Full wwPDB X-ray Structure Validation Report

Feb 19, 2016 – 07:08 PM GMT

PDB ID	:	4RAE
Title	:	Crystal structure of Rv1600 encoded aminotransferase from Mycobacterium tuberculosis
Authors	:	Nasir, N.; Anant, A.; Vyas, R.; Biswal, B.K.
Deposited on	:	2014-09-10
Resolution	:	2.59 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:

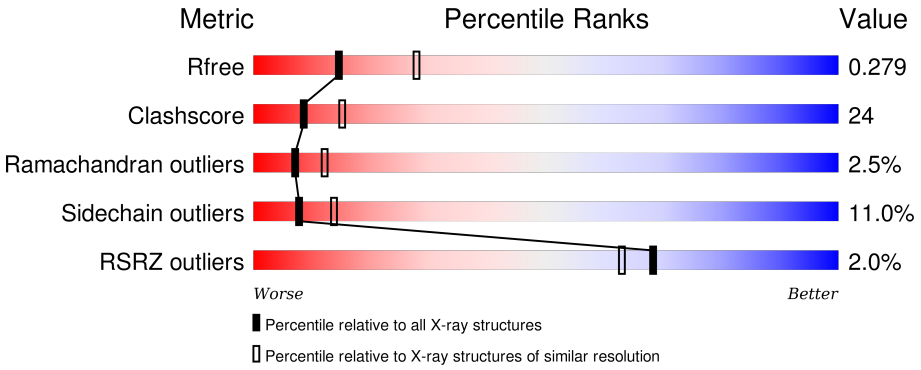
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

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 2.59 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	394	% 55% 31% 8% 7%
1	B	394	3% 56% 31% 6% 7%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 5530 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 Histidinol-phosphate aminotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	367	Total	C	N	O	S	0	0	0
			2772	1753	488	526	5			
1	B	365	Total	C	N	O	S	0	0	0
			2758	1743	486	524	5			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	EXPRESSION TAG	UNP I6XYD8
A	381	LYS	-	EXPRESSION TAG	UNP I6XYD8
A	382	LEU	-	EXPRESSION TAG	UNP I6XYD8
A	383	ALA	-	EXPRESSION TAG	UNP I6XYD8
A	384	ALA	-	EXPRESSION TAG	UNP I6XYD8
A	385	ALA	-	EXPRESSION TAG	UNP I6XYD8
A	386	LEU	-	EXPRESSION TAG	UNP I6XYD8
A	387	GLU	-	EXPRESSION TAG	UNP I6XYD8
A	388	HIS	-	EXPRESSION TAG	UNP I6XYD8
A	389	HIS	-	EXPRESSION TAG	UNP I6XYD8
A	390	HIS	-	EXPRESSION TAG	UNP I6XYD8
A	391	HIS	-	EXPRESSION TAG	UNP I6XYD8
A	392	HIS	-	EXPRESSION TAG	UNP I6XYD8
A	393	HIS	-	EXPRESSION TAG	UNP I6XYD8
B	0	MET	-	EXPRESSION TAG	UNP I6XYD8
B	381	LYS	-	EXPRESSION TAG	UNP I6XYD8
B	382	LEU	-	EXPRESSION TAG	UNP I6XYD8
B	383	ALA	-	EXPRESSION TAG	UNP I6XYD8
B	384	ALA	-	EXPRESSION TAG	UNP I6XYD8
B	385	ALA	-	EXPRESSION TAG	UNP I6XYD8
B	386	LEU	-	EXPRESSION TAG	UNP I6XYD8
B	387	GLU	-	EXPRESSION TAG	UNP I6XYD8
B	388	HIS	-	EXPRESSION TAG	UNP I6XYD8
B	389	HIS	-	EXPRESSION TAG	UNP I6XYD8
B	390	HIS	-	EXPRESSION TAG	UNP I6XYD8

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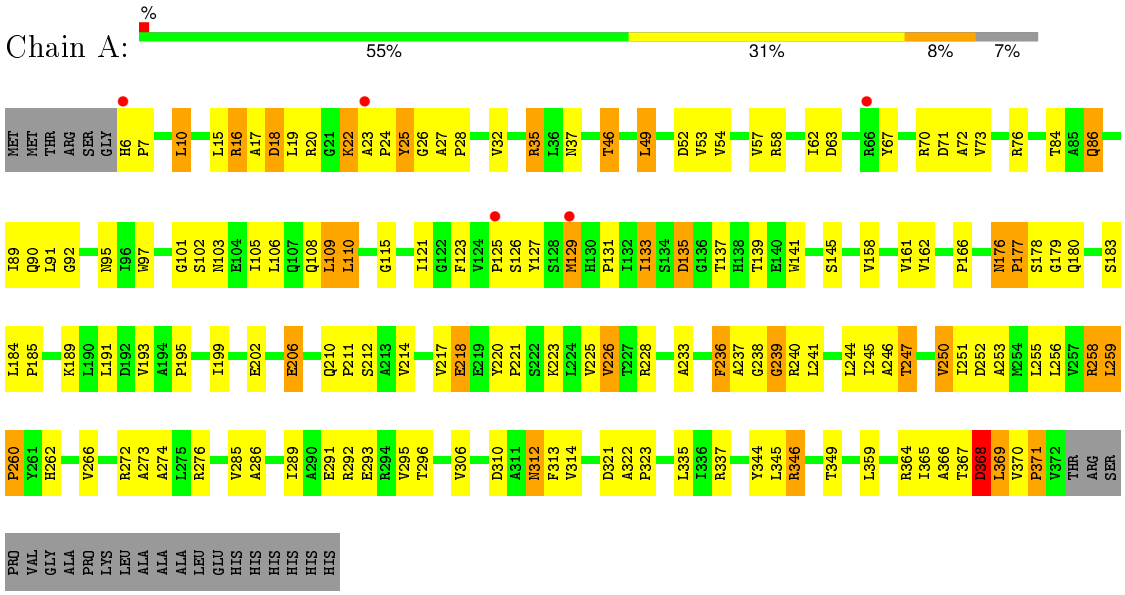
Chain	Residue	Modelled	Actual	Comment	Reference
B	391	HIS	-	EXPRESSION TAG	UNP I6XYD8
B	392	HIS	-	EXPRESSION TAG	UNP I6XYD8
B	393	HIS	-	EXPRESSION TAG	UNP I6XYD8

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.

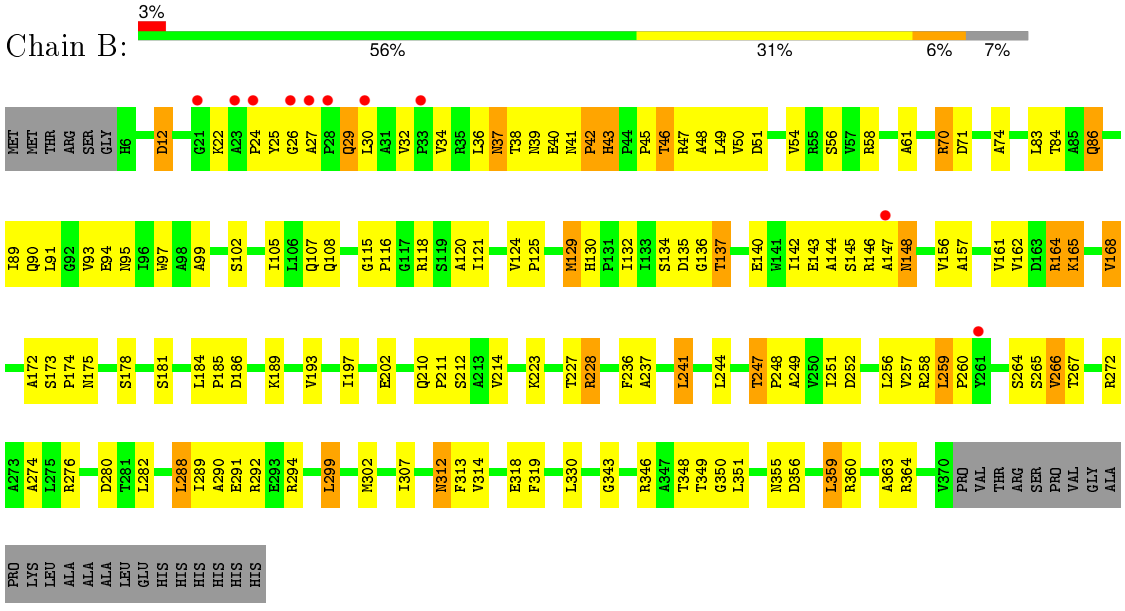
- Molecule 1: Histidinol-phosphate aminotransferase

Chain A:



- Molecule 1: Histidinol-phosphate aminotransferase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	159.94Å 159.94Å 110.32Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	31.52 – 2.59 31.52 – 2.59	Depositor EDS
% Data completeness (in resolution range)	93.9 (31.52-2.59) 94.0 (31.52-2.59)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.16	Depositor
$< I/\sigma(I) >$ [1]	1.60 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.239 , 0.279 0.237 , 0.279	Depositor DCC
R_{free} test set	2406 reflections (5.31%)	DCC
Wilson B-factor (Å^2)	36.8	Xtriage
Anisotropy	0.198	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 10.6	EDS
Estimated twinning fraction	0.059 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.24$	Xtriage
Outliers	0 of 47702 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	5530	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% 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	0.47	0/2831	0.70	0/3871
1	B	0.47	0/2816	0.68	0/3849
All	All	0.47	0/5647	0.69	0/7720

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	2772	0	2763	151	0
1	B	2758	0	2747	133	0
All	All	5530	0	5510	263	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 (263) 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:162:VAL:HG13	1:A:193:VAL:CG1	1.70	1.21
1:A:346:ARG:HH11	1:A:346:ARG:HG2	1.02	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:ASP:HB2	1:A:137:THR:HG22	1.30	1.14
1:A:259:LEU:CD1	1:A:262:HIS:HB3	1.82	1.10
1:A:123:PHE:O	1:A:126:SER:HB2	1.50	1.07
1:A:259:LEU:HD12	1:A:262:HIS:HB3	1.03	1.01
1:A:162:VAL:HG13	1:A:193:VAL:HG11	1.37	1.01
1:A:110:LEU:HG	1:A:137:THR:HG21	1.45	0.98
1:B:264:SER:HB3	1:B:267:THR:OG1	1.65	0.96
1:A:259:LEU:HD12	1:A:262:HIS:CB	1.94	0.96
1:A:125:PRO:HD3	1:A:145:SER:HB3	1.48	0.95
1:A:135:ASP:CB	1:A:137:THR:HG22	1.99	0.92
1:A:16:ARG:HA	1:B:118:ARG:NH2	1.85	0.90
1:A:162:VAL:CG1	1:A:193:VAL:CG1	2.51	0.87
1:A:210:GLN:HG2	1:A:211:PRO:HD2	1.56	0.86
1:A:259:LEU:CD1	1:A:262:HIS:CB	2.54	0.85
1:B:84:THR:HG23	1:B:90:GLN:HA	1.59	0.84
1:B:40:GLU:HG2	1:B:41:ASN:H	1.43	0.83
1:A:346:ARG:HG2	1:A:346:ARG:NH1	1.81	0.83
1:A:58:ARG:NH2	1:B:54:VAL:HG21	1.94	0.82
1:A:365:ILE:O	1:A:368:ASP:HB2	1.80	0.80
1:B:135:ASP:OD1	1:B:137:THR:CG2	2.31	0.79
1:A:321:ASP:OD2	1:A:323:PRO:HD2	1.81	0.78
1:A:312:ASN:HD22	1:A:312:ASN:H	1.32	0.78
1:A:10:LEU:H	1:A:10:LEU:HD12	1.52	0.75
1:B:135:ASP:OD1	1:B:137:THR:HG22	1.86	0.75
1:A:296:THR:HG23	1:A:306:VAL:HG11	1.68	0.75
1:A:129:MET:HE3	1:B:260:PRO:HD3	1.70	0.73
1:B:202:GLU:OE1	1:B:228:ARG:NH1	2.21	0.73
1:A:97:TRP:HE1	1:A:108:GLN:HE22	1.35	0.73
1:A:162:VAL:HG13	1:A:193:VAL:HG13	1.70	0.73
1:A:217:VAL:HG23	1:A:218:GLU:N	2.04	0.72
1:B:247:THR:HG22	1:B:248:PRO:HD2	1.70	0.72
1:A:312:ASN:O	1:A:349:THR:HG22	1.89	0.72
1:B:37:ASN:HD22	1:B:37:ASN:H	1.38	0.71
1:A:176:ASN:O	1:A:177:PRO:C	2.27	0.71
1:B:29:GLN:O	1:B:30:LEU:HD23	1.89	0.71
1:A:162:VAL:CG1	1:A:193:VAL:HG13	2.22	0.70
1:A:16:ARG:NH2	1:B:116:PRO:O	2.24	0.70
1:B:32:VAL:HG23	1:B:32:VAL:O	1.92	0.69
1:A:70:ARG:CZ	1:B:30:LEU:HG	2.22	0.69
1:A:52:ASP:OD2	1:A:276:ARG:NH1	2.26	0.68
1:B:289:ILE:HD12	1:B:290:ALA:N	2.08	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:VAL:HG11	1:B:58:ARG:NH2	2.10	0.67
1:A:158:VAL:HA	1:A:161:VAL:HG12	1.76	0.67
1:B:299:LEU:HD13	1:B:359:LEU:CD1	2.25	0.66
1:B:264:SER:HB3	1:B:267:THR:HG1	1.61	0.66
1:A:92:GLY:H	1:A:95:ASN:HD22	1.43	0.65
1:A:183:SER:HA	1:A:210:GLN:HE22	1.61	0.65
1:B:162:VAL:O	1:B:165:LYS:HE3	1.97	0.65
1:A:23:ALA:HB1	1:A:24:PRO:HA	1.78	0.65
1:B:288:LEU:HD23	1:B:349:THR:HG22	1.79	0.65
1:A:176:ASN:O	1:A:178:SER:N	2.30	0.64
1:A:212:SER:OG	1:A:214:VAL:HG13	1.97	0.64
1:A:346:ARG:CG	1:A:346:ARG:HH11	1.94	0.64
1:A:71:ASP:OD1	1:A:258:ARG:NH2	2.30	0.64
1:A:291:GLU:O	1:A:295:VAL:HG23	1.97	0.64
1:B:40:GLU:CG	1:B:41:ASN:H	2.11	0.64
1:A:237:ALA:HB3	1:A:274:ALA:HB2	1.79	0.64
1:B:144:ALA:HB1	1:B:156:VAL:CG2	2.27	0.63
1:A:217:VAL:HG23	1:A:218:GLU:H	1.64	0.62
1:A:206:GLU:HG3	1:A:233:ALA:HB2	1.79	0.62
1:B:319:PHE:O	1:B:343:GLY:HA2	1.98	0.62
1:A:6:HIS:N	1:A:7:PRO:HD2	2.15	0.62
1:A:70:ARG:NH1	1:B:27:ALA:O	2.32	0.61
1:A:115:GLY:H	1:A:137:THR:HB	1.65	0.61
1:A:366:ALA:O	1:A:368:ASP:N	2.34	0.61
1:A:70:ARG:NH2	1:B:30:LEU:HG	2.15	0.61
1:A:101:GLY:HA3	1:A:240:ARG:CZ	2.30	0.60
1:B:42:PRO:O	1:B:43:HIS:C	2.40	0.60
1:B:94:GLU:O	1:B:248:PRO:HA	2.02	0.60
1:A:252:ASP:HA	1:A:255:LEU:HD12	1.83	0.60
1:B:299:LEU:HD13	1:B:359:LEU:HD12	1.83	0.60
1:A:272:ARG:HG3	1:A:272:ARG:HH11	1.67	0.60
1:A:141:TRP:HE1	1:B:134:SER:HB3	1.67	0.59
1:A:312:ASN:C	1:A:349:THR:HG22	2.22	0.59
1:B:120:ALA:HB2	1:B:168:VAL:HG13	1.82	0.59
1:A:84:THR:HG23	1:A:90:GLN:HA	1.83	0.59
1:B:227:THR:HG22	1:B:228:ARG:N	2.17	0.59
1:B:259:LEU:HB3	1:B:260:PRO:HD2	1.85	0.59
1:B:157:ALA:O	1:B:161:VAL:HG23	2.03	0.59
1:A:313:PHE:CD1	1:A:346:ARG:HD2	2.37	0.58
1:B:99:ALA:HB3	1:B:105:ILE:HG23	1.85	0.58
1:B:144:ALA:HB1	1:B:156:VAL:HG21	1.84	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:LEU:C	1:A:244:LEU:HD12	2.23	0.57
1:A:241:LEU:C	1:A:241:LEU:HD23	2.24	0.57
1:A:86:GLN:HE21	1:A:86:GLN:HA	1.68	0.57
1:B:40:GLU:HG2	1:B:41:ASN:N	2.17	0.57
1:A:184:LEU:N	1:A:185:PRO:HD2	2.20	0.57
1:B:84:THR:CG2	1:B:90:GLN:HA	2.34	0.56
1:B:236:PHE:O	1:B:237:ALA:HB3	2.05	0.56
1:A:46:THR:HB	1:A:49:LEU:H	1.70	0.56
1:B:299:LEU:CD1	1:B:359:LEU:HD12	2.36	0.56
1:A:189:LYS:O	1:A:193:VAL:HG23	2.05	0.56
1:A:312:ASN:HD22	1:A:312:ASN:N	2.00	0.56
1:B:74:ALA:HB3	1:B:272:ARG:HH21	1.71	0.56
1:A:133:ILE:O	1:B:132:ILE:HG13	2.05	0.56
1:A:97:TRP:HE1	1:A:108:GLN:NE2	2.04	0.56
1:A:20:ARG:HD3	1:A:20:ARG:C	2.27	0.55
1:B:264:SER:HB3	1:B:267:THR:CB	2.36	0.55
1:A:322:ALA:HB3	1:A:323:PRO:HD3	1.89	0.55
1:A:273:ALA:HA	1:A:276:ARG:CZ	2.37	0.55
1:B:36:LEU:O	1:B:348:THR:HB	2.07	0.55
1:B:121:ILE:HD12	1:B:142:ILE:HD13	1.89	0.55
1:A:246:ALA:HB3	1:A:250:VAL:CG2	2.37	0.54
1:B:289:ILE:HD12	1:B:290:ALA:H	1.73	0.54
1:A:37:ASN:HD22	1:B:70:ARG:HH12	1.54	0.54
1:A:52:ASP:CG	1:A:276:ARG:HH12	2.11	0.54
1:A:103:ASN:HB2	1:A:240:ARG:HH21	1.73	0.54
1:A:135:ASP:HB2	1:A:137:THR:CG2	2.22	0.54
1:B:74:ALA:HB3	1:B:272:ARG:HE	1.73	0.54
1:B:99:ALA:HB3	1:B:105:ILE:CG2	2.38	0.54
1:A:293:GLU:HA	1:A:293:GLU:OE2	2.07	0.53
1:B:294:ARG:NH2	1:B:356:ASP:OD2	2.41	0.53
1:A:366:ALA:O	1:A:369:LEU:CD1	2.57	0.53
1:B:37:ASN:HD22	1:B:37:ASN:N	2.05	0.53
1:A:131:PRO:HB2	1:A:133:ILE:HD11	1.90	0.53
1:B:125:PRO:HA	1:B:145:SER:HB3	1.91	0.52
1:B:24:PRO:O	1:B:26:GLY:N	2.36	0.52
1:A:202:GLU:OE1	1:A:228:ARG:NH1	2.42	0.52
1:B:74:ALA:CB	1:B:272:ARG:HE	2.22	0.52
1:B:312:ASN:H	1:B:312:ASN:HD22	1.56	0.52
1:B:46:THR:HB	1:B:49:LEU:H	1.75	0.52
1:A:251:ILE:HD12	1:A:251:ILE:N	2.25	0.52
1:A:20:ARG:HD3	1:A:20:ARG:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:TYR:O	1:A:345:LEU:HD12	2.10	0.51
1:B:186:ASP:HA	1:B:189:LYS:HD3	1.91	0.51
1:A:221:PRO:O	1:A:247:THR:HG21	2.11	0.51
1:A:125:PRO:HD3	1:A:145:SER:CB	2.31	0.51
1:A:246:ALA:HB3	1:A:250:VAL:HG22	1.93	0.51
1:B:280:ASP:C	1:B:282:LEU:H	2.15	0.51
1:B:350:GLY:H	1:B:355:ASN:HD21	1.59	0.50
1:A:214:VAL:O	1:A:217:VAL:HG22	2.11	0.50
1:A:217:VAL:CG2	1:A:218:GLU:N	2.73	0.50
1:B:32:VAL:O	1:B:32:VAL:CG2	2.58	0.50
1:A:337:ARG:NH2	1:B:260:PRO:HA	2.27	0.50
1:B:30:LEU:C	1:B:32:VAL:H	2.14	0.50
1:A:214:VAL:HG12	1:A:226:VAL:HG11	1.92	0.50
1:B:124:VAL:O	1:B:143:GLU:HA	2.12	0.50
1:A:129:MET:HG3	1:B:107:GLN:OE1	2.11	0.50
1:B:37:ASN:ND2	1:B:38:THR:N	2.60	0.50
1:A:238:GLY:O	1:A:239:GLY:C	2.50	0.50
1:A:58:ARG:NH1	1:B:51:ASP:OD1	2.39	0.49
1:B:227:THR:CG2	1:B:228:ARG:N	2.74	0.49
1:B:178:SER:HB2	1:B:307:ILE:HG21	1.93	0.49
1:A:53:VAL:HG11	1:A:236:PHE:CE2	2.47	0.49
1:B:94:GLU:N	1:B:94:GLU:OE2	2.39	0.49
1:A:6:HIS:N	1:A:7:PRO:CD	2.76	0.49
1:A:49:LEU:HD12	1:A:49:LEU:C	2.33	0.49
1:A:49:LEU:HD12	1:A:49:LEU:O	2.11	0.49
1:B:49:LEU:HD11	1:B:274:ALA:HA	1.94	0.49
1:A:22:LYS:HE3	1:A:22:LYS:N	2.28	0.49
1:A:71:ASP:O	1:A:76:ARG:HD3	2.14	0.48
1:A:158:VAL:O	1:A:162:VAL:HG22	2.14	0.48
1:A:259:LEU:HD11	1:A:262:HIS:CB	2.40	0.48
1:B:129:MET:HA	1:B:129:MET:CE	2.44	0.48
1:B:247:THR:CG2	1:B:248:PRO:HD2	2.43	0.48
1:B:146:ARG:O	1:B:148:ASN:N	2.47	0.48
1:B:256:LEU:HD12	1:B:257:VAL:HG13	1.95	0.48
1:A:199:ILE:HA	1:A:225:VAL:O	2.14	0.48
1:A:289:ILE:HG23	1:A:292:ARG:NH2	2.28	0.48
1:A:244:LEU:HD12	1:A:245:ILE:N	2.29	0.48
1:A:17:ALA:O	1:A:20:ARG:HB3	2.14	0.47
1:A:177:PRO:O	1:A:313:PHE:HE1	1.97	0.47
1:A:84:THR:HG23	1:A:89:ILE:O	2.14	0.47
1:B:45:PRO:HB3	1:B:49:LEU:HD23	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:292:ARG:HG2	1:B:292:ARG:HH11	1.80	0.47
1:A:191:LEU:O	1:A:223:LYS:NZ	2.47	0.47
1:B:356:ASP:HB3	1:B:360:ARG:NH2	2.29	0.47
1:A:176:ASN:O	1:A:179:GLY:N	2.47	0.47
1:B:299:LEU:HD13	1:B:359:LEU:HD11	1.93	0.47
1:A:221:PRO:O	1:A:247:THR:CG2	2.63	0.47
1:B:12:ASP:OD1	1:B:12:ASP:N	2.47	0.47
1:A:27:ALA:N	1:A:28:PRO:CD	2.78	0.47
1:A:84:THR:CG2	1:A:90:GLN:HA	2.45	0.47
1:B:135:ASP:O	1:B:137:THR:N	2.48	0.47
1:A:58:ARG:HH21	1:B:54:VAL:HG21	1.75	0.46
1:A:70:ARG:NH1	1:B:29:GLN:H	2.13	0.46
1:B:291:GLU:OE2	1:B:294:ARG:NH1	2.48	0.46
1:A:121:ILE:HG12	1:A:166:PRO:HG3	1.98	0.46
1:B:42:PRO:O	1:B:43:HIS:O	2.34	0.46
1:A:109:LEU:HD21	1:A:244:LEU:HD22	1.98	0.46
1:B:70:ARG:HE	1:B:70:ARG:HB3	1.48	0.46
1:B:363:ALA:O	1:B:364:ARG:C	2.53	0.46
1:B:251:ILE:CD1	1:B:251:ILE:N	2.79	0.46
1:A:106:LEU:O	1:A:110:LEU:HD22	2.16	0.45
1:A:57:VAL:O	1:A:58:ARG:C	2.53	0.45
1:B:162:VAL:HG12	1:B:193:VAL:HB	1.99	0.45
1:B:272:ARG:O	1:B:276:ARG:HG3	2.16	0.45
1:B:97:TRP:HB3	1:B:244:LEU:HG	1.99	0.45
1:A:259:LEU:HD11	1:A:262:HIS:HB2	1.98	0.45
1:B:40:GLU:CG	1:B:41:ASN:N	2.78	0.45
1:B:251:ILE:N	1:B:251:ILE:HD12	2.31	0.45
1:B:140:GLU:OE1	1:B:164:ARG:HD3	2.16	0.45
1:A:129:MET:HE2	1:B:260:PRO:HG3	1.97	0.45
1:A:259:LEU:O	1:A:259:LEU:HD12	2.17	0.45
1:B:22:LYS:HD3	1:B:22:LYS:HA	1.76	0.45
1:B:34:VAL:HG12	1:B:36:LEU:HG	1.99	0.45
1:A:250:VAL:HG22	1:A:251:ILE:HD12	1.98	0.45
1:A:289:ILE:HG23	1:A:292:ARG:HH21	1.82	0.45
1:B:184:LEU:HD22	1:B:211:PRO:HB2	1.99	0.45
1:A:370:VAL:HA	1:A:371:PRO:HD2	1.79	0.44
1:B:172:ALA:HB3	1:B:175:ASN:HB3	1.99	0.44
1:A:365:ILE:O	1:A:368:ASP:CB	2.60	0.44
1:B:115:GLY:H	1:B:137:THR:HB	1.83	0.44
1:A:35:ARG:NH2	1:B:70:ARG:HD3	2.33	0.43
1:A:286:ALA:HA	1:A:289:ILE:HD12	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:330:LEU:HA	1:B:330:LEU:HD12	1.71	0.43
1:A:178:SER:HB2	1:A:180:GLN:HG3	2.00	0.43
1:A:253:ALA:O	1:A:256:LEU:HB3	2.19	0.43
1:B:50:VAL:O	1:B:54:VAL:HG22	2.18	0.43
1:A:295:VAL:HG13	1:A:359:LEU:HD21	1.99	0.43
1:B:313:PHE:CD2	1:B:346:ARG:NH2	2.86	0.43
1:B:46:THR:HG22	1:B:48:ALA:H	1.83	0.43
1:B:115:GLY:O	1:B:118:ARG:HB2	2.19	0.43
1:A:141:TRP:HE1	1:B:134:SER:CB	2.29	0.43
1:A:321:ASP:C	1:A:321:ASP:OD2	2.57	0.43
1:A:71:ASP:O	1:A:72:ALA:C	2.57	0.43
1:A:135:ASP:HB2	1:A:137:THR:H	1.84	0.43
1:A:22:LYS:HD3	1:A:22:LYS:HA	1.68	0.43
1:A:32:VAL:HG21	1:A:335:LEU:HB2	2.00	0.43
1:B:95:ASN:O	1:B:251:ILE:HD11	2.18	0.42
1:B:184:LEU:O	1:B:185:PRO:C	2.56	0.42
1:A:102:SER:HA	1:A:105:ILE:HD11	2.01	0.42
1:B:56:SER:OG	1:B:276:ARG:NH2	2.51	0.42
1:B:132:ILE:O	1:B:132:ILE:HD12	2.19	0.42
1:B:71:ASP:OD1	1:B:258:ARG:NH1	2.53	0.42
1:B:86:GLN:OE1	1:B:228:ARG:NH2	2.50	0.42
1:A:285:VAL:O	1:A:289:ILE:HG13	2.19	0.42
1:A:258:ARG:O	1:A:260:PRO:HD3	2.20	0.42
1:A:344:TYR:O	1:A:345:LEU:CD1	2.67	0.42
1:B:249:ALA:O	1:B:252:ASP:HB2	2.19	0.42
1:B:197:ILE:HA	1:B:197:ILE:HD13	1.68	0.42
1:B:312:ASN:N	1:B:312:ASN:HD22	2.16	0.42
1:A:16:ARG:HH11	1:A:18:ASP:CB	2.33	0.42
1:B:61:ALA:HA	1:B:266:VAL:HG12	2.02	0.42
1:A:70:ARG:NH1	1:B:29:GLN:N	2.67	0.42
1:A:15:LEU:C	1:B:118:ARG:HH22	2.22	0.42
1:A:246:ALA:HB3	1:A:250:VAL:HG21	2.02	0.41
1:A:176:ASN:HB3	1:A:177:PRO:CD	2.50	0.41
1:A:369:LEU:H	1:A:369:LEU:HD12	1.86	0.41
1:B:51:ASP:HA	1:B:54:VAL:HG22	2.03	0.41
1:B:37:ASN:H	1:B:37:ASN:ND2	2.13	0.41
1:B:47:ARG:NH1	1:B:47:ARG:HB3	2.35	0.41
1:B:173:SER:HA	1:B:174:PRO:HA	1.94	0.41
1:B:83:LEU:HA	1:B:83:LEU:HD23	1.77	0.41
1:A:179:GLY:O	1:A:310:ASP:N	2.52	0.41
1:A:115:GLY:N	1:A:137:THR:HB	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:LEU:HA	1:A:109:LEU:HD13	1.92	0.41
1:B:241:LEU:HD12	1:B:241:LEU:HA	1.76	0.41
1:A:220:TYR:N	1:A:221:PRO:HD3	2.36	0.41
1:B:124:VAL:HG11	1:B:130:HIS:HB3	2.02	0.41
1:B:37:ASN:HD22	1:B:38:THR:H	1.70	0.40
1:B:30:LEU:C	1:B:32:VAL:N	2.74	0.40
1:A:25:TYR:O	1:A:26:GLY:C	2.60	0.40
1:A:346:ARG:CG	1:A:346:ARG:NH1	2.63	0.40
1:B:108:GLN:HG2	1:B:259:LEU:CD1	2.51	0.40
1:B:302:MET:HE1	1:B:363:ALA:N	2.37	0.40
1:B:197:ILE:HD12	1:B:223:LYS:O	2.22	0.40
1:B:251:ILE:CD1	1:B:251:ILE:H	2.33	0.40
1:B:86:GLN:HE22	1:B:228:ARG:HH22	1.70	0.40
1:B:89:ILE:HG13	1:B:214:VAL:HG23	2.03	0.40
1:A:101:GLY:O	1:A:105:ILE:HG12	2.22	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	365/394 (93%)	319 (87%)	36 (10%)	10 (3%)	6	10
1	B	363/394 (92%)	313 (86%)	42 (12%)	8 (2%)	8	15
All	All	728/788 (92%)	632 (87%)	78 (11%)	18 (2%)	7	12

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	176	ASN
1	A	367	THR
1	A	368	ASP

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Mol	Chain	Res	Type
1	A	371	PRO
1	B	42	PRO
1	B	136	GLY
1	B	147	ALA
1	B	148	ASN
1	B	318	GLU
1	A	18	ASP
1	B	25	TYR
1	B	29	GLN
1	A	236	PHE
1	B	43	HIS
1	A	195	PRO
1	A	239	GLY
1	A	260	PRO
1	A	177	PRO

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	291/312 (93%)	256 (88%)	35 (12%)	6 11
1	B	289/312 (93%)	260 (90%)	29 (10%)	9 18
All	All	580/624 (93%)	516 (89%)	64 (11%)	8 14

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LEU
1	A	16	ARG
1	A	19	LEU
1	A	22	LYS
1	A	25	TYR
1	A	35	ARG
1	A	46	THR
1	A	49	LEU

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Mol	Chain	Res	Type
1	A	62	ILE
1	A	63	ASP
1	A	67	TYR
1	A	73	VAL
1	A	86	GLN
1	A	91	LEU
1	A	109	LEU
1	A	110	LEU
1	A	127	TYR
1	A	129	MET
1	A	133	ILE
1	A	135	ASP
1	A	139	THR
1	A	206	GLU
1	A	218	GLU
1	A	226	VAL
1	A	247	THR
1	A	250	VAL
1	A	258	ARG
1	A	259	LEU
1	A	266	VAL
1	A	312	ASN
1	A	314	VAL
1	A	346	ARG
1	A	364	ARG
1	A	368	ASP
1	A	369	LEU
1	B	12	ASP
1	B	37	ASN
1	B	39	ASN
1	B	46	THR
1	B	70	ARG
1	B	86	GLN
1	B	91	LEU
1	B	93	VAL
1	B	102	SER
1	B	129	MET
1	B	137	THR
1	B	164	ARG
1	B	165	LYS
1	B	168	VAL
1	B	181	SER

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Mol	Chain	Res	Type
1	B	210	GLN
1	B	212	SER
1	B	228	ARG
1	B	241	LEU
1	B	247	THR
1	B	259	LEU
1	B	265	SER
1	B	266	VAL
1	B	288	LEU
1	B	299	LEU
1	B	312	ASN
1	B	314	VAL
1	B	351	LEU
1	B	359	LEU

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	29	GLN
1	A	37	ASN
1	A	39	ASN
1	A	86	GLN
1	A	95	ASN
1	A	108	GLN
1	A	210	GLN
1	A	262	HIS
1	A	300	ASN
1	A	312	ASN
1	B	37	ASN
1	B	39	ASN
1	B	100	ASN
1	B	103	ASN
1	B	277	HIS
1	B	300	ASN
1	B	312	ASN
1	B	355	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	367/394 (93%)	-0.02	5 (1%)	78	74	24, 48, 100, 149	0
1	B	365/394 (92%)	0.08	10 (2%)	58	51	21, 42, 97, 230	0
All	All	732/788 (92%)	0.03	15 (2%)	68	63	21, 45, 100, 230	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	27	ALA	12.4
1	B	28	PRO	6.3
1	B	26	GLY	5.8
1	A	66	ARG	3.7
1	B	21	GLY	3.4
1	A	129	MET	3.4
1	B	24	PRO	3.3
1	A	6	HIS	2.9
1	B	30	LEU	2.8
1	A	125	PRO	2.7
1	B	33	PRO	2.4
1	B	147	ALA	2.4
1	A	23	ALA	2.3
1	B	261	TYR	2.3
1	B	23	ALA	2.2

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.