Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:20 AM GMT

PDB ID	:	3AFE
Title	:	Crystal structure of the HsaA monooxygenase from M.tuberculosis
Authors	:	D'Angelo, I.; Lin, L.Y.; Dresen, C.; Tocheva, E.I.; Eltis, L.D.; Strynadka, N.
Deposited on	:	2010-02-28
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
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:

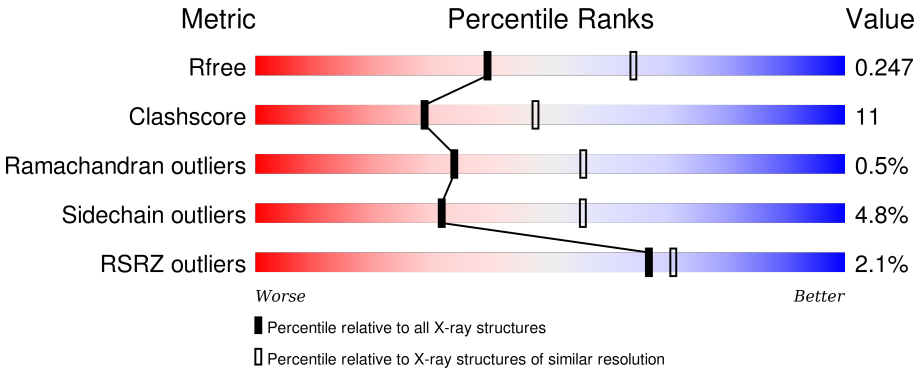
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.50 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}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (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. 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	394	79% 17%
1	B	394	73% 22%
1	C	394	5% 70% 25%
1	D	394	2% 77% 17%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12261 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 Hydroxylase, putative.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	384	Total	C	N	O	S	0	0	0
			2970	1877	537	547	9			
1	B	379	Total	C	N	O	S	0	0	0
			2935	1853	531	542	9			
1	C	381	Total	C	N	O	S	0	0	0
			2948	1860	533	546	9			
1	D	379	Total	C	N	O	S	0	0	0
			2936	1855	532	541	8			

- Molecule 2 is water.

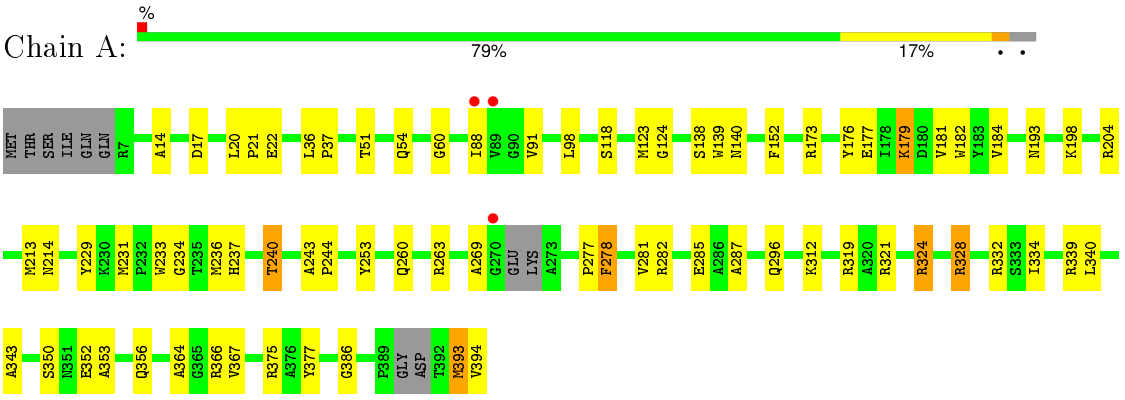
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	158	Total	O	0	0
			158	158		
2	B	114	Total	O	0	0
			114	114		
2	C	90	Total	O	0	0
			90	90		
2	D	110	Total	O	0	0
			110	110		

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.

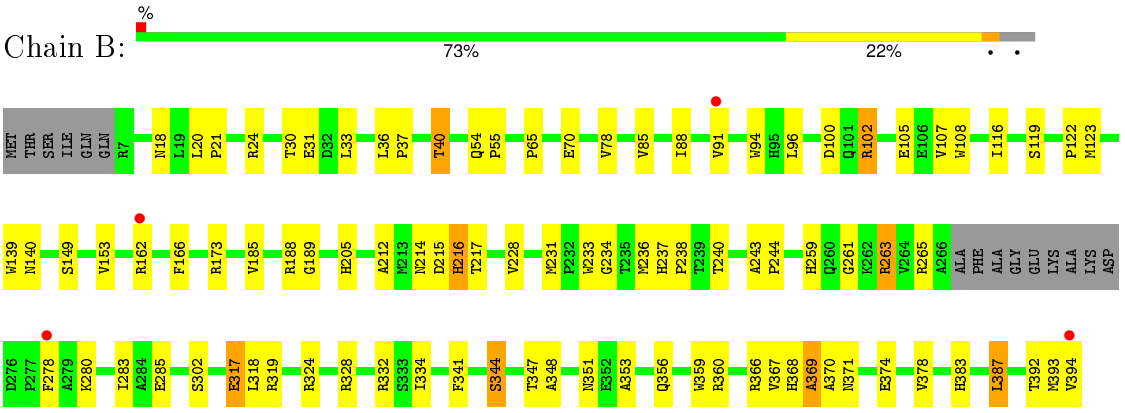
- Molecule 1: Hydroxylase, putative

Chain A:



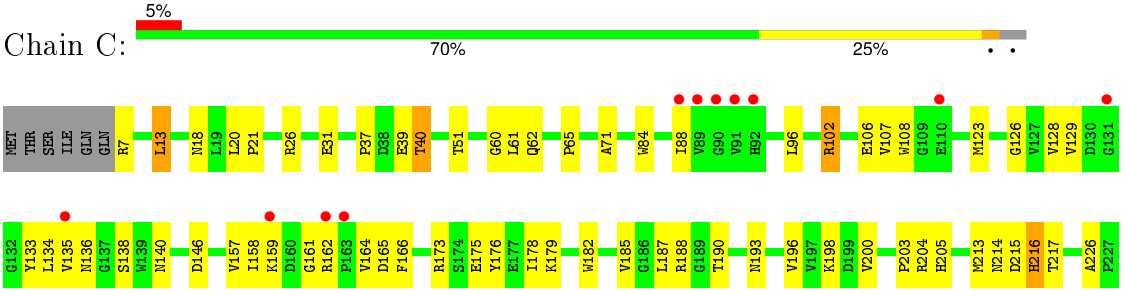
- Molecule 1: Hydroxylase, putative

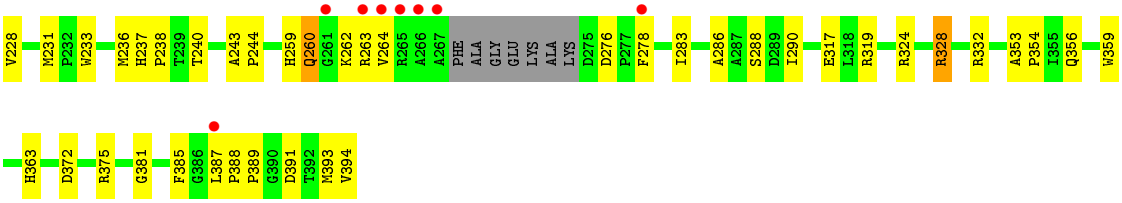
Chain B:



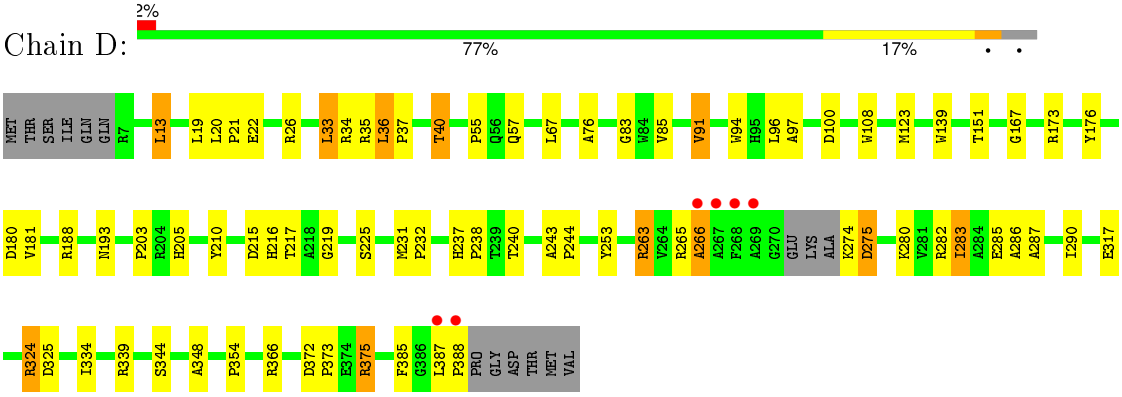
- Molecule 1: Hydroxylase, putative

Chain C:





- Molecule 1: Hydroxylase, putative



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	90.97Å 94.01Å 98.09Å 90.00° 93.94° 90.00°	Depositor
Resolution (Å)	28.80 – 2.50 28.80 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (28.80-2.50) 99.9 (28.80-2.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	2.84 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.191 , 0.258 0.180 , 0.247	Depositor DCC
R_{free} test set	2869 reflections (5.02%)	DCC
Wilson B-factor (Å^2)	38.2	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 29.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Outliers	0 of 57160 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	12261	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.62% 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	0.36	0/3047	0.54	0/4144
1	B	0.37	0/3012	0.56	0/4099
1	C	0.35	0/3025	0.50	0/4117
1	D	0.35	0/3013	0.51	0/4098
All	All	0.36	0/12097	0.53	0/16458

There are no bond length outliers.

There are no bond angle outliers.

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	2970	0	2869	63	0
1	B	2935	0	2833	78	0
1	C	2948	0	2842	80	0
1	D	2936	0	2833	54	0
2	A	158	0	0	7	1
2	B	114	0	0	6	0
2	C	90	0	0	12	0
2	D	110	0	0	5	0
All	All	12261	0	11377	266	1

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 11.

All (266) 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:26:ARG:HH11	1:C:40:THR:HG22	1.12	1.12
1:A:231:MET:HB3	1:A:236:MET:HE1	1.32	1.08
1:A:328:ARG:HH11	1:A:328:ARG:HG2	1.18	1.05
1:B:319:ARG:HH21	1:B:393:MET:HE2	1.26	0.98
1:C:237:HIS:O	1:C:240:THR:HG22	1.63	0.97
1:B:231:MET:CB	1:B:236:MET:HE1	2.01	0.91
1:B:231:MET:HB2	1:B:236:MET:HE1	1.54	0.90
1:B:368:HIS:HA	1:B:369:ALA:HB2	1.54	0.89
1:C:65:PRO:HG3	1:C:228:VAL:HG23	1.55	0.87
1:D:237:HIS:O	1:D:240:THR:HG22	1.74	0.87
1:A:236:MET:O	1:A:240:THR:HG22	1.75	0.86
1:C:214:ASN:HB3	2:C:410:HOH:O	1.75	0.85
1:A:319:ARG:HH21	1:A:393:MET:HE2	1.41	0.85
1:C:328:ARG:HH11	1:C:328:ARG:CG	1.91	0.84
1:B:319:ARG:HH21	1:B:393:MET:CE	1.91	0.84
1:A:231:MET:HB3	1:A:236:MET:CE	2.07	0.83
1:A:319:ARG:HH21	1:A:393:MET:CE	1.92	0.82
1:C:260:GLN:HE21	1:C:260:GLN:HA	1.45	0.81
1:C:328:ARG:HH11	1:C:328:ARG:HG3	1.43	0.81
1:B:88:ILE:HG23	2:B:469:HOH:O	1.79	0.81
1:A:237:HIS:O	1:A:240:THR:HG23	1.81	0.81
1:B:368:HIS:HA	1:B:369:ALA:CB	2.09	0.80
1:B:65:PRO:HG3	1:B:228:VAL:HG23	1.64	0.80
1:D:263:ARG:HH11	1:D:263:ARG:HB3	1.48	0.78
1:B:263:ARG:HG2	1:B:263:ARG:HH11	1.46	0.77
1:B:368:HIS:ND1	1:B:369:ALA:HB3	2.01	0.76
1:A:328:ARG:NH1	1:A:328:ARG:HG2	1.96	0.75
1:D:375:ARG:HG3	2:D:399:HOH:O	1.86	0.74
1:A:231:MET:CB	1:A:236:MET:HE1	2.16	0.74
1:B:185:VAL:HB	2:C:433:HOH:O	1.88	0.74
1:B:96:LEU:HD22	1:B:116:ILE:HD11	1.70	0.73
1:B:231:MET:CB	1:B:236:MET:CE	2.67	0.72
1:C:128:VAL:HG21	1:C:159:LYS:HB2	1.71	0.71
1:D:387:LEU:HB3	1:D:388:PRO:HD2	1.72	0.71
1:C:237:HIS:O	1:C:240:THR:CG2	2.40	0.69
1:C:26:ARG:NH1	1:C:40:THR:HG22	1.97	0.69
1:B:231:MET:HB3	1:B:236:MET:CE	2.22	0.68
1:B:319:ARG:NH2	1:B:393:MET:HE2	2.03	0.68
1:B:214:ASN:HB3	2:B:447:HOH:O	1.93	0.68
1:C:182:TRP:HB2	1:C:193:ASN:ND2	2.09	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:LEU:HD12	1:A:213:MET:CE	2.24	0.67
1:C:353:ALA:O	1:C:356:GLN:HG3	1.94	0.67
1:B:215:ASP:HB3	1:B:217:THR:HG23	1.76	0.66
1:A:22:GLU:HG3	2:A:397:HOH:O	1.96	0.66
1:B:263:ARG:CG	1:B:263:ARG:HH11	2.08	0.66
1:C:96:LEU:HD23	1:C:108:TRP:CH2	2.31	0.65
1:A:328:ARG:HH11	1:A:328:ARG:CG	2.00	0.65
1:B:392:THR:O	1:B:393:MET:HG2	1.96	0.65
1:D:203:PRO:HB2	1:D:205:HIS:CE1	2.33	0.64
1:A:328:ARG:HH12	1:B:285:GLU:HG2	1.62	0.64
1:D:96:LEU:HD23	1:D:108:TRP:CH2	2.33	0.64
1:D:265:ARG:O	1:D:266:ALA:HB3	1.99	0.63
1:B:237:HIS:HB3	1:B:238:PRO:HD3	1.80	0.63
1:B:100:ASP:HB2	2:B:435:HOH:O	1.97	0.63
1:C:328:ARG:CG	1:C:328:ARG:NH1	2.58	0.63
1:D:334:ILE:HD11	1:D:366:ARG:HB2	1.81	0.62
1:C:237:HIS:HB3	1:C:238:PRO:HD3	1.81	0.62
1:C:260:GLN:O	1:C:264:VAL:HG22	1.99	0.62
1:C:161:GLY:O	1:C:162:ARG:HB2	1.99	0.62
1:A:321:ARG:HD3	2:A:414:HOH:O	2.00	0.61
1:C:354:PRO:HD2	2:C:407:HOH:O	2.00	0.61
1:B:280:LYS:O	1:B:283:ILE:HG22	1.99	0.61
1:D:243:ALA:HB3	1:D:244:PRO:HD3	1.82	0.61
1:B:102:ARG:HD2	1:B:205:HIS:NE2	2.16	0.61
1:B:215:ASP:O	1:B:216:HIS:HB2	1.99	0.61
1:D:181:VAL:H	1:D:193:ASN:ND2	1.99	0.60
1:D:57:GLN:HG2	2:D:469:HOH:O	2.01	0.60
1:A:296:GLN:OE1	1:A:332:ARG:NH1	2.32	0.60
1:A:282:ARG:HD3	1:A:343:ALA:HB2	1.83	0.60
1:B:91:VAL:HG11	1:B:240:THR:HG21	1.83	0.59
1:B:368:HIS:CA	1:B:369:ALA:CB	2.80	0.59
1:B:234:GLY:HA3	1:B:393:MET:HG3	1.84	0.59
1:B:231:MET:HB2	1:B:236:MET:CE	2.28	0.59
1:B:139:TRP:CE2	1:B:153:VAL:HB	2.37	0.59
1:A:324:ARG:O	1:A:328:ARG:HB2	2.03	0.59
1:B:102:ARG:HD2	1:B:205:HIS:CD2	2.38	0.58
1:C:319:ARG:HH21	1:C:394:VAL:C	2.07	0.58
1:A:243:ALA:HB3	1:A:244:PRO:HD3	1.85	0.58
1:C:215:ASP:O	1:C:216:HIS:HB2	2.02	0.57
1:A:20:LEU:HB2	1:A:21:PRO:HD3	1.85	0.57
1:B:231:MET:HB3	1:B:236:MET:HE2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:237:HIS:HB3	1:D:238:PRO:HD3	1.85	0.57
1:A:98:LEU:HD12	1:A:213:MET:HE2	1.85	0.57
1:D:282:ARG:HD2	2:D:502:HOH:O	2.04	0.57
1:B:233:TRP:CD1	1:B:394:VAL:HG21	2.39	0.57
1:A:278:PHE:HD2	1:A:282:ARG:NH2	2.04	0.56
1:C:84:TRP:O	1:C:88:ILE:HG13	2.05	0.56
1:B:36:LEU:HD22	1:B:85:VAL:HG11	1.88	0.56
1:C:146:ASP:HA	2:C:430:HOH:O	2.05	0.56
1:A:98:LEU:HD21	1:A:229:TYR:HB3	1.86	0.56
1:C:259:HIS:HB2	2:C:472:HOH:O	2.05	0.56
1:D:354:PRO:HD2	2:D:397:HOH:O	2.06	0.56
1:A:181:VAL:H	1:A:193:ASN:ND2	2.03	0.56
1:B:356:GLN:HE22	1:B:360:ARG:HH21	1.53	0.55
1:C:106:GLU:OE1	1:C:205:HIS:NE2	2.35	0.55
1:C:26:ARG:HD2	1:C:40:THR:HG22	1.88	0.55
1:C:123:MET:HE3	1:C:140:ASN:H	1.71	0.55
1:C:215:ASP:HB3	1:C:217:THR:HG23	1.86	0.55
1:B:96:LEU:HD22	1:B:116:ILE:CD1	2.36	0.55
1:A:328:ARG:NH1	1:A:328:ARG:CG	2.64	0.54
1:B:261:GLY:O	1:B:265:ARG:HD3	2.07	0.54
1:C:372:ASP:OD2	1:C:375:ARG:HB2	2.08	0.54
1:A:98:LEU:HD12	1:A:213:MET:HE3	1.87	0.54
1:D:263:ARG:HH11	1:D:263:ARG:CB	2.19	0.54
1:A:339:ARG:HD2	2:A:421:HOH:O	2.07	0.54
1:B:107:VAL:HG12	1:B:108:TRP:CD1	2.42	0.54
1:A:233:TRP:CD1	1:A:394:VAL:HG21	2.42	0.54
1:C:62:GLN:NE2	1:C:226:ALA:HB2	2.23	0.54
1:B:344:SER:HB3	1:B:348:ALA:HB2	1.90	0.54
1:D:123:MET:HE3	1:D:139:TRP:HA	1.89	0.54
1:D:26:ARG:HH11	1:D:40:THR:HG22	1.72	0.53
1:D:215:ASP:HB3	1:D:217:THR:HG23	1.91	0.53
1:D:265:ARG:O	1:D:266:ALA:CB	2.56	0.53
1:D:96:LEU:HD23	1:D:108:TRP:CZ2	2.43	0.53
1:B:263:ARG:NH1	1:B:263:ARG:CG	2.71	0.53
1:A:253:TYR:HA	1:A:340:LEU:HD13	1.90	0.53
1:B:259:HIS:HD2	2:B:421:HOH:O	1.91	0.53
1:D:13:LEU:HD21	1:D:67:LEU:HB3	1.91	0.52
1:B:236:MET:O	1:B:240:THR:HG23	2.10	0.52
1:A:260:GLN:HE22	1:A:263:ARG:CZ	2.21	0.52
1:A:334:ILE:CD1	1:A:366:ARG:HB2	2.40	0.52
1:D:286:ALA:O	1:D:290:ILE:HG13	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:334:ILE:CD1	1:D:366:ARG:HB2	2.39	0.52
1:D:253:TYR:CE1	1:D:287:ALA:HB2	2.44	0.52
1:B:96:LEU:HD23	1:B:108:TRP:CZ2	2.45	0.51
1:C:203:PRO:HB2	1:C:205:HIS:CE1	2.46	0.51
1:D:181:VAL:H	1:D:193:ASN:HD22	1.57	0.51
1:C:96:LEU:HD23	1:C:108:TRP:CZ2	2.46	0.51
1:B:368:HIS:CG	1:B:369:ALA:HB3	2.45	0.51
1:B:96:LEU:HD23	1:B:108:TRP:CH2	2.46	0.51
1:C:204:ARG:HG3	2:C:402:HOH:O	2.11	0.51
1:C:215:ASP:CB	1:C:217:THR:HG23	2.42	0.50
1:B:319:ARG:HE	1:B:393:MET:HE1	1.76	0.50
1:C:328:ARG:O	1:C:332:ARG:HG2	2.11	0.50
1:C:288:SER:HB2	1:D:324:ARG:HD2	1.94	0.50
1:C:166:PHE:HB3	2:C:418:HOH:O	2.12	0.50
1:B:359:TRP:CZ2	1:C:359:TRP:CZ2	2.99	0.49
1:C:173:ARG:HA	1:C:176:TYR:CZ	2.47	0.49
1:B:243:ALA:HB3	1:B:244:PRO:HD3	1.94	0.49
1:C:26:ARG:HD2	1:C:40:THR:CG2	2.42	0.48
1:A:173:ARG:HA	1:A:176:TYR:CE2	2.49	0.48
1:D:36:LEU:HD22	1:D:85:VAL:HG11	1.95	0.48
1:D:34:ARG:HA	1:D:188:ARG:O	2.12	0.48
1:B:185:VAL:O	1:B:360:ARG:HD2	2.13	0.48
1:C:31:GLU:HG3	1:C:188:ARG:HB2	1.94	0.48
1:A:364:ALA:O	1:A:367:VAL:HG22	2.13	0.48
1:A:51:THR:HB	1:A:60:GLY:HA2	1.96	0.48
1:C:166:PHE:CB	2:C:418:HOH:O	2.61	0.48
1:C:39:GLU:HB2	2:C:455:HOH:O	2.14	0.48
1:D:167:GLY:HA2	1:D:210:TYR:CD1	2.49	0.48
1:A:173:ARG:NH2	2:A:442:HOH:O	2.47	0.47
1:C:381:GLY:HA3	1:D:280:LYS:HB3	1.95	0.47
1:C:126:GLY:CA	1:C:135:VAL:HG22	2.44	0.47
1:B:280:LYS:O	1:B:283:ILE:CG2	2.62	0.47
1:C:136:ASN:OD1	1:C:198:LYS:HA	2.14	0.47
1:D:100:ASP:HB3	1:D:219:GLY:HA3	1.97	0.47
1:C:283:ILE:HD12	1:D:385:PHE:CZ	2.49	0.47
1:A:334:ILE:HD11	1:A:366:ARG:HB2	1.97	0.47
1:C:178:ILE:HD13	2:C:430:HOH:O	2.15	0.47
1:A:182:TRP:HB2	1:A:193:ASN:ND2	2.30	0.47
1:B:317:GLU:HB2	1:B:383:HIS:CE1	2.50	0.46
1:B:334:ILE:CD1	1:B:366:ARG:HB2	2.46	0.46
1:B:91:VAL:O	1:B:94:TRP:HB3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:341:PHE:HE1	1:B:356:GLN:HB3	1.80	0.46
1:C:175:GLU:O	1:C:200:VAL:HG21	2.15	0.46
1:A:277:PRO:O	1:A:281:VAL:HG23	2.15	0.46
1:C:328:ARG:HH12	1:D:285:GLU:HA	1.80	0.46
1:C:107:VAL:HG12	1:C:108:TRP:CD1	2.51	0.46
1:C:102:ARG:O	1:C:106:GLU:HG3	2.14	0.46
1:C:385:PHE:CZ	1:D:283:ILE:HD13	2.51	0.46
1:B:31:GLU:HG3	1:B:188:ARG:HB2	1.98	0.46
1:B:356:GLN:NE2	1:B:360:ARG:HH21	2.14	0.46
1:B:20:LEU:HB2	1:B:21:PRO:HD3	1.97	0.46
1:A:319:ARG:NH2	1:A:393:MET:HE2	2.20	0.45
1:A:312:LYS:HB3	1:A:312:LYS:HE2	1.73	0.45
1:A:253:TYR:CE1	1:A:287:ALA:HB2	2.52	0.45
1:C:13:LEU:HD12	1:C:13:LEU:HA	1.64	0.45
1:B:37:PRO:HD2	1:B:40:THR:CG2	2.47	0.45
1:D:344:SER:HB3	1:D:348:ALA:HB2	1.98	0.45
1:C:138:SER:OG	1:C:196:VAL:HG22	2.17	0.45
1:D:167:GLY:HA2	1:D:210:TYR:CE1	2.52	0.45
1:C:231:MET:CB	1:C:236:MET:HE1	2.46	0.45
1:B:374:GLU:O	1:B:378:VAL:HG23	2.17	0.45
1:B:18:ASN:O	1:B:21:PRO:HD2	2.17	0.44
1:C:20:LEU:HB2	1:C:21:PRO:HD3	1.99	0.44
1:C:243:ALA:HB3	1:C:244:PRO:HD3	1.98	0.44
1:C:286:ALA:O	1:C:290:ILE:HG13	2.16	0.44
1:A:233:TRP:NE1	1:A:394:VAL:HG21	2.32	0.44
1:C:276:ASP:HB3	2:C:434:HOH:O	2.16	0.44
1:C:37:PRO:HB2	1:C:40:THR:HG23	1.99	0.44
1:A:328:ARG:HG2	1:A:377:TYR:OH	2.16	0.44
1:A:173:ARG:NH1	2:A:518:HOH:O	2.44	0.44
1:A:14:ALA:O	1:A:17:ASP:HB2	2.18	0.44
1:A:179:LYS:O	1:A:193:ASN:HB3	2.17	0.44
1:D:324:ARG:HG3	1:D:325:ASP:N	2.32	0.44
1:D:215:ASP:O	1:D:216:HIS:HB2	2.18	0.44
1:B:328:ARG:HD3	2:B:451:HOH:O	2.18	0.44
1:C:236:MET:HE3	1:C:236:MET:HB2	1.70	0.43
1:B:122:PRO:HB3	1:B:166:PHE:CZ	2.53	0.43
1:D:180:ASP:HA	1:D:193:ASN:ND2	2.33	0.43
1:C:231:MET:HB3	1:C:236:MET:CE	2.47	0.43
1:B:123:MET:HE3	1:B:140:ASN:H	1.83	0.43
1:D:387:LEU:CB	1:D:388:PRO:HD2	2.46	0.43
1:B:317:GLU:HG3	1:B:318:LEU:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:231:MET:CB	1:C:236:MET:CE	2.96	0.43
1:C:332:ARG:NH1	2:C:408:HOH:O	2.04	0.43
1:C:185:VAL:O	1:C:185:VAL:HG22	2.19	0.43
1:C:133:TYR:HE1	1:C:157:VAL:CG1	2.31	0.43
1:B:65:PRO:HG3	1:B:228:VAL:CG2	2.41	0.43
1:D:20:LEU:HB2	1:D:21:PRO:HD3	1.99	0.43
1:C:385:PHE:CZ	1:D:283:ILE:CD1	3.02	0.43
1:A:386:GLY:HA2	2:A:476:HOH:O	2.19	0.43
1:C:260:GLN:NE2	1:C:260:GLN:HA	2.23	0.43
1:C:128:VAL:CG2	1:C:159:LYS:HB2	2.45	0.43
1:D:36:LEU:HA	1:D:37:PRO:HD3	1.93	0.43
1:D:274:LYS:O	1:D:275:ASP:HB3	2.19	0.43
1:A:236:MET:HB2	1:A:236:MET:HE3	1.58	0.42
1:A:182:TRP:CZ2	1:A:184:VAL:HG21	2.53	0.42
1:A:123:MET:HE3	1:A:140:ASN:H	1.83	0.42
1:A:177:GLU:OE2	1:A:179:LYS:HE3	2.19	0.42
1:D:19:LEU:O	1:D:22:GLU:HG2	2.19	0.42
1:C:388:PRO:HA	1:C:389:PRO:HD3	1.87	0.42
1:B:280:LYS:C	1:B:283:ILE:HG22	2.39	0.42
1:C:187:LEU:HB3	1:C:190:THR:CG2	2.49	0.42
1:A:36:LEU:HA	1:A:37:PRO:HD3	1.93	0.42
1:B:36:LEU:HA	1:B:37:PRO:HD3	1.95	0.42
1:C:262:LYS:HG3	1:C:263:ARG:H	1.84	0.42
1:B:212:ALA:HA	1:B:215:ASP:HB2	2.00	0.42
1:D:91:VAL:O	1:D:94:TRP:HB3	2.20	0.42
1:D:151:THR:HG22	1:D:176:TYR:CE2	2.54	0.42
1:C:126:GLY:HA2	1:C:135:VAL:HG22	2.01	0.42
1:A:124:GLY:HA3	1:A:139:TRP:CZ2	2.54	0.42
1:D:372:ASP:HA	1:D:373:PRO:HD3	1.88	0.42
1:D:55:PRO:HG3	1:D:97:ALA:HB2	2.01	0.42
1:B:328:ARG:O	1:B:332:ARG:HG3	2.20	0.41
1:D:339:ARG:NE	2:D:418:HOH:O	2.53	0.41
1:A:54:GLN:HB3	1:A:60:GLY:HA3	2.00	0.41
1:C:213:MET:HE2	1:C:233:TRP:HB2	2.03	0.41
1:B:70:GLU:HB2	2:B:418:HOH:O	2.21	0.41
1:A:285:GLU:HB3	1:B:328:ARG:HH21	1.85	0.41
1:A:88:ILE:O	1:A:91:VAL:HG12	2.20	0.41
1:B:353:ALA:O	1:B:356:GLN:HG3	2.20	0.41
1:C:61:LEU:O	1:C:62:GLN:C	2.58	0.41
1:C:18:ASN:HA	1:C:18:ASN:HD22	1.66	0.41
1:A:234:GLY:HA3	1:A:393:MET:SD	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:ARG:CD	1:A:343:ALA:HB2	2.48	0.41
1:B:387:LEU:HD12	1:B:387:LEU:HA	1.72	0.41
1:D:76:ALA:HB2	1:D:83:GLY:HA3	2.03	0.41
1:B:24:ARG:HB2	1:B:78:VAL:HB	2.03	0.41
1:C:158:ILE:HG13	1:C:162:ARG:O	2.21	0.41
1:A:181:VAL:H	1:A:193:ASN:HD22	1.67	0.41
1:D:33:LEU:O	1:D:34:ARG:HB2	2.21	0.41
1:B:30:THR:HG22	1:B:189:GLY:HA3	2.03	0.41
1:A:353:ALA:O	1:A:356:GLN:HG3	2.20	0.41
1:A:277:PRO:HD2	2:A:475:HOH:O	2.20	0.41
1:D:231:MET:HA	1:D:232:PRO:HD3	1.92	0.41
1:B:54:GLN:HA	1:B:55:PRO:HD3	1.95	0.41
1:C:51:THR:HB	1:C:60:GLY:HA2	2.03	0.41
1:A:350:SER:OG	1:A:352:GLU:HG2	2.20	0.41
1:A:118:SER:HA	1:A:152:PHE:O	2.22	0.40
1:A:237:HIS:HA	1:A:240:THR:CG2	2.50	0.40
1:B:119:SER:OG	1:B:139:TRP:HB3	2.20	0.40
1:D:26:ARG:HH11	1:D:40:THR:CG2	2.34	0.40
1:C:359:TRP:O	1:C:363:HIS:HD2	2.05	0.40
1:B:368:HIS:O	1:B:371:ASN:HB2	2.20	0.40
1:C:13:LEU:HD11	1:C:71:ALA:HB2	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:485:HOH:O	2:A:551:HOH:O[2_645]	2.14	0.06

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	378/394 (96%)	371 (98%)	5 (1%)	2 (0%)	34	55
1	B	375/394 (95%)	357 (95%)	15 (4%)	3 (1%)	24	41
1	C	377/394 (96%)	356 (94%)	20 (5%)	1 (0%)	46	68
1	D	375/394 (95%)	360 (96%)	13 (4%)	2 (0%)	34	55
All	All	1505/1576 (96%)	1444 (96%)	53 (4%)	8 (0%)	34	55

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	351	ASN
1	B	369	ALA
1	D	266	ALA
1	A	269	ALA
1	C	391	ASP
1	A	393	MET
1	B	370	ALA
1	D	275	ASP

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	301/310 (97%)	291 (97%)	10 (3%)	45	73
1	B	299/310 (96%)	282 (94%)	17 (6%)	25	46
1	C	300/310 (97%)	283 (94%)	17 (6%)	25	46
1	D	297/310 (96%)	284 (96%)	13 (4%)	35	60
All	All	1197/1240 (96%)	1140 (95%)	57 (5%)	31	55

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	138	SER
1	A	179	LYS
1	A	198	LYS

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Mol	Chain	Res	Type
1	A	204	ARG
1	A	214	ASN
1	A	240	THR
1	A	278	PHE
1	A	324	ARG
1	A	328	ARG
1	A	375	ARG
1	B	33	LEU
1	B	40	THR
1	B	102	ARG
1	B	105	GLU
1	B	149	SER
1	B	162	ARG
1	B	173	ARG
1	B	216	HIS
1	B	263	ARG
1	B	278	PHE
1	B	302	SER
1	B	317	GLU
1	B	324	ARG
1	B	344	SER
1	B	347	THR
1	B	367	VAL
1	B	387	LEU
1	C	7	ARG
1	C	13	LEU
1	C	40	THR
1	C	102	ARG
1	C	129	VAL
1	C	134	LEU
1	C	164	VAL
1	C	165	ASP
1	C	179	LYS
1	C	216	HIS
1	C	260	GLN
1	C	278	PHE
1	C	317	GLU
1	C	324	ARG
1	C	328	ARG
1	C	387	LEU
1	C	393	MET
1	D	13	LEU

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Mol	Chain	Res	Type
1	D	33	LEU
1	D	35	ARG
1	D	36	LEU
1	D	40	THR
1	D	91	VAL
1	D	173	ARG
1	D	225	SER
1	D	263	ARG
1	D	283	ILE
1	D	317	GLU
1	D	324	ARG
1	D	375	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	193	ASN
1	A	260	GLN
1	A	300	ASN
1	A	371	ASN
1	B	193	ASN
1	B	260	GLN
1	B	300	ASN
1	B	356	GLN
1	B	383	HIS
1	C	18	ASN
1	C	193	ASN
1	C	260	GLN
1	C	371	ASN
1	D	18	ASN
1	D	193	ASN
1	D	214	ASN
1	D	371	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	384/394 (97%)	-0.37	3 (0%) 87 89	23, 32, 51, 76	1 (0%)
1	B	379/394 (96%)	-0.32	4 (1%) 82 84	24, 35, 57, 77	1 (0%)
1	C	381/394 (96%)	0.04	19 (4%) 32 37	28, 45, 69, 89	1 (0%)
1	D	379/394 (96%)	-0.26	6 (1%) 74 78	23, 36, 60, 93	1 (0%)
All	All	1523/1576 (96%)	-0.23	32 (2%) 67 71	23, 37, 63, 93	4 (0%)

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	268	PHE	4.2
1	D	269	ALA	4.0
1	B	394	VAL	3.8
1	C	88	ILE	3.7
1	C	266	ALA	3.5
1	C	89	VAL	3.3
1	D	266	ALA	3.2
1	C	90	GLY	3.1
1	C	131	GLY	3.1
1	D	267	ALA	3.0
1	C	162	ARG	2.8
1	C	91	VAL	2.8
1	C	267	ALA	2.8
1	A	89	VAL	2.8
1	D	388	PRO	2.5
1	C	159	LYS	2.5
1	C	110	GLU	2.5
1	B	278	PHE	2.4
1	C	264	VAL	2.4
1	C	263	ARG	2.4
1	C	135	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	265	ARG	2.3
1	C	278	PHE	2.2
1	A	88	ILE	2.2
1	A	270	GLY	2.2
1	B	162	ARG	2.2
1	C	387	LEU	2.1
1	D	387	LEU	2.1
1	C	261	GLY	2.1
1	C	92	HIS	2.1
1	B	91	VAL	2.0
1	C	163	PRO	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.