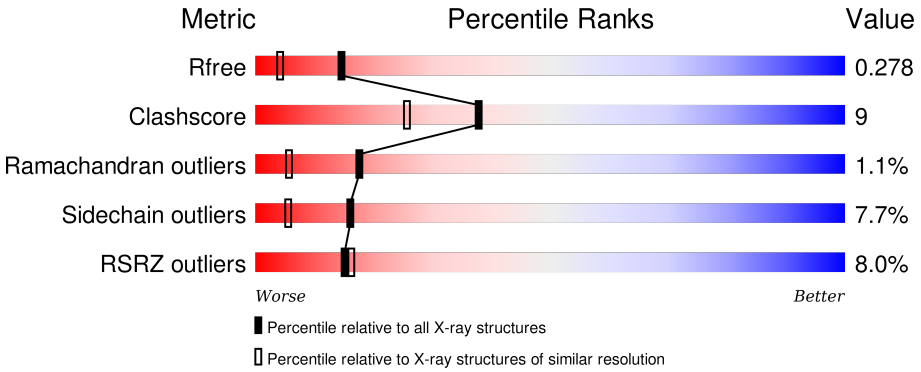
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 1.88 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}	91344	6965 (1.90-1.86)
Clashscore	102246	7778 (1.90-1.86)
Ramachandran outliers	100387	7691 (1.90-1.86)
Sidechain outliers	100360	7692 (1.90-1.86)
RSRZ outliers	91569	6979 (1.90-1.86)

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 <=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	525	6% 71% 15% • 10%
1	B	525	4% 70% 14% • • 12%
1	C	525	8% 74% 14% • 11%
1	D	525	10% 67% 17% • 13%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13673 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 Type I polyketide synthase PikAII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	470	Total	C	N	O	S	0	0	0
			3390	2118	620	647	5			
1	B	460	Total	C	N	O	S	0	0	0
			3317	2075	605	632	5			
1	C	465	Total	C	N	O	S	0	0	0
			3340	2088	609	638	5			
1	D	457	Total	C	N	O	S	0	0	0
			3283	2055	597	626	5			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	EXPRESSION TAG	UNP Q9ZGI4
A	-19	GLY	-	EXPRESSION TAG	UNP Q9ZGI4
A	-18	SER	-	EXPRESSION TAG	UNP Q9ZGI4
A	-17	SER	-	EXPRESSION TAG	UNP Q9ZGI4
A	-16	HIS	-	EXPRESSION TAG	UNP Q9ZGI4
A	-15	HIS	-	EXPRESSION TAG	UNP Q9ZGI4
A	-14	HIS	-	EXPRESSION TAG	UNP Q9ZGI4
A	-13	HIS	-	EXPRESSION TAG	UNP Q9ZGI4
A	-12	HIS	-	EXPRESSION TAG	UNP Q9ZGI4
A	-11	HIS	-	EXPRESSION TAG	UNP Q9ZGI4
A	-10	SER	-	EXPRESSION TAG	UNP Q9ZGI4
A	-9	SER	-	EXPRESSION TAG	UNP Q9ZGI4
A	-8	GLY	-	EXPRESSION TAG	UNP Q9ZGI4
A	-7	LEU	-	EXPRESSION TAG	UNP Q9ZGI4
A	-6	VAL	-	EXPRESSION TAG	UNP Q9ZGI4
A	-5	PRO	-	EXPRESSION TAG	UNP Q9ZGI4
A	-4	ARG	-	EXPRESSION TAG	UNP Q9ZGI4
A	-3	GLY	-	EXPRESSION TAG	UNP Q9ZGI4
A	-2	SER	-	EXPRESSION TAG	UNP Q9ZGI4
A	-1	HIS	-	EXPRESSION TAG	UNP Q9ZGI4
A	0	MET	-	EXPRESSION TAG	UNP Q9ZGI4

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-20	MET	-	EXPRESSION TAG	UNP Q9ZGI4
B	-19	GLY	-	EXPRESSION TAG	UNP Q9ZGI4
B	-18	SER	-	EXPRESSION TAG	UNP Q9ZGI4
B	-17	SER	-	EXPRESSION TAG	UNP Q9ZGI4
B	-16	HIS	-	EXPRESSION TAG	UNP Q9ZGI4
B	-15	HIS	-	EXPRESSION TAG	UNP Q9ZGI4
B	-14	HIS	-	EXPRESSION TAG	UNP Q9ZGI4
B	-13	HIS	-	EXPRESSION TAG	UNP Q9ZGI4
B	-12	HIS	-	EXPRESSION TAG	UNP Q9ZGI4
B	-11	HIS	-	EXPRESSION TAG	UNP Q9ZGI4
B	-10	SER	-	EXPRESSION TAG	UNP Q9ZGI4
B	-9	SER	-	EXPRESSION TAG	UNP Q9ZGI4
B	-8	GLY	-	EXPRESSION TAG	UNP Q9ZGI4
B	-7	LEU	-	EXPRESSION TAG	UNP Q9ZGI4
B	-6	VAL	-	EXPRESSION TAG	UNP Q9ZGI4
B	-5	PRO	-	EXPRESSION TAG	UNP Q9ZGI4
B	-4	ARG	-	EXPRESSION TAG	UNP Q9ZGI4
B	-3	GLY	-	EXPRESSION TAG	UNP Q9ZGI4
B	-2	SER	-	EXPRESSION TAG	UNP Q9ZGI4
B	-1	HIS	-	EXPRESSION TAG	UNP Q9ZGI4
B	0	MET	-	EXPRESSION TAG	UNP Q9ZGI4
C	-20	MET	-	EXPRESSION TAG	UNP Q9ZGI4
C	-19	GLY	-	EXPRESSION TAG	UNP Q9ZGI4
C	-18	SER	-	EXPRESSION TAG	UNP Q9ZGI4
C	-17	SER	-	EXPRESSION TAG	UNP Q9ZGI4
C	-16	HIS	-	EXPRESSION TAG	UNP Q9ZGI4
C	-15	HIS	-	EXPRESSION TAG	UNP Q9ZGI4
C	-14	HIS	-	EXPRESSION TAG	UNP Q9ZGI4
C	-13	HIS	-	EXPRESSION TAG	UNP Q9ZGI4
C	-12	HIS	-	EXPRESSION TAG	UNP Q9ZGI4
C	-11	HIS	-	EXPRESSION TAG	UNP Q9ZGI4
C	-10	SER	-	EXPRESSION TAG	UNP Q9ZGI4
C	-9	SER	-	EXPRESSION TAG	UNP Q9ZGI4
C	-8	GLY	-	EXPRESSION TAG	UNP Q9ZGI4
C	-7	LEU	-	EXPRESSION TAG	UNP Q9ZGI4
C	-6	VAL	-	EXPRESSION TAG	UNP Q9ZGI4
C	-5	PRO	-	EXPRESSION TAG	UNP Q9ZGI4
C	-4	ARG	-	EXPRESSION TAG	UNP Q9ZGI4
C	-3	GLY	-	EXPRESSION TAG	UNP Q9ZGI4
C	-2	SER	-	EXPRESSION TAG	UNP Q9ZGI4
C	-1	HIS	-	EXPRESSION TAG	UNP Q9ZGI4
C	0	MET	-	EXPRESSION TAG	UNP Q9ZGI4

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	-20	MET	-	EXPRESSION TAG	UNP Q9ZGI4
D	-19	GLY	-	EXPRESSION TAG	UNP Q9ZGI4
D	-18	SER	-	EXPRESSION TAG	UNP Q9ZGI4
D	-17	SER	-	EXPRESSION TAG	UNP Q9ZGI4
D	-16	HIS	-	EXPRESSION TAG	UNP Q9ZGI4
D	-15	HIS	-	EXPRESSION TAG	UNP Q9ZGI4
D	-14	HIS	-	EXPRESSION TAG	UNP Q9ZGI4
D	-13	HIS	-	EXPRESSION TAG	UNP Q9ZGI4
D	-12	HIS	-	EXPRESSION TAG	UNP Q9ZGI4
D	-11	HIS	-	EXPRESSION TAG	UNP Q9ZGI4
D	-10	SER	-	EXPRESSION TAG	UNP Q9ZGI4
D	-9	SER	-	EXPRESSION TAG	UNP Q9ZGI4
D	-8	GLY	-	EXPRESSION TAG	UNP Q9ZGI4
D	-7	LEU	-	EXPRESSION TAG	UNP Q9ZGI4
D	-6	VAL	-	EXPRESSION TAG	UNP Q9ZGI4
D	-5	PRO	-	EXPRESSION TAG	UNP Q9ZGI4
D	-4	ARG	-	EXPRESSION TAG	UNP Q9ZGI4
D	-3	GLY	-	EXPRESSION TAG	UNP Q9ZGI4
D	-2	SER	-	EXPRESSION TAG	UNP Q9ZGI4
D	-1	HIS	-	EXPRESSION TAG	UNP Q9ZGI4
D	0	MET	-	EXPRESSION TAG	UNP Q9ZGI4

- Molecule 2 is water.

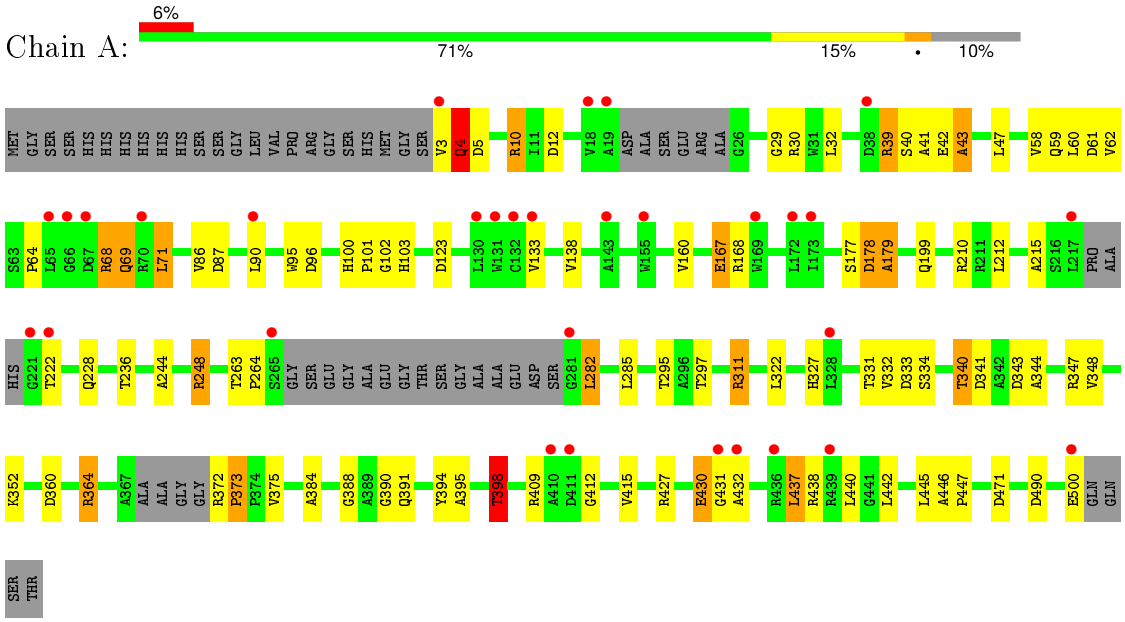
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	120	Total O 120 120	0	0
2	B	99	Total O 99 99	0	0
2	C	69	Total O 69 69	0	0
2	D	55	Total O 55 55	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

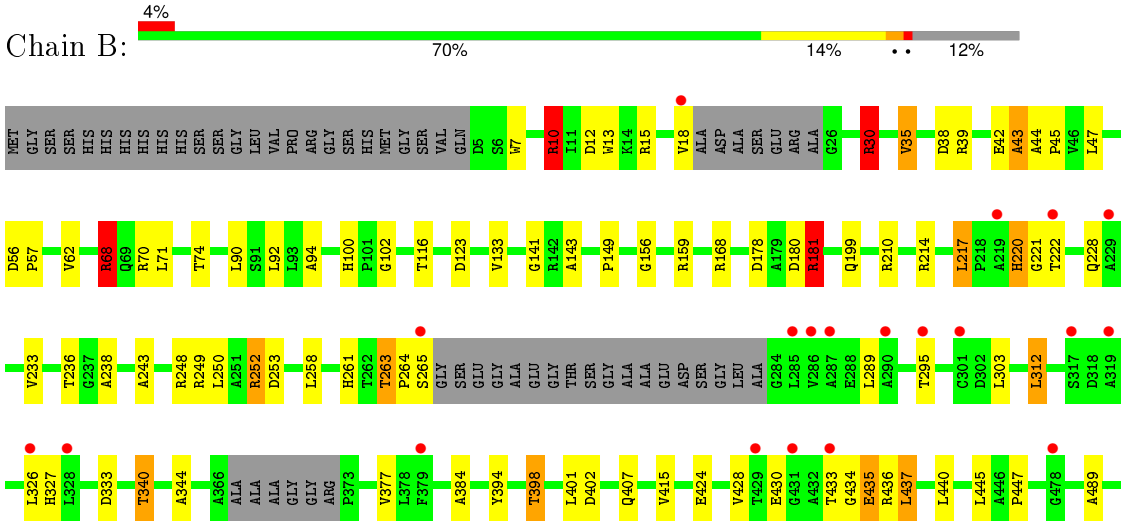
- Molecule 1: Type I polyketide synthase PikAII

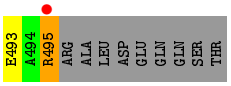
Chain A:



- Molecule 1: Type I polyketide synthase PikAII

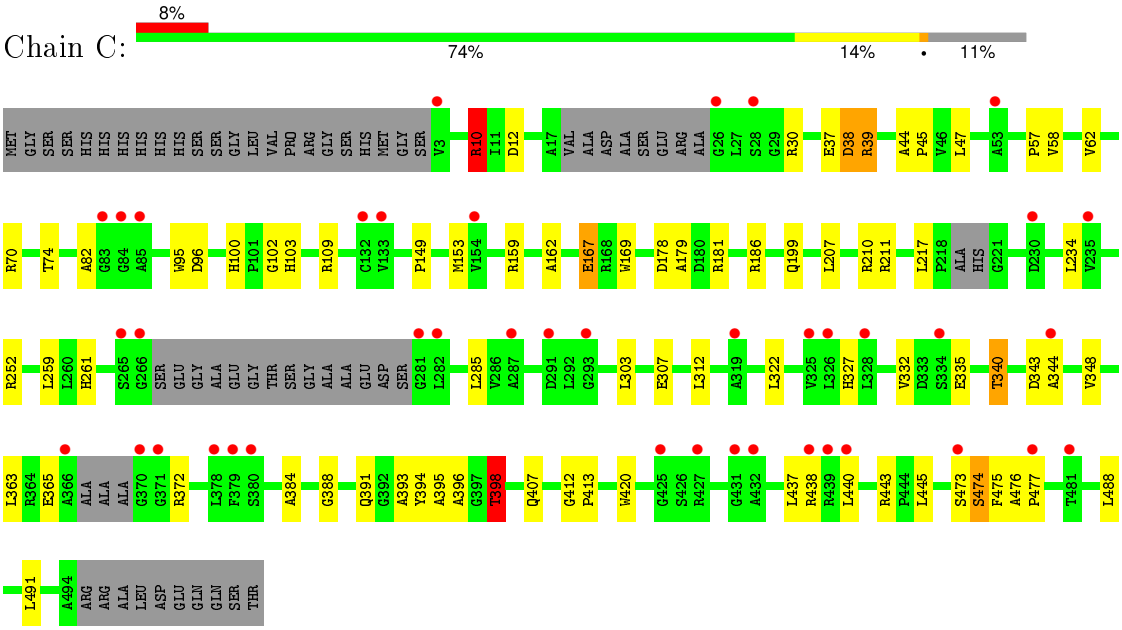
Chain B:





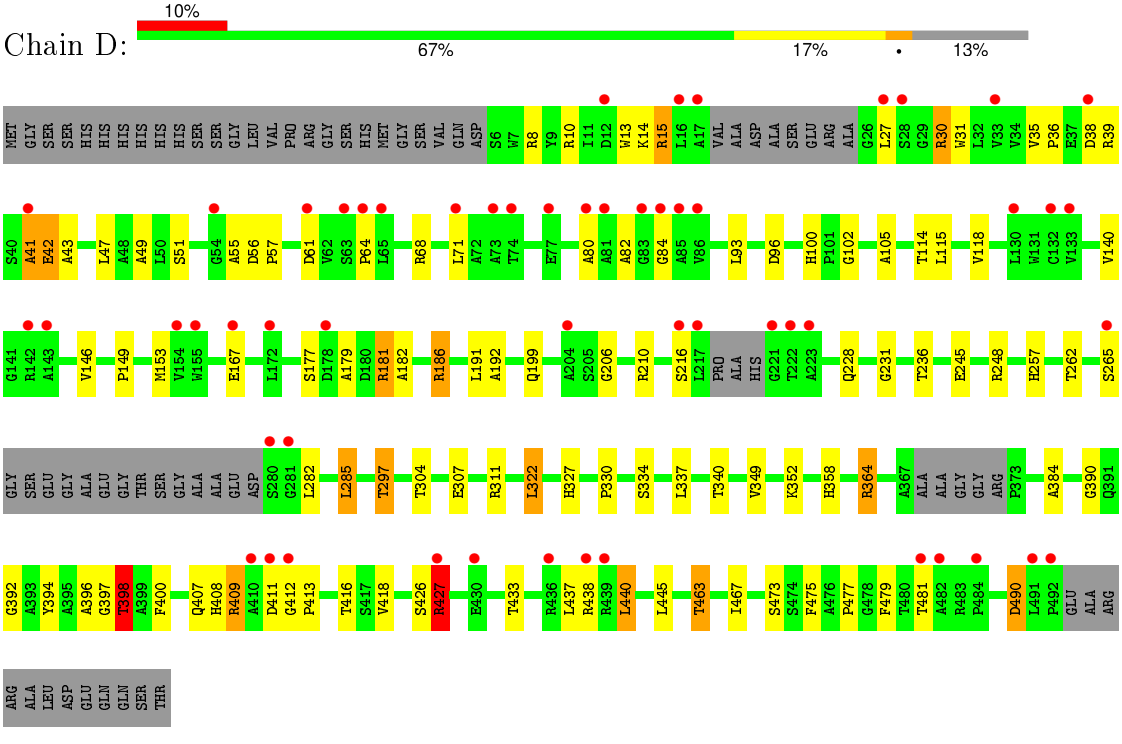
• Molecule 1: Type I polyketide synthase PikAII

Chain C:



• Molecule 1: Type I polyketide synthase PikAII

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	79.64Å 150.09Å 86.87Å 90.00° 105.12° 90.00°	Depositor
Resolution (Å)	31.23 – 1.88 31.23 – 1.88	Depositor EDS
% Data completeness (in resolution range)	91.0 (31.23-1.88) 91.0 (31.23-1.88)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.55 (at 1.88Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.227 , 0.276 0.228 , 0.278	Depositor DCC
R_{free} test set	7250 reflections (5.27%)	DCC
Wilson B-factor (Å^2)	32.7	Xtriage
Anisotropy	0.117	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 46.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 144759 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	13673	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.95% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	1.16	5/3457 (0.1%)	1.06	10/4737 (0.2%)
1	B	1.16	8/3387 (0.2%)	1.10	20/4645 (0.4%)
1	C	0.97	1/3408 (0.0%)	0.98	6/4671 (0.1%)
1	D	1.03	2/3350 (0.1%)	0.99	6/4592 (0.1%)
All	All	1.08	16/13602 (0.1%)	1.03	42/18645 (0.2%)

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	D	1	0

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	398	THR	CB-CG2	-9.73	1.20	1.52
1	B	415	VAL	CB-CG1	7.50	1.68	1.52
1	A	160	VAL	CB-CG1	7.04	1.67	1.52
1	A	138	VAL	CB-CG1	6.45	1.66	1.52
1	B	94	ALA	CA-CB	6.32	1.65	1.52
1	B	13	TRP	CE3-CZ3	6.02	1.48	1.38
1	A	167	GLU	CG-CD	5.99	1.60	1.51
1	C	420	TRP	CB-CG	-5.90	1.39	1.50
1	A	167	GLU	CB-CG	5.86	1.63	1.52
1	B	156	GLY	N-CA	5.75	1.54	1.46
1	B	143	ALA	CA-CB	5.65	1.64	1.52
1	A	415	VAL	CB-CG1	5.48	1.64	1.52
1	B	30	ARG	CG-CD	5.42	1.65	1.51
1	D	105	ALA	CA-CB	5.32	1.63	1.52
1	B	141	GLY	N-CA	5.18	1.53	1.46
1	B	35	VAL	CB-CG1	5.13	1.63	1.52

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	10	ARG	NE-CZ-NH1	-10.38	115.11	120.30
1	B	10	ARG	NE-CZ-NH2	10.22	125.41	120.30
1	C	10	ARG	NE-CZ-NH1	-9.62	115.49	120.30
1	B	68	ARG	NE-CZ-NH1	9.11	124.86	120.30
1	B	68	ARG	NE-CZ-NH2	-8.20	116.20	120.30
1	A	248	ARG	NE-CZ-NH1	-7.49	116.56	120.30
1	B	181	ARG	NE-CZ-NH2	-7.33	116.64	120.30
1	D	408	HIS	CB-CA-C	7.28	124.96	110.40
1	B	39	ARG	NE-CZ-NH1	-7.18	116.71	120.30
1	A	398	THR	CA-CB-CG2	7.16	122.42	112.40
1	D	322	LEU	CA-CB-CG	7.11	131.65	115.30
1	D	285	LEU	CB-CG-CD2	7.08	123.04	111.00
1	C	10	ARG	NE-CZ-NH2	7.05	123.83	120.30
1	A	490	ASP	CB-CG-OD1	7.02	124.62	118.30
1	C	96	ASP	CB-CG-OD1	6.91	124.52	118.30
1	B	15	ARG	NE-CZ-NH2	-6.90	116.85	120.30
1	A	471	ASP	CB-CG-OD1	6.65	124.28	118.30
1	C	211	ARG	NE-CZ-NH2	6.54	123.57	120.30
1	A	10	ARG	NE-CZ-NH2	6.33	123.47	120.30
1	A	347	ARG	NE-CZ-NH2	6.23	123.41	120.30
1	A	282	LEU	CA-CB-CG	6.16	129.47	115.30
1	D	398	THR	N-CA-CB	-6.07	98.77	110.30
1	B	180	ASP	CB-CG-OD1	5.99	123.69	118.30
1	B	30	ARG	NE-CZ-NH1	-5.96	117.32	120.30
1	B	168	ARG	NE-CZ-NH1	-5.64	117.48	120.30
1	C	398	THR	CA-CB-CG2	5.63	120.28	112.40
1	D	407	GLN	C-N-CA	-5.48	108.00	121.70
1	B	30	ARG	NE-CZ-NH2	5.44	123.02	120.30
1	B	181	ARG	CG-CD-NE	5.40	123.14	111.80
1	B	437	LEU	CA-CB-CG	5.38	127.68	115.30
1	D	10	ARG	NE-CZ-NH1	-5.35	117.62	120.30
1	B	181	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	B	253	ASP	CB-CG-OD2	-5.31	113.52	118.30
1	A	311	ARG	NE-CZ-NH2	5.31	122.96	120.30
1	C	109	ARG	NE-CZ-NH1	-5.31	117.64	120.30
1	B	217	LEU	CA-CB-CG	5.27	127.42	115.30
1	B	253	ASP	CB-CG-OD1	5.13	122.92	118.30
1	A	212	LEU	CB-CG-CD1	-5.12	102.30	111.00
1	B	15	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	B	402	ASP	CB-CG-OD2	5.07	122.86	118.30
1	B	401	LEU	CB-CG-CD1	-5.05	102.41	111.00
1	A	347	ARG	NE-CZ-NH1	-5.01	117.80	120.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	D	408	HIS	CA

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	3390	0	3364	63	0
1	B	3317	0	3287	61	0
1	C	3340	0	3309	54	0
1	D	3283	0	3259	72	0
2	A	120	0	0	1	0
2	B	99	0	0	1	0
2	C	69	0	0	1	0
2	D	55	0	0	5	0
All	All	13673	0	13219	243	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 9.

All (243) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:384:ALA:HB2	1:C:398:THR:HG23	1.16	1.16
1:A:384:ALA:HB2	1:A:398:THR:HG23	1.34	1.08
1:B:384:ALA:HB2	1:B:398:THR:HG23	1.34	1.07
1:A:29:GLY:HA3	1:A:87:ASP:OD2	1.55	1.06
1:D:384:ALA:HB2	1:D:398:THR:CG2	1.90	1.02
1:B:434:GLY:HA2	1:B:436:ARG:N	1.74	1.02
1:D:186:ARG:HG3	1:D:186:ARG:HH11	1.24	1.01
1:A:334:SER:HB2	1:A:390:GLY:O	1.60	0.98
1:C:384:ALA:HB2	1:C:398:THR:CG2	1.93	0.98
1:B:384:ALA:HB2	1:B:398:THR:CG2	1.93	0.97
1:A:384:ALA:HB2	1:A:398:THR:CG2	1.96	0.95

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:42:GLU:O	1:B:43:ALA:HB3	1.64	0.93
1:B:42:GLU:O	1:B:43:ALA:CB	2.12	0.92
1:D:384:ALA:HB2	1:D:398:THR:HG22	1.52	0.90
1:D:49:ALA:HA	1:D:181:ARG:NH2	1.86	0.89
1:C:384:ALA:CB	1:C:398:THR:HG23	2.01	0.88
1:D:199:GLN:NE2	1:D:210:ARG:HD3	1.90	0.86
1:D:49:ALA:HA	1:D:181:ARG:HH21	1.40	0.86
1:B:384:ALA:CB	1:B:398:THR:HG23	2.05	0.86
1:D:228:GLN:HG3	2:D:525:HOH:O	1.77	0.84
1:B:434:GLY:CA	1:B:437:LEU:H	1.92	0.82
1:B:149:PRO:HG3	1:B:407:GLN:NE2	1.94	0.82
1:A:384:ALA:CB	1:A:398:THR:HG23	2.10	0.81
1:D:384:ALA:HB2	1:D:398:THR:HG23	1.62	0.81
1:D:334:SER:HB2	1:D:390:GLY:O	1.81	0.80
1:D:427:ARG:HH11	1:D:427:ARG:HG2	1.48	0.79
1:D:186:ARG:CG	1:D:186:ARG:HH11	1.97	0.78
1:B:68:ARG:HD2	1:B:123:ASP:OD1	1.82	0.78
1:D:36:PRO:HD3	1:D:93:LEU:HD23	1.66	0.76
1:C:100:HIS:HD2	1:C:102:GLY:H	1.30	0.76
1:C:303:LEU:HD21	1:C:312:LEU:HD22	1.68	0.76
1:B:434:GLY:CA	1:B:436:ARG:N	2.50	0.74
1:C:149:PRO:HG3	1:C:407:GLN:NE2	2.01	0.74
1:A:103:HIS:HE1	1:A:343:ASP:OD2	1.69	0.74
1:B:434:GLY:HA2	1:B:435:GLU:C	2.07	0.73
1:A:42:GLU:O	1:A:43:ALA:CB	2.37	0.72
1:D:426:SER:O	1:D:427:ARG:HB3	1.90	0.71
1:B:70:ARG:NH2	1:C:38:ASP:HB3	2.07	0.69
1:D:153:MET:HE1	1:D:397:GLY:HA2	1.75	0.69
1:A:68:ARG:HD2	1:A:123:ASP:OD1	1.92	0.69
1:A:10:ARG:HG2	1:A:215:ALA:HB2	1.74	0.69
1:D:245:GLU:OE2	1:D:248:ARG:NH2	2.27	0.68
1:C:100:HIS:CD2	1:C:102:GLY:H	2.10	0.68
1:B:489:ALA:O	1:B:495:ARG:NH1	2.27	0.68
1:D:262:THR:HG21	1:D:282:LEU:HD11	1.77	0.66
1:A:236:THR:OG1	1:A:327:HIS:HD2	1.79	0.65
1:D:199:GLN:HE21	1:D:210:ARG:HD3	1.61	0.65
1:B:434:GLY:HA3	1:B:437:LEU:H	1.62	0.65
1:D:153:MET:CE	1:D:397:GLY:HA2	2.27	0.65
1:C:340:THR:HG22	1:C:344:ALA:HB3	1.78	0.65
1:C:186:ARG:HB3	1:C:207:LEU:HD21	1.78	0.63
1:D:100:HIS:HD2	1:D:102:GLY:H	1.44	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:236:THR:OG1	1:B:327:HIS:HD2	1.81	0.63
1:B:434:GLY:HA2	1:B:437:LEU:N	2.14	0.62
1:C:30:ARG:HH11	1:C:82:ALA:HA	1.65	0.62
1:C:476:ALA:HB3	1:C:477:PRO:HD3	1.81	0.62
1:D:297:THR:HB	2:D:508:HOH:O	1.98	0.62
1:D:327:HIS:HE1	2:D:507:HOH:O	1.81	0.61
1:C:234:LEU:HD13	1:C:259:LEU:HD23	1.83	0.61
1:C:303:LEU:HD21	1:C:312:LEU:CD2	2.31	0.61
1:B:70:ARG:HH12	1:C:38:ASP:HA	1.66	0.61
1:A:340:THR:HG22	1:A:344:ALA:HB3	1.83	0.60
1:D:433:THR:O	1:D:437:LEU:HD13	2.01	0.60
1:C:149:PRO:HG3	1:C:407:GLN:HE21	1.67	0.60
1:B:100:HIS:HD2	1:B:102:GLY:H	1.49	0.60
1:D:409:ARG:HD3	1:D:413:PRO:O	2.01	0.60
1:D:394:TYR:O	1:D:398:THR:HB	2.02	0.60
1:A:30:ARG:HD3	1:A:58:VAL:HG23	1.84	0.59
1:D:153:MET:CE	1:D:400:PHE:HB2	2.32	0.59
1:B:434:GLY:CA	1:B:437:LEU:N	2.65	0.59
1:D:153:MET:HE2	1:D:400:PHE:HB2	1.83	0.59
1:A:90:LEU:HD11	1:A:133:VAL:CG2	2.33	0.59
1:C:394:TYR:O	1:C:398:THR:HB	2.03	0.58
1:C:335:GLU:OE2	1:C:340:THR:HG23	2.03	0.58
1:A:199:GLN:HE21	1:A:210:ARG:HD3	1.66	0.58
1:B:261:HIS:HE1	1:B:263:THR:HG23	1.68	0.58
1:A:340:THR:HG22	1:A:341:ASP:H	1.67	0.58
1:A:69:GLN:HE21	1:A:69:GLN:HA	1.68	0.58
1:A:69:GLN:NE2	1:A:69:GLN:HA	2.18	0.58
1:A:3:VAL:HG12	1:A:4:GLN:N	2.17	0.58
1:B:149:PRO:HG3	1:B:407:GLN:HE21	1.65	0.58
1:C:327:HIS:HE1	2:C:509:HOH:O	1.86	0.58
1:A:39:ARG:NH2	1:A:95:TRP:O	2.37	0.58
1:D:47:LEU:HD22	1:D:57:PRO:HB2	1.85	0.57
1:A:427:ARG:O	1:A:430:GLU:HB3	2.04	0.57
1:D:186:ARG:HG3	1:D:186:ARG:NH1	2.03	0.57
1:D:30:ARG:NH1	1:D:56:ASP:OD2	2.37	0.57
1:B:434:GLY:HA2	1:B:437:LEU:H	1.66	0.57
1:B:220:HIS:CD2	1:B:221:GLY:H	2.23	0.57
1:B:70:ARG:CZ	1:C:38:ASP:HB3	2.35	0.56
1:D:199:GLN:HE22	1:D:210:ARG:HH21	1.53	0.56
1:C:159:ARG:HD3	1:C:199:GLN:HE22	1.71	0.56
1:D:30:ARG:HD3	1:D:56:ASP:O	2.05	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:340:THR:HG22	1:B:344:ALA:HB3	1.87	0.56
1:D:384:ALA:CB	1:D:398:THR:HG23	2.35	0.56
1:C:30:ARG:HH21	1:C:58:VAL:HG21	1.71	0.56
1:A:59:GLN:NE2	1:A:61:ASP:OD1	2.38	0.56
1:A:42:GLU:O	1:A:43:ALA:HB3	2.07	0.55
1:D:15:ARG:HH21	1:D:206:GLY:HA3	1.71	0.55
1:A:100:HIS:CD2	1:A:102:GLY:H	2.24	0.55
1:D:42:GLU:O	1:D:43:ALA:HB3	2.06	0.55
1:B:220:HIS:CG	1:B:221:GLY:H	2.25	0.55
1:A:10:ARG:NH2	1:A:12:ASP:OD1	2.40	0.54
1:A:332:VAL:HG21	1:A:348:VAL:HG13	1.88	0.54
1:C:363:LEU:HB2	1:C:413:PRO:HG3	1.88	0.54
1:D:364:ARG:HG2	1:D:412:GLY:O	2.07	0.54
1:B:7:TRP:CZ3	1:B:445:LEU:HG	2.42	0.54
1:A:430:GLU:HG3	1:A:432:ALA:H	1.73	0.54
1:A:100:HIS:HD2	1:A:102:GLY:H	1.54	0.54
1:B:181:ARG:HH11	1:B:181:ARG:HG3	1.72	0.54
1:D:236:THR:OG1	1:D:327:HIS:HD2	1.91	0.53
1:B:44:ALA:N	1:B:45:PRO:CD	2.72	0.53
1:D:228:GLN:CG	2:D:525:HOH:O	2.48	0.53
1:D:427:ARG:CG	1:D:427:ARG:HH11	2.21	0.53
1:C:162:ALA:HB2	1:C:169:TRP:CD1	2.45	0.52
1:B:303:LEU:HD21	1:B:312:LEU:HD22	1.90	0.52
1:B:70:ARG:HH22	1:C:38:ASP:HB3	1.72	0.52
1:B:199:GLN:HE21	1:B:210:ARG:HD3	1.75	0.52
1:B:384:ALA:HB2	1:B:398:THR:HG22	1.83	0.52
1:D:186:ARG:CG	1:D:186:ARG:NH1	2.66	0.52
1:B:434:GLY:H	1:B:436:ARG:H	1.57	0.52
1:D:440:LEU:O	1:D:475:PHE:HA	2.10	0.52
1:C:153:MET:HG2	1:C:396:ALA:O	2.10	0.52
1:B:100:HIS:CD2	1:B:102:GLY:H	2.27	0.51
1:C:10:ARG:HD2	1:C:12:ASP:OD2	2.10	0.51
1:A:62:VAL:HG21	1:A:71:LEU:HG	1.93	0.51
1:B:38:ASP:HB2	1:C:70:ARG:NH2	2.24	0.51
1:A:90:LEU:HD11	1:A:133:VAL:HG23	1.93	0.51
1:A:228:GLN:OE1	1:A:372:ARG:HD3	2.11	0.51
1:C:100:HIS:HD2	1:C:102:GLY:N	2.06	0.50
1:A:167:GLU:OE2	1:A:168:ARG:HG2	2.10	0.50
1:B:70:ARG:O	1:B:74:THR:HG23	2.12	0.50
1:A:384:ALA:HB2	1:A:398:THR:HG22	1.88	0.50
1:D:64:PRO:HG2	1:D:96:ASP:OD2	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:431:GLY:HA2	1:A:438:ARG:HH12	1.77	0.50
1:B:70:ARG:NH1	1:C:38:ASP:HA	2.26	0.49
1:D:199:GLN:HE22	1:D:210:ARG:NH2	2.10	0.49
1:D:182:ALA:O	1:D:186:ARG:HG2	2.12	0.49
1:C:199:GLN:NE2	1:C:210:ARG:HD3	2.27	0.49
1:D:146:VAL:HG12	1:D:149:PRO:HD3	1.93	0.49
1:D:13:TRP:CD1	1:D:140:VAL:HA	2.47	0.49
1:A:437:LEU:HD13	1:A:442:LEU:HD12	1.94	0.49
1:C:30:ARG:NH2	1:C:58:VAL:HG21	2.28	0.49
1:A:431:GLY:HA2	1:A:438:ARG:NH1	2.28	0.48
1:A:30:ARG:HD2	1:A:58:VAL:HG21	1.93	0.48
1:B:90:LEU:HD11	1:B:133:VAL:CG2	2.43	0.48
1:C:412:GLY:HA2	1:C:413:PRO:C	2.33	0.48
1:C:395:ALA:HA	1:C:398:THR:HG22	1.95	0.48
1:A:236:THR:OG1	1:A:327:HIS:CD2	2.62	0.48
1:A:327:HIS:HE1	2:A:522:HOH:O	1.97	0.48
1:D:307:GLU:HG2	1:D:311:ARG:HH22	1.77	0.48
1:C:37:GLU:HG3	1:C:62:VAL:O	2.14	0.48
1:B:159:ARG:HD3	1:B:199:GLN:HE22	1.79	0.48
1:B:327:HIS:HE1	2:B:526:HOH:O	1.96	0.48
1:A:395:ALA:HA	1:A:398:THR:HG22	1.96	0.48
1:A:394:TYR:O	1:A:398:THR:HB	2.14	0.47
1:A:178:ASP:O	1:A:179:ALA:HB3	2.15	0.47
1:C:199:GLN:HE22	1:C:210:ARG:NH2	2.13	0.47
1:C:39:ARG:HH11	1:C:39:ARG:HG3	1.79	0.47
1:C:44:ALA:HB3	1:C:45:PRO:HD3	1.97	0.47
1:B:249:ARG:HD3	1:B:252:ARG:HD2	1.97	0.46
1:B:70:ARG:NH1	1:C:38:ASP:HB3	2.31	0.46
1:A:90:LEU:HD11	1:A:133:VAL:HG21	1.96	0.46
1:D:153:MET:HE1	1:D:349:VAL:HG13	1.97	0.46
1:D:418:VAL:CG1	1:D:467:ILE:HD12	2.46	0.46
1:B:199:GLN:NE2	1:B:210:ARG:HD3	2.30	0.45
1:D:8:ARG:HG2	2:D:526:HOH:O	2.16	0.45
1:D:337:LEU:HD21	1:D:392:GLY:HA3	1.98	0.45
1:B:434:GLY:N	1:B:436:ARG:H	2.14	0.45
1:C:488:LEU:HD12	1:C:488:LEU:N	2.31	0.45
1:A:199:GLN:NE2	1:A:210:ARG:HD3	2.31	0.45
1:C:167:GLU:CD	1:C:167:GLU:H	2.20	0.45
1:B:326:LEU:HD23	1:B:377:VAL:HB	1.99	0.45
1:A:360:ASP:O	1:A:364:ARG:HB2	2.17	0.45
1:C:437:LEU:HA	1:C:440:LEU:HG	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:307:GLU:HG2	1:D:311:ARG:NH2	2.32	0.45
1:A:3:VAL:HG12	1:A:4:GLN:H	1.82	0.45
1:D:27:LEU:HD12	1:D:192:ALA:HA	1.99	0.45
1:A:42:GLU:O	1:A:43:ALA:HB2	2.15	0.44
1:A:352:LYS:HE2	1:A:394:TYR:HE1	1.82	0.44
1:B:47:LEU:CD1	1:B:57:PRO:HB2	2.47	0.44
1:D:153:MET:HG2	1:D:396:ALA:O	2.18	0.44
1:B:424:GLU:HB2	1:B:447:PRO:HD3	2.00	0.44
1:C:47:LEU:HD22	1:C:57:PRO:HB2	1.99	0.44
1:B:394:TYR:O	1:B:398:THR:HB	2.18	0.44
1:B:10:ARG:HD2	1:B:12:ASP:OD2	2.17	0.44
1:B:47:LEU:HD13	1:B:57:PRO:HB2	1.99	0.43
1:C:443:ARG:HD3	1:C:443:ARG:N	2.33	0.43
1:D:35:VAL:HG12	1:D:36:PRO:O	2.19	0.43
1:D:304:THR:O	1:D:358:HIS:HE1	2.01	0.43
1:D:115:LEU:HD21	1:D:340:THR:HG23	2.00	0.43
1:D:149:PRO:HB2	1:D:400:PHE:CE1	2.53	0.43
1:B:42:GLU:HG3	1:B:42:GLU:H	1.63	0.43
1:B:30:ARG:NH1	1:B:56:ASP:OD2	2.51	0.43
1:C:440:LEU:O	1:C:475:PHE:HA	2.19	0.43
1:B:258:LEU:HD12	1:B:289:LEU:HD13	2.00	0.43
1:A:199:GLN:HE22	1:A:210:ARG:NH2	2.16	0.43
1:C:95:TRP:N	1:C:95:TRP:CD1	2.87	0.43
1:C:473:SER:O	1:C:474:SER:HB3	2.18	0.43
1:B:428:VAL:O	1:B:433:THR:O	2.36	0.43
1:C:332:VAL:HG21	1:C:348:VAL:HG13	2.01	0.43
1:D:39:ARG:NH1	1:D:42:GLU:OE2	2.52	0.42
1:D:418:VAL:HG11	1:D:467:ILE:HD12	2.01	0.42
1:D:334:SER:CB	1:D:390:GLY:O	2.60	0.42
1:A:388:GLY:HA3	1:A:391:GLN:NE2	2.34	0.42
1:D:114:THR:O	1:D:118:VAL:HG23	2.19	0.42
1:D:55:ALA:O	1:D:57:PRO:HD3	2.19	0.42
1:A:446:ALA:HA	1:A:447:PRO:HD3	1.87	0.42
1:A:68:ARG:HH11	1:A:123:ASP:CG	2.23	0.42
1:C:159:ARG:HD3	1:C:199:GLN:NE2	2.33	0.42
1:C:332:VAL:HG11	1:C:348:VAL:HG13	2.02	0.42
1:D:416:THR:HA	1:D:463:THR:O	2.20	0.42
1:C:348:VAL:HB	1:C:393:ALA:HB1	2.01	0.42
1:A:64:PRO:HG2	1:A:96:ASP:OD2	2.20	0.42
1:D:477:PRO:C	1:D:479:PHE:H	2.23	0.42
1:D:186:ARG:CZ	1:D:206:GLY:HA2	2.50	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:LEU:HD13	1:A:60:LEU:HD11	2.03	0.41
1:D:153:MET:CE	1:D:349:VAL:HG13	2.51	0.41
1:A:263:THR:HA	1:A:264:PRO:HD3	1.92	0.41
1:D:231:GLY:O	1:D:257:HIS:HB2	2.20	0.41
1:A:199:GLN:HE22	1:A:210:ARG:HH21	1.69	0.41
1:D:31:TRP:CZ3	1:D:191:LEU:HD22	2.55	0.41
1:B:68:ARG:HB2	1:B:116:THR:HG23	2.03	0.41
1:A:373:PRO:HB3	1:A:412:GLY:HA3	2.02	0.41
1:D:282:LEU:N	1:D:282:LEU:HD12	2.35	0.41
1:A:372:ARG:HH11	1:A:372:ARG:HG2	1.85	0.41
1:B:35:VAL:HG22	1:B:92:LEU:HD12	2.03	0.41
1:C:103:HIS:HE1	1:C:343:ASP:OD2	2.04	0.41
1:A:30:ARG:CD	1:A:58:VAL:HG23	2.49	0.41
1:A:90:LEU:HD12	1:A:90:LEU:HA	1.92	0.41
1:D:41:ALA:HB3	1:D:42:GLU:OE1	2.21	0.41
1:A:360:ASP:OD2	1:A:409:ARG:NE	2.51	0.41
1:C:388:GLY:HA3	1:C:391:GLN:HE21	1.86	0.41
1:C:388:GLY:CA	1:C:391:GLN:HE21	2.34	0.41
1:A:244:ALA:O	1:A:248:ARG:HG3	2.21	0.41
1:A:30:ARG:HG2	1:A:86:VAL:HG22	2.03	0.41
1:B:258:LEU:CD1	1:B:289:LEU:HD13	2.51	0.41
1:B:238:ALA:HA	1:B:243:ALA:CB	2.51	0.41
1:D:80:ALA:C	1:D:82:ALA:H	2.24	0.41
1:B:238:ALA:HA	1:B:243:ALA:HB3	2.03	0.40
1:D:330:PRO:O	1:D:352:LYS:HE2	2.21	0.40
1:B:233:VAL:HG11	1:B:250:LEU:HD13	2.03	0.40
1:A:100:HIS:HA	1:A:101:PRO:HD3	1.91	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	460/525 (88%)	441 (96%)	13 (3%)	6 (1%)	15 4
1	B	452/525 (86%)	433 (96%)	14 (3%)	5 (1%)	17 6
1	C	455/525 (87%)	441 (97%)	12 (3%)	2 (0%)	39 25
1	D	447/525 (85%)	420 (94%)	20 (4%)	7 (2%)	12 3
All	All	1814/2100 (86%)	1735 (96%)	59 (3%)	20 (1%)	17 6

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	430	GLU
1	B	220	HIS
1	B	435	GLU
1	C	179	ALA
1	C	474	SER
1	D	84	GLY
1	D	490	ASP
1	A	41	ALA
1	A	43	ALA
1	B	43	ALA
1	D	42	GLU
1	D	179	ALA
1	D	427	ARG
1	B	222	THR
1	D	41	ALA
1	D	481	THR
1	A	177	SER
1	B	264	PRO
1	A	179	ALA

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	328/365 (90%)	301 (92%)	27 (8%)	14 5

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	322/365 (88%)	298 (92%)	24 (8%)	17 6
1	C	323/365 (88%)	303 (94%)	20 (6%)	23 9
1	D	318/365 (87%)	290 (91%)	28 (9%)	12 4
All	All	1291/1460 (88%)	1192 (92%)	99 (8%)	16 5

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	5	ASP
1	A	39	ARG
1	A	40	SER
1	A	47	LEU
1	A	68	ARG
1	A	69	GLN
1	A	71	LEU
1	A	178	ASP
1	A	222	THR
1	A	282	LEU
1	A	285	LEU
1	A	295	THR
1	A	297	THR
1	A	311	ARG
1	A	322	LEU
1	A	331	THR
1	A	333	ASP
1	A	340	THR
1	A	364	ARG
1	A	373	PRO
1	A	375	VAL
1	A	398	THR
1	A	437	LEU
1	A	440	LEU
1	A	445	LEU
1	A	500	GLU
1	B	10	ARG
1	B	18	VAL
1	B	30	ARG
1	B	62	VAL
1	B	68	ARG
1	B	71	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	178	ASP
1	B	181	ARG
1	B	214	ARG
1	B	217	LEU
1	B	228	GLN
1	B	248	ARG
1	B	252	ARG
1	B	263	THR
1	B	265	SER
1	B	295	THR
1	B	312	LEU
1	B	333	ASP
1	B	340	THR
1	B	398	THR
1	B	430	GLU
1	B	440	LEU
1	B	493	GLU
1	B	495	ARG
1	C	10	ARG
1	C	38	ASP
1	C	39	ARG
1	C	74	THR
1	C	167	GLU
1	C	178	ASP
1	C	181	ARG
1	C	217	LEU
1	C	252	ARG
1	C	261	HIS
1	C	285	LEU
1	C	307	GLU
1	C	322	LEU
1	C	340	THR
1	C	365	GLU
1	C	372	ARG
1	C	398	THR
1	C	438	ARG
1	C	445	LEU
1	C	491	LEU
1	D	14	LYS
1	D	15	ARG
1	D	30	ARG
1	D	38	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	51	SER
1	D	61	ASP
1	D	68	ARG
1	D	71	LEU
1	D	167	GLU
1	D	177	SER
1	D	181	ARG
1	D	186	ARG
1	D	216	SER
1	D	265	SER
1	D	285	LEU
1	D	297	THR
1	D	322	LEU
1	D	364	ARG
1	D	398	THR
1	D	409	ARG
1	D	411	ASP
1	D	427	ARG
1	D	438	ARG
1	D	440	LEU
1	D	445	LEU
1	D	463	THR
1	D	473	SER
1	D	490	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	69	GLN
1	A	100	HIS
1	A	103	HIS
1	A	199	GLN
1	A	228	GLN
1	A	257	HIS
1	A	327	HIS
1	A	358	HIS
1	A	391	GLN
1	B	100	HIS
1	B	103	HIS
1	B	199	GLN
1	B	327	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	358	HIS
1	B	391	GLN
1	B	407	GLN
1	C	100	HIS
1	C	103	HIS
1	C	199	GLN
1	C	257	HIS
1	C	327	HIS
1	C	391	GLN
1	C	407	GLN
1	D	100	HIS
1	D	103	HIS
1	D	199	GLN
1	D	228	GLN
1	D	327	HIS
1	D	358	HIS

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

There are no ligands in this entry.

5.7 Other polymers

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	470/525 (89%)	0.19	31 (6%) 22 23	21, 36, 59, 75	0
1	B	460/525 (87%)	0.15	21 (4%) 36 38	19, 37, 63, 72	0
1	C	465/525 (88%)	0.46	41 (8%) 12 13	24, 47, 68, 80	0
1	D	457/525 (87%)	0.58	55 (12%) 6 6	22, 48, 80, 88	0
All	All	1852/2100 (88%)	0.34	148 (7%) 15 16	19, 40, 70, 88	0

All (148) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	266	GLY	8.1
1	D	221	GLY	7.3
1	D	85	ALA	6.9
1	D	410	ALA	5.8
1	C	432	ALA	5.4
1	C	265	SER	5.4
1	A	221	GLY	5.4
1	D	482	ALA	5.3
1	D	41	ALA	5.1
1	A	19	ALA	4.8
1	D	217	LEU	4.7
1	D	491	LEU	4.7
1	C	281	GLY	4.7
1	B	265	SER	4.6
1	D	83	GLY	4.4
1	A	222	THR	4.2
1	C	370	GLY	4.1
1	D	80	ALA	4.0
1	D	74	THR	4.0
1	D	65	LEU	3.9
1	A	18	VAL	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	3	VAL	3.8
1	C	334	SER	3.6
1	D	132	CYS	3.6
1	C	282	LEU	3.6
1	D	216	SER	3.6
1	D	265	SER	3.6
1	D	64	PRO	3.5
1	D	222	THR	3.5
1	B	18	VAL	3.5
1	A	132	CYS	3.5
1	A	66	GLY	3.4
1	D	280	SER	3.4
1	A	65	LEU	3.4
1	A	431	GLY	3.4
1	C	431	GLY	3.4
1	C	473	SER	3.4
1	A	90	LEU	3.4
1	C	326	LEU	3.4
1	D	411	ASP	3.4
1	D	436	ARG	3.3
1	C	371	GLY	3.2
1	A	133	VAL	3.2
1	D	154	VAL	3.1
1	D	16	LEU	3.1
1	D	133	VAL	3.1
1	B	286	VAL	3.1
1	D	172	LEU	3.0
1	C	427	ARG	3.0
1	B	379	PHE	3.0
1	A	265	SER	3.0
1	C	83	GLY	3.0
1	D	81	ALA	3.0
1	A	172	LEU	2.9
1	D	28	SER	2.9
1	B	222	THR	2.9
1	B	295	THR	2.9
1	B	317	SER	2.9
1	C	85	ALA	2.9
1	D	143	ALA	2.8
1	D	155	TRP	2.8
1	A	143	ALA	2.8
1	C	287	ALA	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	366	ALA	2.8
1	D	38	ASP	2.7
1	C	481	THR	2.7
1	C	438	ARG	2.7
1	A	3	VAL	2.7
1	C	84	GLY	2.7
1	B	326	LEU	2.7
1	A	173	ILE	2.6
1	B	429	THR	2.6
1	D	61	ASP	2.6
1	A	410	ALA	2.6
1	C	378	LEU	2.6
1	C	439	ARG	2.6
1	C	132	CYS	2.6
1	D	481	THR	2.6
1	A	130	LEU	2.6
1	D	63	SER	2.6
1	A	131	TRP	2.6
1	B	319	ALA	2.6
1	B	478	GLY	2.6
1	C	133	VAL	2.6
1	C	328	LEU	2.5
1	D	17	ALA	2.5
1	A	70	ARG	2.5
1	C	319	ALA	2.5
1	D	223	ALA	2.5
1	D	86	VAL	2.5
1	D	427	ARG	2.5
1	C	440	LEU	2.5
1	D	27	LEU	2.5
1	C	379	PHE	2.5
1	D	178	ASP	2.5
1	A	281	GLY	2.5
1	D	84	GLY	2.5
1	D	430	GLU	2.4
1	A	155	TRP	2.4
1	C	293	GLY	2.4
1	D	77	GLU	2.4
1	D	484	PRO	2.4
1	B	290	ALA	2.4
1	D	167	GLU	2.4
1	B	495	ARG	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	71	LEU	2.4
1	D	439	ARG	2.4
1	D	142	ARG	2.4
1	D	438	ARG	2.3
1	C	380	SER	2.3
1	C	235	VAL	2.3
1	A	411	ASP	2.3
1	C	230	ASP	2.3
1	A	169	TRP	2.3
1	B	287	ALA	2.3
1	D	73	ALA	2.3
1	B	431	GLY	2.3
1	C	325	VAL	2.3
1	D	281	GLY	2.3
1	C	291	ASP	2.3
1	D	412	GLY	2.3
1	C	53	ALA	2.3
1	B	229	ALA	2.2
1	B	285	LEU	2.2
1	B	301	CYS	2.2
1	A	432	ALA	2.2
1	A	436	ARG	2.2
1	C	26	GLY	2.2
1	D	54	GLY	2.2
1	A	67	ASP	2.2
1	D	33	VAL	2.2
1	C	344	ALA	2.1
1	A	439	ARG	2.1
1	C	28	SER	2.1
1	A	217	LEU	2.1
1	B	219	ALA	2.1
1	A	38	ASP	2.1
1	A	328	LEU	2.1
1	B	328	LEU	2.1
1	D	130	LEU	2.1
1	D	492	PRO	2.1
1	D	204	ALA	2.1
1	C	154	VAL	2.1
1	C	425	GLY	2.1
1	A	500	GLU	2.0
1	D	12	ASP	2.0
1	B	433	THR	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	477	PRO	2.0

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

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.