Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 09:27 pm BST

PDB ID	:	4OB9
Title	:	Crystal structure of chorismate synthase from Acinetobacter baumannii at 2.50A resolution
Authors	:	Shukla, P.K.; Chaudhary, A.; Singh, N.; Sinha, M.; Bhushan, A.; Kaur, P.; Sharma, S.; Singh, T.P.
Deposited on	:	2014-01-07
Resolution	:	2.50 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 following versions of software and data (see references ①) were used in the production of this report:

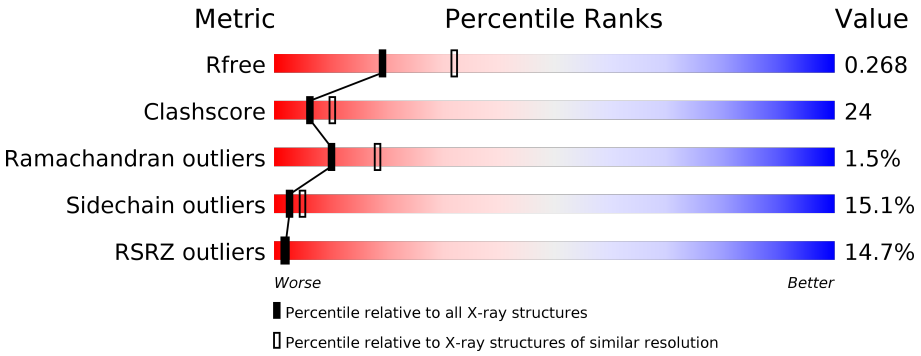
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 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	363	11% 53% 26% 7% 14%
1	B	363	14% 55% 23% 8% 14%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 4881 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 Chorismate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	313	Total	C	N	O	S	0	0	0
			2335	1463	421	440	11			
1	B	313	Total	C	N	O	S	0	0	0
			2335	1463	421	440	11			

- Molecule 2 is water.

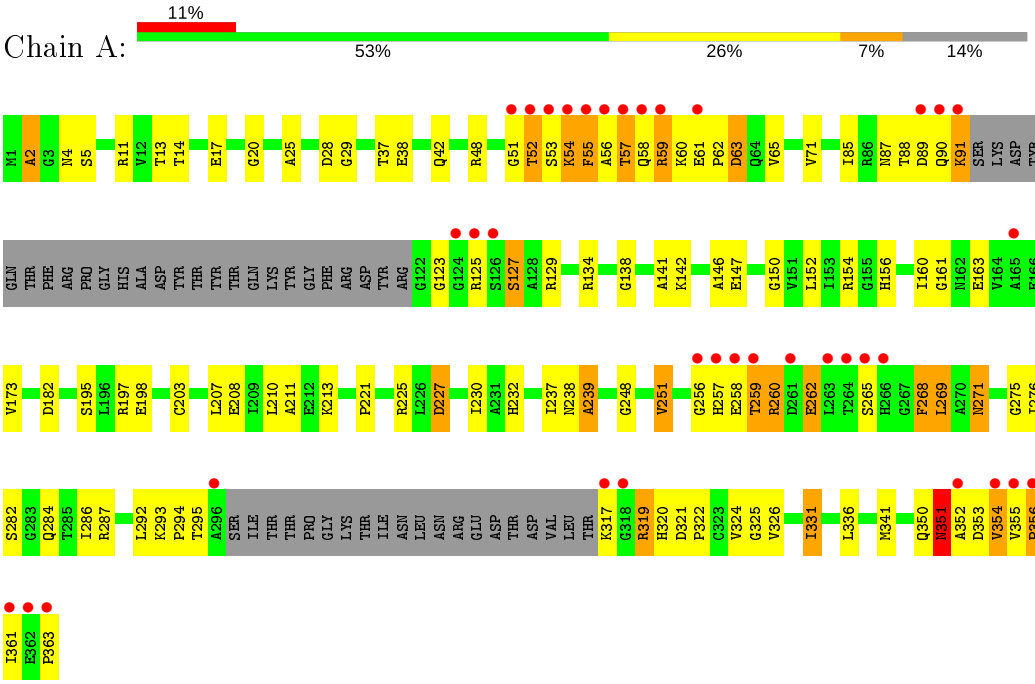
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	107	Total	O	0	0
			107	107		
2	B	104	Total	O	0	0
			104	104		

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 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.

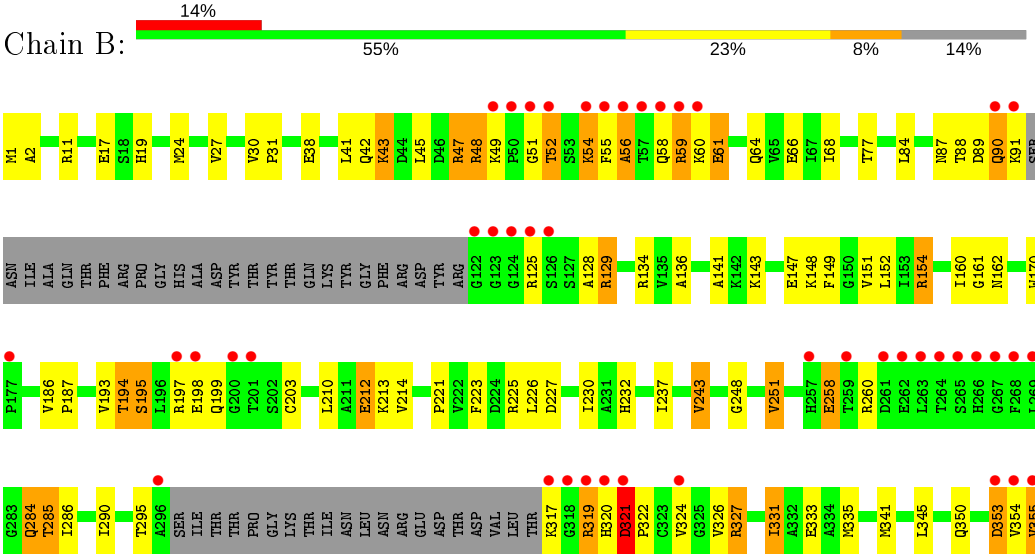
- Molecule 1: Chorismate synthase

Chain A:



- Molecule 1: Chorismate synthase

Chain B:




P360
I361
E362
P363

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 2 21	Depositor
Cell constants a, b, c, α, β, γ	72.98Å 89.79Å 108.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.19 – 2.50 50.19 – 2.50	Depositor EDS
% Data completeness (in resolution range)	91.2 (50.19-2.50) 91.2 (50.19-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.18	Depositor
$< I/\sigma(I) >$ [1]	2.10 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.218 , 0.264 0.220 , 0.268	Depositor DCC
R_{free} test set	1166 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	37.3	Xtriage
Anisotropy	0.589	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 53.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	4881	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.17% 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	0.88	1/2376 (0.0%)	1.00	5/3211 (0.2%)
1	B	0.87	0/2376	0.96	4/3211 (0.1%)
All	All	0.87	1/4752 (0.0%)	0.98	9/6422 (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	A	0	3
1	B	0	3
All	All	0	6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	170	TRP	CD2-CE2	6.63	1.49	1.41

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	55	PHE	CB-CA-C	-13.73	82.94	110.40
1	B	355	VAL	C-N-CD	-6.14	107.09	120.60
1	B	282	SER	CB-CA-C	-6.00	98.70	110.10
1	A	57	THR	CB-CA-C	-5.89	95.70	111.60
1	A	29	GLY	N-CA-C	5.48	126.80	113.10
1	A	295	THR	CB-CA-C	-5.36	97.12	111.60
1	A	351	ASN	O-C-N	5.17	130.97	122.70
1	B	56	ALA	N-CA-C	-5.12	97.19	111.00
1	B	319	ARG	N-CA-C	-5.08	97.28	111.00

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2	ALA	Peptide
1	A	256	GLY	Peptide
1	A	269	LEU	Peptide
1	B	321	ASP	Mainchain,Peptide
1	B	360	PRO	Peptide

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	2335	0	2342	119	0
1	B	2335	0	2342	118	0
2	A	107	0	0	5	0
2	B	104	0	0	7	0
All	All	4881	0	4684	225	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 24.

All (225) 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:356:PRO:CB	1:B:357:PRO:HA	1.72	1.20
1:B:357:PRO:O	1:B:358:PHE:HD1	1.22	1.19
1:B:59:ARG:NE	1:B:59:ARG:HA	1.45	1.17
1:B:51:GLY:HA3	1:B:55:PHE:CB	1.75	1.16
1:B:357:PRO:O	1:B:358:PHE:CD1	2.00	1.15
1:B:51:GLY:CA	1:B:55:PHE:HB2	1.81	1.09
1:A:260:ARG:H	1:A:265:SER:HB3	1.15	1.06
1:B:52:THR:OG1	1:B:54:LYS:HB2	1.53	1.06
1:A:262:GLU:HA	1:A:262:GLU:OE2	1.51	1.05
1:A:90:GLN:O	1:A:91:LYS:HB2	1.54	1.05
1:B:355:VAL:O	1:B:355:VAL:HG23	1.59	1.02
1:A:59:ARG:HH21	1:A:59:ARG:CG	1.73	1.01
1:A:55:PHE:CD2	1:A:56:ALA:N	2.29	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:356:PRO:HB2	1:B:357:PRO:HA	1.41	1.00
1:A:259:THR:HA	1:A:260:ARG:HD2	1.43	0.99
1:A:259:THR:HG23	1:A:260:ARG:HB2	1.46	0.98
1:A:268:PHE:CD1	1:A:268:PHE:N	2.29	0.98
1:B:356:PRO:CB	1:B:357:PRO:CA	2.44	0.96
1:B:362:GLU:O	1:B:363:PRO:OXT	1.85	0.95
1:B:356:PRO:HB3	1:B:357:PRO:HA	1.48	0.94
1:B:59:ARG:HE	1:B:59:ARG:CA	1.81	0.94
1:A:55:PHE:HD2	1:A:56:ALA:N	1.63	0.93
1:A:293:LYS:HA	1:B:251:VAL:HG13	1.50	0.93
1:B:359:ALA:HB1	1:B:360:PRO:CD	1.98	0.92
1:A:211:ALA:HB3	1:A:286:ILE:HB	1.54	0.90
1:A:268:PHE:H	1:A:268:PHE:HD1	0.93	0.87
1:A:260:ARG:H	1:A:265:SER:CB	1.88	0.87
1:A:260:ARG:N	1:A:265:SER:HB3	1.88	0.86
1:A:260:ARG:CG	1:A:260:ARG:HH11	1.87	0.86
1:B:59:ARG:HE	1:B:59:ARG:HA	1.10	0.85
1:A:2:ALA:HB1	2:B:412:HOH:O	1.75	0.85
1:A:268:PHE:N	1:A:268:PHE:HD1	1.69	0.85
1:B:357:PRO:C	1:B:358:PHE:CD1	2.50	0.85
1:A:59:ARG:HH21	1:A:59:ARG:HG2	1.41	0.83
1:B:359:ALA:HB1	1:B:360:PRO:HD3	1.60	0.81
1:B:90:GLN:HE21	1:B:90:GLN:H	1.29	0.81
1:A:269:LEU:HG	1:A:284:GLN:HE21	1.46	0.79
1:A:90:GLN:O	1:A:91:LYS:CB	2.30	0.79
1:A:262:GLU:CA	1:A:262:GLU:OE2	2.30	0.79
1:A:269:LEU:HG	1:A:284:GLN:NE2	1.97	0.79
1:A:351:ASN:N	1:A:351:ASN:ND2	2.31	0.79
1:A:20:GLY:HA3	2:A:417:HOH:O	1.82	0.78
1:A:319:ARG:HH11	1:A:319:ARG:HG3	1.48	0.78
1:A:238:ASN:O	1:A:239:ALA:HB3	1.83	0.78
1:B:355:VAL:O	1:B:355:VAL:CG2	2.32	0.77
1:B:186:VAL:HB	1:B:187:PRO:HD2	1.66	0.77
1:B:51:GLY:HA3	1:B:55:PHE:HB2	0.87	0.77
1:A:260:ARG:HG3	1:A:260:ARG:HH11	1.49	0.76
1:A:59:ARG:HH21	1:A:59:ARG:HG3	1.50	0.76
1:A:350:GLN:HB3	1:A:351:ASN:ND2	2.00	0.76
1:B:42:GLN:OE1	1:B:64:GLN:HA	1.86	0.75
1:A:260:ARG:HG3	1:A:260:ARG:NH1	2.00	0.75
1:A:60:LYS:HG3	1:A:61:GLU:H	1.52	0.75
1:B:356:PRO:HB3	1:B:357:PRO:CA	2.15	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:LYS:HA	1:B:251:VAL:CG1	2.19	0.73
1:A:351:ASN:N	1:A:351:ASN:HD22	1.86	0.72
1:B:285:THR:HG21	2:B:421:HOH:O	1.92	0.69
1:A:238:ASN:O	1:A:239:ALA:CB	2.38	0.69
1:A:89:ASP:O	1:A:90:GLN:HB2	1.93	0.69
1:A:59:ARG:NH2	1:A:59:ARG:CG	2.45	0.69
1:A:208:GLU:OE1	1:A:287:ARG:HD3	1.93	0.68
1:B:52:THR:C	1:B:54:LYS:H	1.97	0.68
1:B:160:ILE:HG22	1:B:203:CYS:SG	2.35	0.67
1:B:359:ALA:CB	1:B:360:PRO:CD	2.71	0.67
1:A:182:ASP:C	1:A:182:ASP:OD1	2.30	0.66
1:B:90:GLN:NE2	1:B:90:GLN:H	1.94	0.65
1:B:237:ILE:HG12	1:B:331:ILE:HD11	1.79	0.65
1:B:90:GLN:HE21	1:B:90:GLN:N	1.94	0.65
1:A:355:VAL:O	1:A:356:PRO:O	2.15	0.65
1:B:52:THR:C	1:B:54:LYS:N	2.50	0.64
1:B:61:GLU:OE1	1:B:61:GLU:HA	1.96	0.64
1:A:319:ARG:NH1	1:A:319:ARG:HG3	2.10	0.64
1:A:42:GLN:OE1	1:A:65:VAL:HG12	1.98	0.63
1:B:356:PRO:HB2	1:B:357:PRO:CA	2.21	0.63
1:A:269:LEU:CG	1:A:284:GLN:HE21	2.12	0.63
1:B:89:ASP:O	1:B:90:GLN:C	2.37	0.63
1:B:17:GLU:HG3	2:B:467:HOH:O	1.98	0.63
1:B:160:ILE:CG2	1:B:203:CYS:SG	2.87	0.63
1:B:186:VAL:HB	1:B:187:PRO:CD	2.28	0.62
1:B:55:PHE:CD2	1:B:55:PHE:C	2.73	0.62
1:A:221:PRO:O	1:B:2:ALA:HA	1.99	0.62
1:A:355:VAL:HB	1:A:356:PRO:HD2	1.81	0.62
1:B:56:ALA:HB3	1:B:59:ARG:HB2	1.82	0.61
1:A:350:GLN:C	1:A:351:ASN:HD22	2.02	0.61
1:B:353:ASP:C	1:B:353:ASP:OD1	2.38	0.61
1:B:321:ASP:HB3	2:B:496:HOH:O	2.00	0.61
1:B:225:ARG:HB3	1:B:227:ASP:OD1	2.00	0.61
1:A:127:SER:C	1:A:129:ARG:H	2.05	0.60
1:A:87:ASN:HB3	1:A:89:ASP:OD1	2.02	0.60
1:B:186:VAL:CB	1:B:187:PRO:CD	2.80	0.59
1:B:282:SER:HB3	1:B:284:GLN:HG2	1.84	0.59
1:A:350:GLN:HG3	1:B:1:MET:SD	2.42	0.59
1:A:59:ARG:NH2	1:A:59:ARG:HG3	2.15	0.59
1:B:59:ARG:CZ	1:B:59:ARG:HA	2.28	0.59
1:B:359:ALA:HB1	1:B:360:PRO:HD2	1.80	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:LYS:CA	1:B:251:VAL:HG13	2.29	0.58
1:A:257:HIS:ND1	1:A:258:GLU:C	2.57	0.58
1:A:225:ARG:HG2	1:A:279:GLY:HA3	1.85	0.58
1:B:68:ILE:HD11	1:B:84:LEU:HB3	1.84	0.58
1:B:353:ASP:OD1	1:B:354:VAL:N	2.37	0.57
1:B:143:LYS:O	1:B:147:GLU:HG3	2.04	0.57
1:A:150:GLY:O	1:A:213:LYS:HD3	2.04	0.57
1:A:293:LYS:CA	1:B:251:VAL:CG1	2.83	0.57
1:B:87:ASN:HB3	1:B:129:ARG:NH2	2.19	0.57
1:A:57:THR:HG23	1:A:58:GLN:N	2.18	0.57
1:B:258:GLU:HG2	2:B:478:HOH:O	2.03	0.56
1:B:38:GLU:HB2	2:B:418:HOH:O	2.05	0.56
1:A:52:THR:O	1:A:59:ARG:HD3	2.05	0.56
1:A:232:HIS:HB2	1:B:232:HIS:HB2	1.87	0.56
1:B:210:LEU:HA	1:B:286:ILE:O	2.05	0.56
1:B:186:VAL:HG12	1:B:187:PRO:HD3	1.87	0.56
1:A:156:HIS:NE2	1:A:208:GLU:OE2	2.37	0.56
1:B:66:GLU:O	1:B:68:ILE:HD12	2.05	0.56
1:A:320:HIS:CE1	2:A:414:HOH:O	2.58	0.55
1:A:317:LYS:HE2	1:A:317:LYS:HA	1.88	0.55
1:B:243:VAL:HG13	1:B:290:ILE:HG22	1.88	0.55
1:A:269:LEU:CD2	1:A:284:GLN:HE21	2.20	0.55
1:B:359:ALA:O	1:B:361:ILE:HA	2.06	0.55
1:A:170:TRP:O	1:A:173:VAL:HG22	2.06	0.55
1:B:227:ASP:N	1:B:227:ASP:OD1	2.40	0.54
1:B:361:ILE:O	1:B:362:GLU:HG3	2.08	0.54
1:A:11:ARG:HB3	1:A:28:ASP:HB2	1.90	0.54
1:A:293:LYS:HB3	1:B:251:VAL:HG11	1.89	0.54
1:A:350:GLN:HB3	1:A:351:ASN:HD21	1.72	0.53
1:A:13:THR:O	1:A:25:ALA:HA	2.09	0.52
1:A:257:HIS:ND1	1:A:258:GLU:N	2.58	0.52
1:A:195:SER:O	1:A:198:GLU:HG3	2.09	0.52
1:B:356:PRO:HB3	1:B:358:PHE:N	2.24	0.52
1:A:248:GLY:O	1:A:251:VAL:HB	2.10	0.52
1:B:148:LYS:HG2	1:B:149:PHE:CE2	2.45	0.51
1:A:230:ILE:HD13	1:A:336:LEU:CD1	2.40	0.51
1:A:259:THR:HA	1:A:260:ARG:CD	2.27	0.51
1:A:59:ARG:NH2	1:A:59:ARG:HG2	2.18	0.51
1:A:227:ASP:N	1:A:227:ASP:OD1	2.33	0.51
1:A:2:ALA:HA	1:B:221:PRO:O	2.10	0.51
1:A:260:ARG:HG2	1:A:260:ARG:HH11	1.73	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:SER:C	1:A:129:ARG:N	2.63	0.51
1:A:356:PRO:HA	1:A:357:PRO:C	2.30	0.51
1:B:320:HIS:O	1:B:321:ASP:C	2.48	0.51
1:B:68:ILE:CD1	1:B:84:LEU:HB3	2.41	0.51
1:A:51:GLY:HA3	1:A:54:LYS:HB2	1.92	0.51
1:A:88:THR:C	1:A:90:GLN:N	2.63	0.50
1:B:160:ILE:O	1:B:161:GLY:C	2.48	0.50
1:B:335:MET:HE2	1:B:335:MET:N	2.26	0.50
1:A:55:PHE:HB2	1:A:59:ARG:HG2	1.94	0.50
1:B:186:VAL:HG12	1:B:187:PRO:CD	2.41	0.50
1:B:248:GLY:O	1:B:251:VAL:HB	2.12	0.50
1:A:63:ASP:HB2	2:A:476:HOH:O	2.12	0.49
1:A:138:GLY:O	1:A:142:LYS:HB2	2.12	0.49
1:A:60:LYS:HG3	1:A:61:GLU:N	2.26	0.49
1:A:352:ALA:O	1:A:353:ASP:OD1	2.30	0.49
1:A:259:THR:CG2	1:A:260:ARG:HB2	2.31	0.49
1:B:356:PRO:HB3	1:B:357:PRO:C	2.34	0.48
1:B:356:PRO:HA	1:B:358:PHE:CE1	2.47	0.48
1:A:17:GLU:HA	2:A:428:HOH:O	2.13	0.48
1:A:356:PRO:HB3	2:A:420:HOH:O	2.14	0.48
1:A:146:ALA:O	1:A:150:GLY:HA2	2.14	0.48
1:A:355:VAL:O	1:A:356:PRO:C	2.52	0.47
1:B:41:LEU:HD22	1:B:136:ALA:O	2.14	0.47
1:A:271:ASN:ND2	1:A:275:GLY:H	2.13	0.47
1:B:321:ASP:HB2	1:B:322:PRO:HA	1.95	0.47
1:B:282:SER:CB	1:B:284:GLN:HG2	2.44	0.47
1:A:320:HIS:O	1:A:322:PRO:CD	2.63	0.47
1:A:134:ARG:HD3	1:B:223:PHE:HE1	1.80	0.47
1:B:134:ARG:HG2	1:B:335:MET:HE1	1.96	0.46
1:B:173:VAL:HG22	1:B:174:PRO:HD3	1.97	0.46
1:B:195:SER:O	1:B:199:GLN:HG2	2.16	0.46
1:A:225:ARG:HB3	1:A:227:ASP:OD1	2.16	0.46
1:B:48:ARG:NH1	1:B:128:ALA:O	2.40	0.46
1:B:43:LYS:HE3	1:B:43:LYS:HB2	1.45	0.46
1:A:207:LEU:HD13	1:A:292:LEU:HD13	1.98	0.45
1:A:293:LYS:HB3	1:B:251:VAL:CG1	2.47	0.45
1:A:197:ARG:NH1	1:A:320:HIS:O	2.49	0.45
1:B:320:HIS:O	1:B:321:ASP:O	2.34	0.45
1:B:11:ARG:O	1:B:27:VAL:HA	2.15	0.45
1:A:275:GLY:C	1:A:276:ILE:HG13	2.36	0.45
1:A:65:VAL:HA	1:A:85:ILE:HG12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:VAL:HA	1:B:31:PRO:HD3	1.80	0.45
1:B:359:ALA:CB	1:B:360:PRO:HD2	2.44	0.45
1:B:59:ARG:HE	1:B:59:ARG:N	2.11	0.45
1:B:151:VAL:HA	1:B:212:GLU:O	2.17	0.44
1:B:214:VAL:HG21	1:B:286:ILE:HD12	1.98	0.44
1:B:42:GLN:OE1	1:B:64:GLN:CA	2.59	0.44
1:A:141:ALA:HB1	1:A:341:MET:HB2	1.99	0.44
1:B:61:GLU:OE1	1:B:61:GLU:CA	2.63	0.44
1:A:257:HIS:CG	1:A:258:GLU:N	2.85	0.43
1:A:167:LYS:HB2	1:A:167:LYS:HE2	1.57	0.43
1:A:355:VAL:HB	1:A:356:PRO:CD	2.47	0.43
1:B:356:PRO:HA	1:B:358:PHE:CZ	2.53	0.43
1:B:19:HIS:H	1:B:19:HIS:CD2	2.36	0.43
1:B:141:ALA:HB1	1:B:341:MET:HB2	2.01	0.43
1:B:47:ARG:NH1	1:B:333:GLU:OE1	2.43	0.43
1:B:359:ALA:O	1:B:360:PRO:C	2.57	0.43
1:B:327:ARG:NH1	2:B:462:HOH:O	2.52	0.43
1:B:362:GLU:HA	1:B:363:PRO:HD2	1.71	0.43
1:B:237:ILE:HG12	1:B:331:ILE:CD1	2.48	0.42
1:B:225:ARG:HG2	1:B:279:GLY:HA3	2.02	0.42
1:B:154:ARG:HA	1:B:333:GLU:OE2	2.20	0.42
1:B:88:THR:HG22	1:B:88:THR:O	2.18	0.42
1:A:4:ASN:HB2	1:A:14:THR:O	2.19	0.42
1:B:197:ARG:HD2	1:B:320:HIS:ND1	2.34	0.42
1:A:230:ILE:CD1	1:A:336:LEU:CD1	2.97	0.42
1:A:230:ILE:HD13	1:A:336:LEU:HD13	2.00	0.42
1:B:170:TRP:HZ2	1:B:210:LEU:HD12	1.83	0.42
1:B:1:MET:O	1:B:2:ALA:HB2	2.20	0.42
1:B:45:LEU:O	1:B:48:ARG:HB2	2.19	0.42
1:A:71:VAL:O	1:A:71:VAL:HG23	2.18	0.42
1:B:226:LEU:O	1:B:230:ILE:HG13	2.20	0.42
1:A:293:LYS:HB2	1:A:294:PRO:CD	2.50	0.42
1:A:167:LYS:O	1:A:182:ASP:HB2	2.20	0.42
1:A:237:ILE:HG12	1:A:331:ILE:HG12	2.02	0.41
1:A:160:ILE:HG22	1:A:203:CYS:SG	2.61	0.41
1:B:194:THR:O	1:B:198:GLU:HG3	2.21	0.41
1:A:170:TRP:HZ2	1:A:210:LEU:HD12	1.86	0.41
1:A:57:THR:CG2	1:A:58:GLN:N	2.82	0.41
1:A:88:THR:C	1:A:90:GLN:H	2.22	0.41
1:B:335:MET:HE2	1:B:335:MET:CA	2.50	0.41
1:A:320:HIS:O	1:A:322:PRO:HD2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:ARG:HD3	1:B:223:PHE:CE1	2.55	0.41
1:A:354:VAL:C	1:A:355:VAL:HG13	2.40	0.41
1:A:147:GLU:O	1:A:363:PRO:HA	2.20	0.41
1:B:284:GLN:HG2	1:B:284:GLN:H	1.49	0.40
1:B:345:LEU:HD23	1:B:345:LEU:HA	1.87	0.40
1:A:260:ARG:HA	1:A:260:ARG:HD2	1.90	0.40
1:A:282:SER:HB3	1:A:284:GLN:HG3	2.03	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	307/363 (85%)	285 (93%)	14 (5%)	8 (3%)	5 8
1	B	307/363 (85%)	287 (94%)	19 (6%)	1 (0%)	41 61
All	All	614/726 (85%)	572 (93%)	33 (5%)	9 (2%)	10 18

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	62	PRO
1	B	356	PRO
1	A	325	GLY
1	A	356	PRO
1	A	360	PRO
1	A	123	GLY
1	A	239	ALA
1	A	359	ALA
1	A	161	GLY

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	242/286 (85%)	210 (87%)	32 (13%)	4 7
1	B	242/286 (85%)	201 (83%)	41 (17%)	2 3
All	All	484/572 (85%)	411 (85%)	73 (15%)	3 5

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	SER
1	A	37	THR
1	A	38	GLU
1	A	48	ARG
1	A	52	THR
1	A	53	SER
1	A	54	LYS
1	A	59	ARG
1	A	63	ASP
1	A	91	LYS
1	A	125	ARG
1	A	127	SER
1	A	152	LEU
1	A	154	ARG
1	A	163	GLU
1	A	167	LYS
1	A	227	ASP
1	A	251	VAL
1	A	259	THR
1	A	260	ARG
1	A	262	GLU
1	A	268	PHE
1	A	271	ASN
1	A	280	ILE
1	A	319	ARG
1	A	321	ASP
1	A	324	VAL

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Mol	Chain	Res	Type
1	A	326	VAL
1	A	331	ILE
1	A	351	ASN
1	A	354	VAL
1	A	361	ILE
1	B	24	MET
1	B	43	LYS
1	B	47	ARG
1	B	48	ARG
1	B	49	LYS
1	B	52	THR
1	B	54	LYS
1	B	58	GLN
1	B	59	ARG
1	B	60	LYS
1	B	61	GLU
1	B	77	THR
1	B	90	GLN
1	B	91	LYS
1	B	125	ARG
1	B	129	ARG
1	B	152	LEU
1	B	154	ARG
1	B	162	ASN
1	B	193	VAL
1	B	194	THR
1	B	195	SER
1	B	212	GLU
1	B	213	LYS
1	B	243	VAL
1	B	251	VAL
1	B	258	GLU
1	B	260	ARG
1	B	284	GLN
1	B	285	THR
1	B	295	THR
1	B	317	LYS
1	B	319	ARG
1	B	321	ASP
1	B	324	VAL
1	B	326	VAL
1	B	327	ARG

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Mol	Chain	Res	Type
1	B	331	ILE
1	B	350	GLN
1	B	353	ASP
1	B	361	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	175	ASN
1	A	199	GLN
1	A	271	ASN
1	A	284	GLN
1	A	351	ASN
1	B	19	HIS
1	B	90	GLN
1	B	175	ASN
1	B	238	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

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	313/363 (86%)	0.58	40 (12%)	3	3	17, 31, 102, 150	30 (9%)
1	B	313/363 (86%)	0.95	52 (16%)	1	1	18, 36, 116, 158	24 (7%)
All	All	626/726 (86%)	0.76	92 (14%)	2	2	17, 33, 111, 158	54 (8%)

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	55	PHE	13.2
1	B	355	VAL	11.7
1	B	359	ALA	11.4
1	A	257	HIS	10.7
1	B	57	THR	10.6
1	B	358	PHE	10.5
1	B	263	LEU	10.2
1	A	354	VAL	10.0
1	B	59	ARG	9.9
1	A	363	PRO	9.9
1	B	56	ALA	9.8
1	B	356	PRO	9.6
1	B	357	PRO	9.3
1	B	55	PHE	9.0
1	A	265	SER	8.1
1	A	59	ARG	7.6
1	A	53	SER	7.6
1	A	263	LEU	7.3
1	B	58	GLN	7.3
1	B	52	THR	7.2
1	A	361	ILE	6.9
1	A	259	THR	6.9
1	B	363	PRO	6.8
1	B	354	VAL	6.8

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Mol	Chain	Res	Type	RSRZ
1	A	52	THR	6.7
1	B	360	PRO	6.7
1	A	56	ALA	6.7
1	B	262	GLU	6.7
1	B	319	ARG	6.6
1	A	124	GLY	6.4
1	B	267	GLY	6.3
1	B	266	HIS	6.2
1	B	264	THR	6.1
1	A	58	GLN	6.1
1	A	126	SER	5.5
1	B	124	GLY	5.5
1	B	265	SER	5.4
1	A	318	GLY	5.3
1	A	358	PHE	5.3
1	B	296	ALA	5.1
1	B	268	PHE	5.1
1	B	91	LYS	5.0
1	B	261	ASP	5.0
1	B	318	GLY	5.0
1	A	264	THR	5.0
1	A	359	ALA	4.7
1	A	266	HIS	4.6
1	B	51	GLY	4.5
1	A	261	ASP	4.5
1	B	125	ARG	4.3
1	A	357	PRO	4.1
1	B	60	LYS	4.1
1	A	57	THR	4.1
1	A	90	GLN	4.1
1	A	317	LYS	3.9
1	A	256	GLY	3.9
1	B	353	ASP	3.9
1	A	54	LYS	3.9
1	B	126	SER	3.9
1	B	54	LYS	3.8
1	B	197	ARG	3.7
1	A	89	ASP	3.7
1	B	361	ILE	3.7
1	A	51	GLY	3.7
1	A	91	LYS	3.5
1	B	90	GLN	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	200	GLY	3.4
1	B	269	LEU	3.4
1	A	61	GLU	3.4
1	B	123	GLY	3.4
1	B	317	LYS	3.3
1	A	360	PRO	3.1
1	A	258	GLU	3.1
1	B	257	HIS	3.1
1	A	355	VAL	2.9
1	B	201	THR	2.8
1	B	122	GLY	2.8
1	A	125	ARG	2.7
1	B	259	THR	2.6
1	A	362	GLU	2.6
1	B	49	LYS	2.6
1	B	362	GLU	2.6
1	B	320	HIS	2.5
1	A	352	ALA	2.4
1	A	356	PRO	2.3
1	A	296	ALA	2.3
1	B	50	PRO	2.2
1	B	321	ASP	2.1
1	B	177	PRO	2.1
1	B	198	GLU	2.1
1	B	324	VAL	2.1
1	A	165	ALA	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 carbohydrates 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.