Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 12:46 AM GMT

PDB ID	:	2BGH
Title	:	Crystal structure of Vinorine Synthase
Authors	:	Ma, X.; Koepke, J.; Panjikar, S.; Fritzsch, G.; Stoeckigt, J.
Deposited on	:	2004-12-22
Resolution	:	2.60 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:

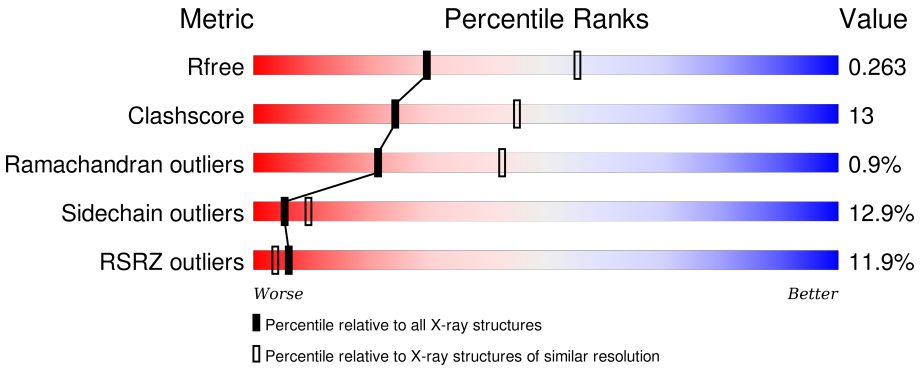
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.60 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	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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	421	9% 71% 22%
1	B	421	14% 67% 25% 6%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6608 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 VINORINE SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	413	Total	C	N	O	S	0	0	0
			3240	2076	538	609	17			
1	B	412	Total	C	N	O	S	0	0	0
			3225	2068	536	604	17			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	200	VAL	ALA	CONFLICT	UNP Q70PR7
B	200	VAL	ALA	CONFLICT	UNP Q70PR7

- Molecule 2 is water.

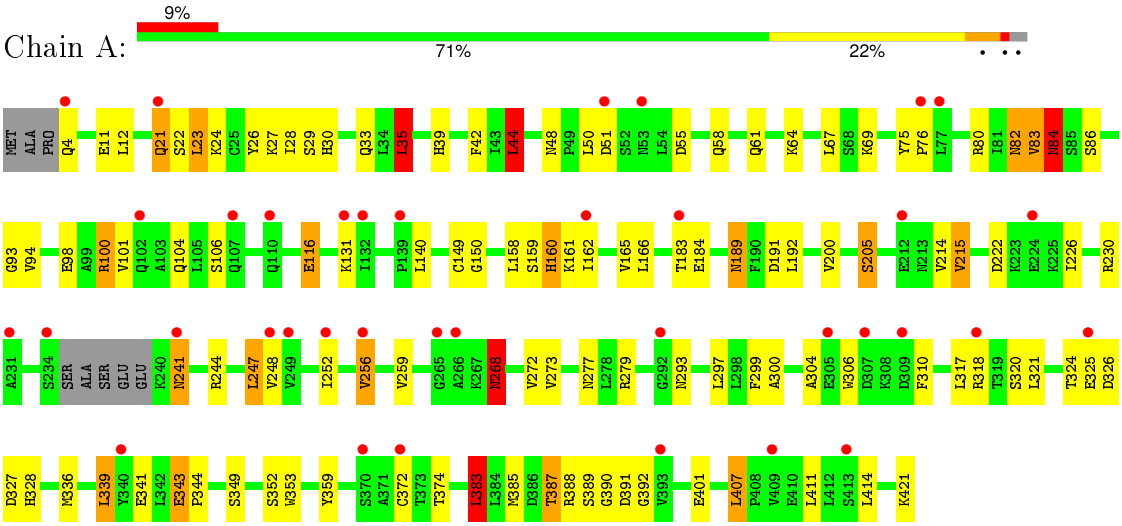
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	101	Total	O	0	0
			101	101		
2	B	42	Total	O	0	0
			42	42		

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.

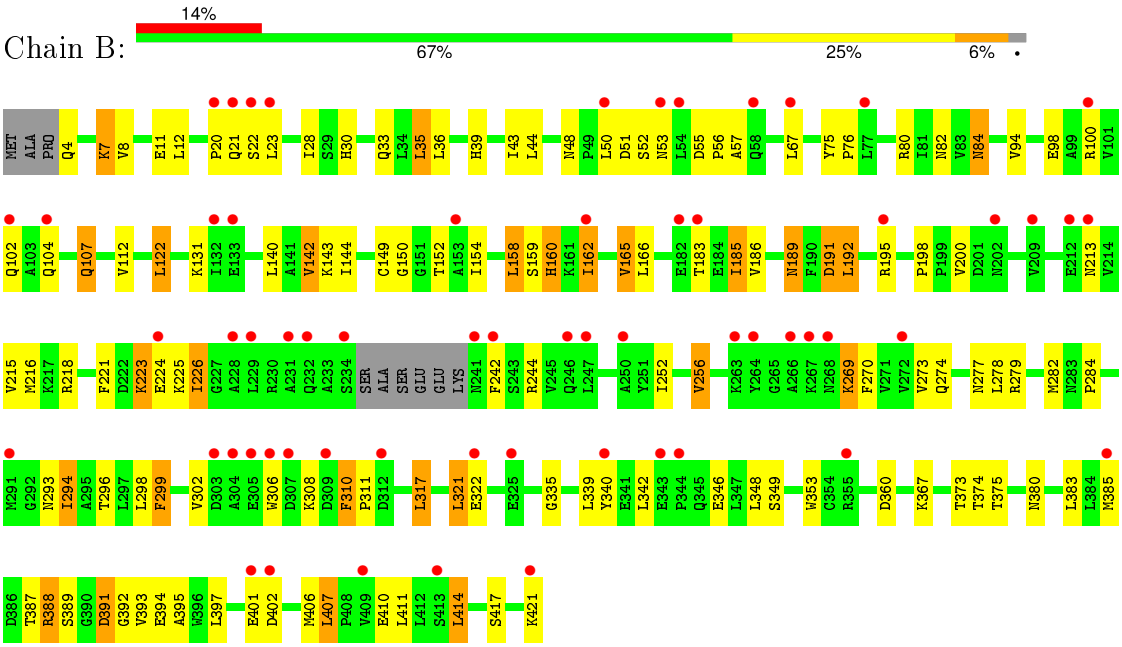
- Molecule 1: VINORINE SYNTHASE

Chain A:



- Molecule 1: VINORINE SYNTHASE

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	82.72Å 90.45Å 136.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.60 19.99 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.6 (20.00-2.60) 98.6 (19.99-2.60)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	6.38 (at 2.59Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.211 , 0.272 0.207 , 0.263	Depositor DCC
R_{free} test set	1004 reflections (3.27%)	DCC
Wilson B-factor (Å^2)	64.1	Xtriage
Anisotropy	0.133	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 70.5	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 31717 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6608	wwPDB-VP
Average B, all atoms (Å^2)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 51.11 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 5.8791e-05.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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	0.68	1/3318 (0.0%)	0.79	4/4516 (0.1%)
1	B	0.59	2/3303 (0.1%)	0.73	4/4497 (0.1%)
All	All	0.64	3/6621 (0.0%)	0.76	8/9013 (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	1	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	53	ASN	CG-ND2	9.32	1.56	1.32
1	B	53	ASN	CG-OD1	7.90	1.41	1.24
1	A	372	CYS	CB-SG	-5.15	1.73	1.81

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	383	LEU	CA-CB-CG	8.16	134.07	115.30
1	A	84	ASN	N-CA-C	6.01	127.23	111.00
1	A	35	LEU	CA-CB-CG	-5.96	101.59	115.30
1	B	84	ASN	N-CA-C	5.62	126.18	111.00
1	B	158	LEU	CA-CB-CG	5.58	128.14	115.30
1	A	44	LEU	CA-CB-CG	5.39	127.70	115.30
1	B	80	ARG	NE-CZ-NH2	5.29	122.95	120.30
1	B	321	LEU	CA-CB-CG	5.03	126.87	115.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	84	ASN	CA

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	22	SER	Peptide
1	A	83	VAL	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3240	0	3220	89	0
1	B	3225	0	3203	82	0
2	A	101	0	0	12	0
2	B	42	0	0	14	0
All	All	6608	0	6423	168	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 13.

All (168) 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:A:160:HIS:HD2	2:A:2043:HOH:O	1.13	1.25
1:A:21:GLN:HE21	1:A:21:GLN:HA	1.14	1.07
1:A:100:ARG:HH11	1:A:100:ARG:HG3	1.26	1.01
1:A:160:HIS:CD2	2:A:2043:HOH:O	1.94	0.98
1:A:318:ARG:HH11	1:A:318:ARG:HG3	1.37	0.88
1:A:21:GLN:HA	1:A:21:GLN:NE2	1.91	0.85
1:A:226:ILE:CD1	1:A:392:GLY:HA2	2.06	0.85
1:B:284:PRO:HD3	2:B:2028:HOH:O	1.84	0.76
1:A:324:THR:HG22	1:A:326:ASP:H	1.51	0.74
1:B:385:MET:HE3	2:B:2037:HOH:O	1.88	0.74
1:A:27:LYS:HA	2:A:2012:HOH:O	1.88	0.74
1:A:116:GLU:HA	1:A:116:GLU:OE2	1.90	0.72
1:A:226:ILE:HD11	1:A:392:GLY:HA2	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:GLN:HE22	1:A:200:VAL:H	1.39	0.69
1:B:28:ILE:HD11	1:B:162:ILE:HD11	1.74	0.69
1:B:278:LEU:HD13	1:B:296:THR:HB	1.75	0.68
1:A:165:VAL:HG11	1:A:353:TRP:NE1	2.09	0.67
1:B:39:HIS:HD2	1:B:159:SER:HA	1.57	0.67
1:A:407:LEU:HG	1:A:411:LEU:HD23	1.79	0.65
1:A:189:ASN:ND2	1:A:191:ASP:H	1.93	0.65
1:B:317:LEU:HB3	2:B:2033:HOH:O	1.96	0.65
1:A:39:HIS:HD2	1:A:159:SER:HA	1.63	0.64
1:B:149:CYS:HA	2:B:2016:HOH:O	1.97	0.64
1:B:410:GLU:HG3	2:B:2042:HOH:O	1.97	0.64
1:A:256:VAL:HA	1:A:259:VAL:HG22	1.81	0.63
1:B:8:VAL:CG2	1:B:98:GLU:HB3	2.29	0.63
1:B:189:ASN:ND2	1:B:191:ASP:H	1.97	0.63
1:B:33:GLN:HE22	1:B:200:VAL:H	1.47	0.62
1:A:189:ASN:HD22	1:A:189:ASN:C	2.03	0.62
1:B:30:HIS:CD2	1:B:200:VAL:HG23	2.34	0.62
1:B:339:LEU:HD12	1:B:342:LEU:HD12	1.82	0.61
1:A:23:LEU:O	1:A:24:LYS:HB2	2.00	0.60
1:A:42:PHE:CE1	1:A:44:LEU:HD22	2.36	0.60
1:B:107:GLN:HB2	2:B:2009:HOH:O	2.00	0.60
1:B:348:LEU:HD12	1:B:380:ASN:HB3	1.83	0.59
1:A:104:GLN:HG2	1:A:149:CYS:HB3	1.84	0.59
1:A:30:HIS:HA	1:A:33:GLN:HE21	1.67	0.59
1:A:100:ARG:HD3	2:A:2029:HOH:O	2.03	0.58
1:A:64:LYS:NZ	1:A:98:GLU:OE2	2.33	0.58
1:B:28:ILE:CD1	1:B:162:ILE:HD11	2.33	0.57
1:B:82:ASN:HB2	2:B:2007:HOH:O	2.05	0.57
1:A:277:ASN:ND2	1:A:279:ARG:H	2.02	0.57
1:B:75:TYR:CG	1:B:76:PRO:HD3	2.39	0.57
1:B:35:LEU:HD13	1:B:293:ASN:CG	2.26	0.57
1:B:8:VAL:HG22	1:B:98:GLU:HB3	1.87	0.56
1:A:42:PHE:HE1	1:A:44:LEU:CD2	2.18	0.56
1:A:83:VAL:HG13	1:A:84:ASN:H	1.69	0.56
1:A:28:ILE:HG12	1:A:86:SER:HA	1.87	0.56
1:A:161:LYS:NZ	1:A:205:SER:HB3	2.21	0.56
1:B:279:ARG:NH2	1:B:294:ILE:HB	2.21	0.55
1:A:268:ASN:O	1:A:304:ALA:HB2	2.06	0.55
1:A:318:ARG:NH1	1:A:318:ARG:HG3	2.11	0.55
1:A:244:ARG:NH1	1:A:390:GLY:O	2.39	0.55
1:A:11:GLU:OE1	1:B:11:GLU:OE1	2.25	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:226:ILE:HD13	1:B:392:GLY:HA2	1.88	0.54
1:A:343:GLU:HG3	1:A:344:PRO:HD2	1.90	0.54
1:A:80:ARG:NH1	1:A:93:GLY:O	2.36	0.53
1:A:388:ARG:NH2	1:A:421:LYS:OXT	2.41	0.53
1:B:306:TRP:CZ2	1:B:308:LYS:HB2	2.44	0.52
1:A:83:VAL:CG1	1:A:84:ASN:H	2.22	0.52
1:A:55:ASP:H	1:A:58:GLN:NE2	2.07	0.52
1:A:324:THR:CG2	1:A:325:GLU:N	2.72	0.52
1:A:248:VAL:O	1:A:252:ILE:HG13	2.10	0.52
1:B:421:LYS:HB3	1:B:421:LYS:NZ	2.25	0.52
1:B:189:ASN:ND2	1:B:192:LEU:HD22	2.25	0.52
1:A:324:THR:HG22	1:A:325:GLU:N	2.25	0.51
1:B:221:PHE:HB3	1:B:226:ILE:HD12	1.91	0.51
1:A:317:LEU:O	1:A:320:SER:HB3	2.11	0.51
1:B:407:LEU:HG	1:B:411:LEU:HD23	1.91	0.51
1:A:388:ARG:NH2	1:A:421:LYS:O	2.43	0.51
1:B:142:VAL:HG23	1:B:143:LYS:N	2.25	0.51
1:B:385:MET:HB2	1:B:394:GLU:HB2	1.93	0.50
1:A:215:VAL:HG22	1:A:401:GLU:HG2	1.93	0.50
1:A:42:PHE:CE1	1:A:44:LEU:CD2	2.94	0.50
1:B:35:LEU:HD22	1:B:160:HIS:ND1	2.26	0.50
1:A:35:LEU:HD13	1:A:293:ASN:CG	2.32	0.50
1:B:402:ASP:O	1:B:406:MET:HG3	2.11	0.50
1:B:48:ASN:HD22	1:B:150:GLY:HA3	1.76	0.50
1:A:61:GLN:NE2	1:B:57:ALA:HA	2.27	0.50
1:A:387:THR:HG23	2:A:2095:HOH:O	2.11	0.49
1:B:144:ILE:HD11	1:B:152:THR:HB	1.93	0.49
1:B:273:VAL:HG12	1:B:349:SER:HB3	1.93	0.49
1:B:391:ASP:OD1	1:B:391:ASP:N	2.44	0.49
1:B:277:ASN:ND2	1:B:279:ARG:H	2.10	0.49
1:B:104:GLN:HB2	2:B:2009:HOH:O	2.13	0.48
1:A:100:ARG:NH1	1:A:100:ARG:HG3	2.06	0.48
1:A:82:ASN:C	1:A:82:ASN:HD22	2.17	0.48
1:B:269:LYS:O	1:B:346:GLU:HG2	2.13	0.48
1:B:385:MET:HE2	2:B:2039:HOH:O	2.13	0.48
1:B:28:ILE:HD11	1:B:162:ILE:CD1	2.42	0.48
1:B:186:VAL:O	1:B:186:VAL:HG13	2.14	0.48
1:A:230:ARG:HA	1:A:247:LEU:HD21	1.96	0.47
1:A:241:ASN:HA	2:A:2059:HOH:O	2.13	0.47
1:B:28:ILE:CD1	1:B:162:ILE:CD1	2.91	0.47
1:A:272:VAL:HG11	1:A:317:LEU:HD21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:ILE:HD13	1:A:392:GLY:HA2	1.95	0.47
1:B:299:PHE:CD2	1:B:299:PHE:N	2.83	0.47
1:B:75:TYR:CD1	1:B:76:PRO:HD3	2.50	0.46
1:A:26:TYR:O	2:A:2010:HOH:O	2.20	0.46
1:B:189:ASN:C	1:B:189:ASN:HD22	2.18	0.46
1:B:216:MET:HE2	1:B:375:THR:HA	1.97	0.46
1:A:189:ASN:C	1:A:189:ASN:ND2	2.69	0.46
1:A:83:VAL:CG1	1:A:84:ASN:N	2.77	0.46
1:B:395:ALA:HB1	2:B:2040:HOH:O	2.15	0.46
1:A:222:ASP:OD2	1:A:222:ASP:N	2.40	0.46
1:A:35:LEU:HD22	1:A:160:HIS:ND1	2.31	0.46
1:A:272:VAL:HG12	1:A:300:ALA:HB3	1.97	0.46
1:B:310:PHE:N	1:B:311:PRO:HD2	2.31	0.46
1:B:397:LEU:HB2	2:B:2040:HOH:O	2.16	0.46
1:A:42:PHE:HE1	1:A:44:LEU:HD22	1.76	0.46
1:B:277:ASN:ND2	1:B:279:ARG:HH21	2.14	0.46
1:A:387:THR:HG22	1:A:389:SER:H	1.81	0.46
1:A:12:LEU:HB2	1:B:12:LEU:HB2	1.98	0.46
1:A:160:HIS:CE1	1:A:293:ASN:HD21	2.33	0.45
1:B:55:ASP:HB2	1:B:56:PRO:HD2	1.97	0.45
1:A:21:GLN:HB2	2:A:2009:HOH:O	2.16	0.45
1:A:353:TRP:CE2	1:A:383:LEU:HD11	2.52	0.45
1:A:318:ARG:NH1	1:A:318:ARG:CG	2.78	0.45
1:B:373:THR:HG21	1:B:383:LEU:HD12	1.99	0.45
1:B:360:ASP:HA	1:B:367:LYS:HD3	1.98	0.45
1:A:30:HIS:HA	1:A:33:GLN:NE2	2.32	0.44
1:B:252:ILE:O	1:B:256:VAL:HG13	2.17	0.44
1:A:48:ASN:HD22	1:A:150:GLY:HA3	1.82	0.44
1:A:336:MET:HB3	2:A:2078:HOH:O	2.18	0.43
1:A:39:HIS:CD2	1:A:159:SER:HA	2.49	0.43
1:B:411:LEU:HB2	2:B:2042:HOH:O	2.18	0.43
1:A:75:TYR:CG	1:A:76:PRO:HD3	2.53	0.43
1:B:225:LYS:HE2	1:B:414:LEU:HD21	1.99	0.43
1:A:385:MET:HE2	2:A:2090:HOH:O	2.18	0.43
1:A:161:LYS:HZ1	1:A:205:SER:HB3	1.83	0.43
1:A:55:ASP:H	1:A:58:GLN:HE21	1.65	0.43
1:A:48:ASN:ND2	1:A:150:GLY:HA3	2.33	0.43
1:B:273:VAL:CG1	1:B:349:SER:HB3	2.49	0.43
1:B:30:HIS:HB2	1:B:198:PRO:O	2.18	0.43
1:B:226:ILE:HG12	1:B:244:ARG:HG3	2.00	0.43
1:B:299:PHE:HE1	1:B:339:LEU:HD13	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:75:TYR:N	1:B:76:PRO:CD	2.82	0.42
1:B:387:THR:HG22	1:B:388:ARG:N	2.34	0.42
1:A:21:GLN:NE2	1:A:21:GLN:CA	2.72	0.42
1:B:270:PHE:HB2	1:B:302:VAL:HG23	2.01	0.42
1:A:39:HIS:HD2	1:A:159:SER:CA	2.30	0.42
1:A:42:PHE:HE1	1:A:44:LEU:HD21	1.85	0.42
1:B:112:VAL:O	1:B:417:SER:HB2	2.20	0.42
1:B:218:ARG:HD2	1:B:394:GLU:CD	2.40	0.42
1:B:191:ASP:HB3	1:B:195:ARG:HE	1.83	0.42
1:B:144:ILE:HD13	1:B:154:ILE:HG12	2.01	0.42
1:A:35:LEU:HD13	1:A:293:ASN:ND2	2.35	0.42
1:B:7:LYS:HE2	1:B:7:LYS:HB3	1.91	0.42
1:A:273:VAL:HG12	1:A:349:SER:HB3	2.02	0.41
1:A:299:PHE:HE1	1:A:339:LEU:HD13	1.84	0.41
1:A:359:TYR:CD2	1:A:388:ARG:HG3	2.56	0.41
1:B:142:VAL:CG2	1:B:143:LYS:N	2.83	0.41
1:B:299:PHE:CE2	1:B:335:GLY:HA2	2.55	0.41
1:A:392:GLY:N	2:A:2096:HOH:O	2.28	0.41
1:B:273:VAL:HA	1:B:298:LEU:O	2.20	0.41
1:B:43:ILE:HD11	1:B:122:LEU:HD13	2.02	0.41
1:B:185:ILE:HD12	1:B:185:ILE:HA	1.75	0.41
1:A:299:PHE:CE1	1:A:339:LEU:HD13	2.56	0.41
1:B:274:GLN:HG3	2:B:2031:HOH:O	2.21	0.41
1:B:20:PRO:O	1:B:22:SER:N	2.54	0.41
1:A:324:THR:HG22	1:A:326:ASP:N	2.29	0.41
1:B:104:GLN:HG2	1:B:149:CYS:HB3	2.03	0.40
1:B:215:VAL:HG22	1:B:401:GLU:HG2	2.03	0.40
1:B:165:VAL:HG11	1:B:353:TRP:CD1	2.56	0.40
1:B:223:LYS:HB3	2:B:2022:HOH:O	2.22	0.40
1:A:29:SER:O	1:A:33:GLN:HG3	2.21	0.40
1:A:387:THR:HB	1:A:391:ASP:O	2.21	0.40
1:A:321:LEU:HD13	2:A:2074: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	409/421 (97%)	391 (96%)	15 (4%)	3 (1%)	26 51
1	B	408/421 (97%)	377 (92%)	27 (7%)	4 (1%)	19 39
All	All	817/842 (97%)	768 (94%)	42 (5%)	7 (1%)	21 42

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	21	GLN
1	B	269	LYS
1	A	84	ASN
1	B	84	ASN
1	A	268	ASN
1	A	306	TRP
1	B	183	THR

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	362/368 (98%)	317 (88%)	45 (12%)	6 11
1	B	359/368 (98%)	311 (87%)	48 (13%)	5 8
All	All	721/736 (98%)	628 (87%)	93 (13%)	5 9

All (93) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	21	GLN
1	A	23	LEU
1	A	35	LEU
1	A	44	LEU

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Mol	Chain	Res	Type
1	A	50	LEU
1	A	51	ASP
1	A	67	LEU
1	A	69	LYS
1	A	82	ASN
1	A	94	VAL
1	A	100	ARG
1	A	101	VAL
1	A	106	SER
1	A	116	GLU
1	A	131	LYS
1	A	140	LEU
1	A	158	LEU
1	A	160	HIS
1	A	162	ILE
1	A	166	LEU
1	A	183	THR
1	A	184	GLU
1	A	189	ASN
1	A	192	LEU
1	A	205	SER
1	A	214	VAL
1	A	215	VAL
1	A	241	ASN
1	A	247	LEU
1	A	256	VAL
1	A	268	ASN
1	A	297	LEU
1	A	310	PHE
1	A	327	ASP
1	A	328	HIS
1	A	339	LEU
1	A	341	GLU
1	A	343	GLU
1	A	352	SER
1	A	374	THR
1	A	383	LEU
1	A	387	THR
1	A	407	LEU
1	A	414	LEU
1	B	4	GLN
1	B	7	LYS

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Mol	Chain	Res	Type
1	B	23	LEU
1	B	35	LEU
1	B	36	LEU
1	B	44	LEU
1	B	50	LEU
1	B	51	ASP
1	B	52	SER
1	B	67	LEU
1	B	94	VAL
1	B	100	ARG
1	B	102	GLN
1	B	107	GLN
1	B	122	LEU
1	B	131	LYS
1	B	140	LEU
1	B	142	VAL
1	B	158	LEU
1	B	160	HIS
1	B	162	ILE
1	B	165	VAL
1	B	166	LEU
1	B	185	ILE
1	B	189	ASN
1	B	191	ASP
1	B	192	LEU
1	B	213	ASN
1	B	223	LYS
1	B	224	GLU
1	B	226	ILE
1	B	242	PHE
1	B	256	VAL
1	B	282	MET
1	B	294	ILE
1	B	299	PHE
1	B	310	PHE
1	B	317	LEU
1	B	321	LEU
1	B	322	GLU
1	B	340	TYR
1	B	374	THR
1	B	388	ARG
1	B	389	SER

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Mol	Chain	Res	Type
1	B	391	ASP
1	B	393	VAL
1	B	407	LEU
1	B	414	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	GLN
1	A	33	GLN
1	A	39	HIS
1	A	48	ASN
1	A	58	GLN
1	A	61	GLN
1	A	82	ASN
1	A	189	ASN
1	A	277	ASN
1	A	293	ASN
1	B	30	HIS
1	B	33	GLN
1	B	39	HIS
1	B	48	ASN
1	B	62	HIS
1	B	73	HIS
1	B	82	ASN
1	B	102	GLN
1	B	104	GLN
1	B	135	ASN
1	B	189	ASN
1	B	274	GLN
1	B	277	ASN
1	B	293	ASN

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

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	413/421 (98%)	0.54	37 (8%)	12	8	55, 63, 78, 89	0
1	B	412/421 (97%)	0.85	61 (14%)	3	2	55, 64, 72, 79	0
All	All	825/842 (97%)	0.69	98 (11%)	6	4	55, 63, 74, 89	0

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	242	PHE	13.0
1	B	305	GLU	6.1
1	B	132	ILE	5.7
1	B	241	ASN	5.2
1	B	267	LYS	5.1
1	B	228	ALA	5.0
1	B	224	GLU	4.8
1	B	304	ALA	4.8
1	B	229	LEU	4.7
1	B	264	TYR	4.6
1	B	340	TYR	4.4
1	A	241	ASN	4.4
1	A	340	TYR	4.3
1	B	54	LEU	4.1
1	A	249	VAL	4.0
1	B	213	ASN	3.9
1	B	266	ALA	3.9
1	B	212	GLU	3.8
1	B	402	ASP	3.7
1	A	21	GLN	3.6
1	A	325	GLU	3.6
1	A	224	GLU	3.5
1	B	209	VAL	3.5
1	A	183	THR	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	231	ALA	3.5
1	B	250	ALA	3.5
1	A	53	ASN	3.4
1	B	246	GLN	3.4
1	A	256	VAL	3.4
1	A	51	ASP	3.4
1	B	104	GLN	3.2
1	B	312	ASP	3.2
1	B	162	ILE	3.2
1	A	4	GLN	3.1
1	B	309	ASP	3.1
1	B	263	LYS	3.1
1	A	231	ALA	3.1
1	A	139	PRO	3.1
1	B	401	GLU	3.1
1	B	202	ASN	3.0
1	B	102	GLN	3.0
1	B	50	LEU	3.0
1	B	322	GLU	2.9
1	A	248	VAL	2.9
1	B	77	LEU	2.9
1	B	409	VAL	2.8
1	B	183	THR	2.8
1	A	234	SER	2.8
1	B	20	PRO	2.8
1	A	102	GLN	2.8
1	A	131	LYS	2.8
1	A	409	VAL	2.8
1	B	307	ASP	2.7
1	B	268	ASN	2.7
1	A	309	ASP	2.7
1	A	212	GLU	2.7
1	B	133	GLU	2.7
1	B	247	LEU	2.7
1	A	252	ILE	2.6
1	B	413	SER	2.6
1	A	132	ILE	2.6
1	A	77	LEU	2.6
1	A	393	VAL	2.6
1	A	413	SER	2.6
1	B	355	ARG	2.6
1	A	372	CYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	182	GLU	2.6
1	A	265	GLY	2.6
1	B	343	GLU	2.6
1	B	23	LEU	2.5
1	B	303	ASP	2.5
1	B	421	LYS	2.5
1	B	58	GLN	2.5
1	B	325	GLU	2.5
1	B	153	ALA	2.4
1	B	344	PRO	2.4
1	B	234	SER	2.3
1	A	266	ALA	2.3
1	A	307	ASP	2.3
1	A	110	GLN	2.3
1	B	291	MET	2.3
1	A	318	ARG	2.3
1	B	100	ARG	2.3
1	B	21	GLN	2.3
1	B	53	ASN	2.2
1	B	306	TRP	2.2
1	A	76	PRO	2.2
1	A	305	GLU	2.2
1	A	370	SER	2.2
1	B	22	SER	2.1
1	B	67	LEU	2.1
1	B	195	ARG	2.1
1	A	162	ILE	2.1
1	A	292	GLY	2.1
1	B	232	GLN	2.0
1	B	272	VAL	2.0
1	B	385	MET	2.0
1	A	107	GLN	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

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.