Full wwPDB X-ray Structure Validation Report (i)

Jun 16, 2024 – 06:57 AM EDT

PDB ID	:	1YBT
Title	:	MYCOBACTERIUM TUBERCULOSIS ADENYLYL CYCLASE, RV1900C CHD
Authors	:	Sinha, S.C.; Wetterer, M.; Sprang, S.R.; Schultz, J.E.; Linder, J.U.
Deposited on	:	2004-12-21
Resolution	:	2.31 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

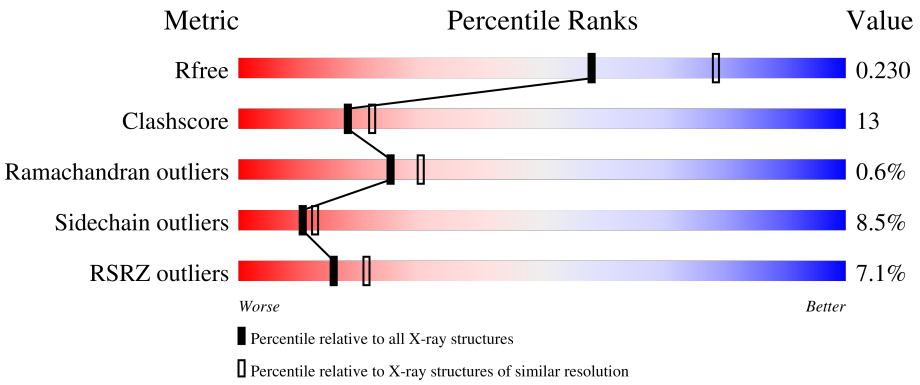
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.31 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	5974 (2.34-2.30)
Clashscore	141614	6604 (2.34-2.30)
Ramachandran outliers	138981	6523 (2.34-2.30)
Sidechain outliers	138945	6523 (2.34-2.30)
RSRZ outliers	127900	5855 (2.34-2.30)

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 of 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	184	2%, 66%, 21%, •, 9%
1	B	184	11%, 67%, 23%, •, 7%
1	C	184	10%, 71%, 21%, •, 7%
1	D	184	2%, 65%, 23%, •, 9%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 5213 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 hydrolase, alpha/beta hydrolase fold family.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	167	1244	764	234	239	4	3	0	0	0
1	B	172	1286	787	245	247	4	3	0	0	0
1	C	172	1286	787	245	247	4	3	0	0	0
1	D	167	1244	764	234	239	4	3	0	0	0

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	279	MSE	-	CLONING ARTIFACT	UNP O07732
A	280	ARG	-	CLONING ARTIFACT	UNP O07732
A	281	GLY	-	CLONING ARTIFACT	UNP O07732
A	282	SER	-	CLONING ARTIFACT	UNP O07732
A	283	HIS	-	EXPRESSION TAG	UNP O07732
A	284	HIS	-	EXPRESSION TAG	UNP O07732
A	285	HIS	-	EXPRESSION TAG	UNP O07732
A	286	HIS	-	EXPRESSION TAG	UNP O07732
A	287	HIS	-	EXPRESSION TAG	UNP O07732
A	288	HIS	-	EXPRESSION TAG	UNP O07732
A	289	GLY	-	CLONING ARTIFACT	UNP O07732
A	290	SER	-	CLONING ARTIFACT	UNP O07732
A	294	MSE	MET	MODIFIED RESIDUE	UNP O07732
A	299	MSE	MET	MODIFIED RESIDUE	UNP O07732
A	454	MSE	MET	MODIFIED RESIDUE	UNP O07732
B	279	MSE	-	CLONING ARTIFACT	UNP O07732
B	280	ARG	-	CLONING ARTIFACT	UNP O07732
B	281	GLY	-	CLONING ARTIFACT	UNP O07732
B	282	SER	-	CLONING ARTIFACT	UNP O07732
B	283	HIS	-	EXPRESSION TAG	UNP O07732
B	284	HIS	-	EXPRESSION TAG	UNP O07732

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Chain	Residue	Modelled	Actual	Comment	Reference
B	285	HIS	-	EXPRESSION TAG	UNP O07732
B	286	HIS	-	EXPRESSION TAG	UNP O07732
B	287	HIS	-	EXPRESSION TAG	UNP O07732
B	288	HIS	-	EXPRESSION TAG	UNP O07732
B	289	GLY	-	CLONING ARTIFACT	UNP O07732
B	290	SER	-	CLONING ARTIFACT	UNP O07732
B	294	MSE	MET	MODIFIED RESIDUE	UNP O07732
B	299	MSE	MET	MODIFIED RESIDUE	UNP O07732
B	454	MSE	MET	MODIFIED RESIDUE	UNP O07732
C	279	MSE	-	CLONING ARTIFACT	UNP O07732
C	280	ARG	-	CLONING ARTIFACT	UNP O07732
C	281	GLY	-	CLONING ARTIFACT	UNP O07732
C	282	SER	-	CLONING ARTIFACT	UNP O07732
C	283	HIS	-	EXPRESSION TAG	UNP O07732
C	284	HIS	-	EXPRESSION TAG	UNP O07732
C	285	HIS	-	EXPRESSION TAG	UNP O07732
C	286	HIS	-	EXPRESSION TAG	UNP O07732
C	287	HIS	-	EXPRESSION TAG	UNP O07732
C	288	HIS	-	EXPRESSION TAG	UNP O07732
C	289	GLY	-	CLONING ARTIFACT	UNP O07732
C	290	SER	-	CLONING ARTIFACT	UNP O07732
C	294	MSE	MET	CLONING ARTIFACT	UNP O07732
C	299	MSE	MET	MODIFIED RESIDUE	UNP O07732
C	454	MSE	MET	MODIFIED RESIDUE	UNP O07732
D	279	MSE	-	MODIFIED RESIDUE	UNP O07732
D	280	ARG	-	CLONING ARTIFACT	UNP O07732
D	281	GLY	-	CLONING ARTIFACT	UNP O07732
D	282	SER	-	CLONING ARTIFACT	UNP O07732
D	283	HIS	-	EXPRESSION TAG	UNP O07732
D	284	HIS	-	EXPRESSION TAG	UNP O07732
D	285	HIS	-	EXPRESSION TAG	UNP O07732
D	286	HIS	-	EXPRESSION TAG	UNP O07732
D	287	HIS	-	EXPRESSION TAG	UNP O07732
D	288	HIS	-	EXPRESSION TAG	UNP O07732
D	289	GLY	-	CLONING ARTIFACT	UNP O07732
D	290	SER	-	CLONING ARTIFACT	UNP O07732
D	294	MSE	MET	MODIFIED RESIDUE	UNP O07732
D	299	MSE	MET	MODIFIED RESIDUE	UNP O07732
D	454	MSE	MET	MODIFIED RESIDUE	UNP O07732

- Molecule 2 is water.

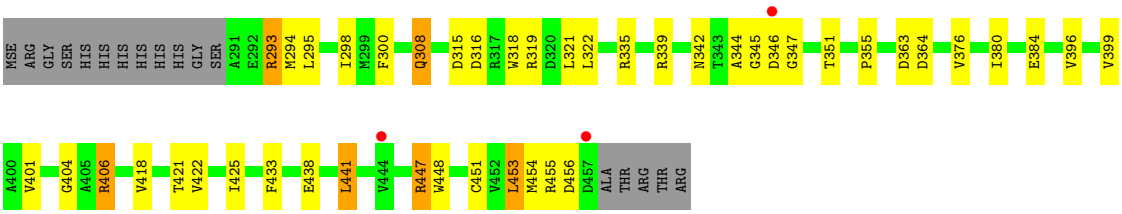
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	43	43	43	0	0
			Total	O		
2	B	35	35	35	0	0
			Total	O		
2	C	37	37	37	0	0
			Total	O		
2	D	38	38	38	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

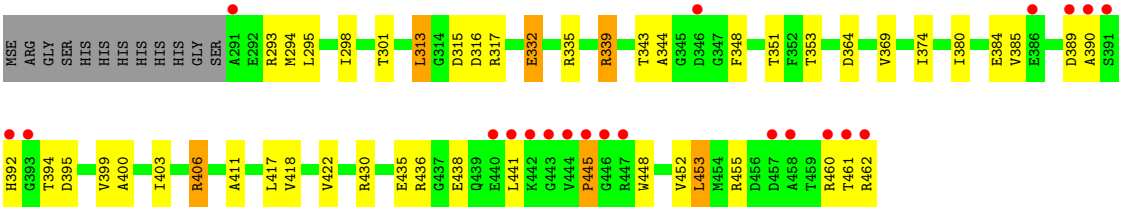
• Molecule 1: hydrolase, alpha/beta hydrolase fold family

Chain A:



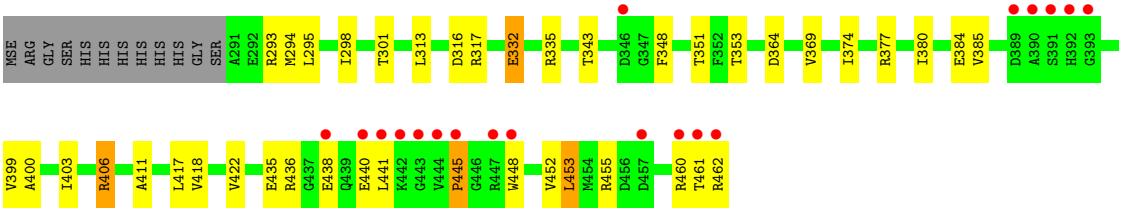
• Molecule 1: hydrolase, alpha/beta hydrolase fold family

Chain B:



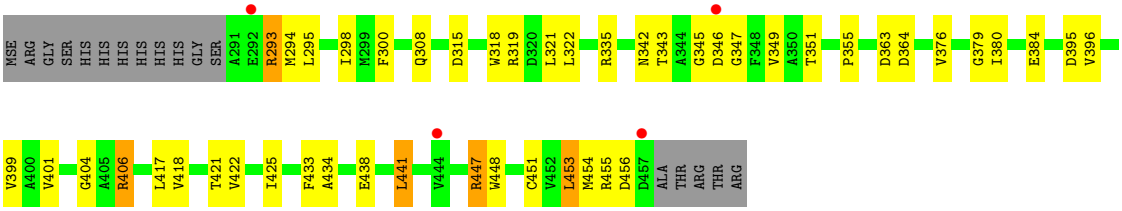
• Molecule 1: hydrolase, alpha/beta hydrolase fold family

Chain C:



• Molecule 1: hydrolase, alpha/beta hydrolase fold family

Chain D:


MSE
ARG
GLY
SER
HIS
HIS
HIS
HIS
HIS
GLY
SER
A291
E292
R293
M294
L295
I298
M299
F300
Q308
D315
W318
R319
D320
L321
L322
R335
N342
T343
A344
G345
D346
G347
F348
V349
A350
T351
P355
D363
D364
V376
G379
I380
E384
D395
V396
V399
A400
V401
G404
A405
R406
L417
V418
T421
V422
I425
F433
A434
E438
L441
V444
R447
W448
C451
V452
L453
M454
R455
D456
D457
ALA
THR
ARG
THR
ARG

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	90.70Å 44.39Å 80.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.94 – 2.31 19.93 – 2.32	Depositor EDS
% Data completeness (in resolution range)	99.1 (19.94-2.31) 99.1 (19.93-2.32)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	2.56 (at 2.33Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.194 , 0.230 0.195 , 0.230	Depositor DCC
R_{free} test set	1401 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	39.3	Xtriage
Anisotropy	0.448	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 40.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.479 for -h,-k,l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	5213	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.14% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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	0.55	0/1259	0.78	1/1702 (0.1%)
1	B	0.53	0/1301	0.82	2/1757 (0.1%)
1	C	0.54	0/1301	0.80	2/1757 (0.1%)
1	D	0.55	0/1259	0.78	1/1702 (0.1%)
All	All	0.54	0/5120	0.79	6/6918 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	445	PRO	CA-N-CD	-8.89	99.06	111.50
1	B	445	PRO	CA-N-CD	-7.92	100.42	111.50
1	B	453	LEU	CA-CB-CG	6.29	129.77	115.30
1	C	453	LEU	CA-CB-CG	5.82	128.68	115.30
1	D	453	LEU	CA-CB-CG	5.39	127.69	115.30
1	A	453	LEU	CA-CB-CG	5.03	126.88	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1244	0	1216	39	0
1	B	1286	0	1261	35	0
1	C	1286	0	1261	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1244	0	1216	37	0
2	A	43	0	0	1	0
2	B	35	0	0	2	0
2	C	37	0	0	1	0
2	D	38	0	0	0	0
All	All	5213	0	4954	135	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 (135) 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:344:ALA:HB2	2:B:109:HOH:O	1.76	0.85
1:C:377:ARG:NH1	1:C:411:ALA:O	2.22	0.72
1:C:436:ARG:HH21	1:C:460:ARG:HB3	1.56	0.70
1:A:438:GLU:HG2	1:A:447:ARG:NH1	2.06	0.70
1:D:345:GLY:O	1:D:347:GLY:N	2.25	0.69
1:B:436:ARG:HH21	1:B:460:ARG:HB3	1.56	0.69
1:C:436:ARG:NH2	1:C:460:ARG:HB3	2.08	0.69
1:D:438:GLU:HG2	1:D:447:ARG:NH1	2.07	0.69
1:B:436:ARG:NH2	1:B:460:ARG:HB3	2.08	0.69
1:D:298:ILE:HD12	1:D:351:THR:HG22	1.74	0.69
1:C:332:GLU:HA	1:C:332:GLU:OE1	1.93	0.68
1:A:345:GLY:O	1:A:347:GLY:N	2.25	0.68
1:A:344:ALA:HB2	1:B:395:ASP:OD2	1.93	0.68
1:B:406:ARG:NH1	1:B:441:LEU:HA	2.09	0.68
1:A:298:ILE:HD12	1:A:351:THR:HG22	1.76	0.68
1:A:293:ARG:HH11	1:A:293:ARG:HG3	1.59	0.67
1:B:332:GLU:OE1	1:B:335:ARG:HD3	1.95	0.66
1:A:293:ARG:HG3	1:A:293:ARG:NH1	2.11	0.66
1:C:406:ARG:NH1	1:C:441:LEU:HA	2.10	0.66
1:A:421:THR:O	1:A:425:ILE:HG12	1.96	0.65
1:C:332:GLU:OE1	1:C:335:ARG:HD3	1.95	0.65
1:D:406:ARG:HH11	1:D:406:ARG:HG3	1.61	0.64
1:B:332:GLU:OE1	1:B:332:GLU:HA	1.96	0.64
1:D:421:THR:O	1:D:425:ILE:HG12	1.98	0.63
1:A:406:ARG:HH11	1:A:406:ARG:HG3	1.61	0.63
1:D:355:PRO:HG2	1:D:425:ILE:HG21	1.80	0.62
1:B:313:LEU:HD13	1:D:434:ALA:HB1	1.80	0.62
1:A:355:PRO:HG2	1:A:425:ILE:HG21	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:453:LEU:CD1	1:B:455:ARG:HG2	2.30	0.62
1:D:293:ARG:HG3	1:D:293:ARG:NH1	2.15	0.61
1:D:293:ARG:HG3	1:D:293:ARG:HH11	1.65	0.60
1:C:462:ARG:HG3	2:C:143:HOH:O	2.00	0.60
1:D:406:ARG:HG3	1:D:406:ARG:NH1	2.15	0.60
1:A:406:ARG:HG3	1:A:406:ARG:NH1	2.17	0.60
1:C:435:GLU:O	1:C:461:THR:HG21	2.02	0.59
1:B:380:ILE:HB	1:B:418:VAL:HG12	1.84	0.58
1:D:363:ASP:OD2	1:D:455:ARG:HG2	2.03	0.58
1:B:435:GLU:O	1:B:461:THR:HG21	2.04	0.57
1:C:380:ILE:HB	1:C:418:VAL:HG12	1.85	0.57
1:B:461:THR:O	1:B:462:ARG:HB2	2.04	0.57
1:C:453:LEU:CD1	1:C:455:ARG:HG2	2.34	0.57
1:D:308:GLN:CD	1:D:308:GLN:N	2.59	0.56
1:C:461:THR:O	1:C:462:ARG:HB2	2.05	0.56
1:C:417:LEU:CD1	1:C:452:VAL:HG22	2.36	0.55
1:A:318:TRP:CZ2	1:A:322:LEU:HD13	2.42	0.55
1:D:335:ARG:HH11	1:D:335:ARG:HG3	1.71	0.55
1:C:436:ARG:O	1:C:436:ARG:HG3	2.07	0.54
1:A:298:ILE:CD1	1:A:351:THR:HG22	2.37	0.54
1:A:335:ARG:HH11	1:A:335:ARG:HG3	1.72	0.54
1:D:315:ASP:OD1	1:D:319:ARG:NH1	2.41	0.54
1:D:298:ILE:CD1	1:D:351:THR:HG22	2.37	0.54
1:B:453:LEU:HD13	1:B:455:ARG:HG2	1.89	0.53
1:A:339:ARG:HB2	1:A:339:ARG:NH1	2.24	0.53
1:A:315:ASP:OD1	1:A:319:ARG:NH1	2.41	0.52
1:C:453:LEU:HD13	1:C:455:ARG:HG2	1.90	0.52
1:B:436:ARG:O	1:B:436:ARG:HG3	2.09	0.52
1:D:315:ASP:O	1:D:319:ARG:HD3	2.09	0.52
1:D:318:TRP:CZ2	1:D:322:LEU:HD13	2.44	0.52
1:B:417:LEU:CD1	1:B:452:VAL:HG22	2.40	0.52
1:B:294:MSE:O	1:B:384:GLU:HA	2.09	0.52
1:C:411:ALA:HA	1:C:417:LEU:HD22	1.92	0.51
1:A:315:ASP:O	1:A:319:ARG:HD3	2.11	0.51
1:D:441:LEU:HD22	1:D:448:TRP:CD1	2.46	0.51
1:D:454:MSE:HA	1:D:454:MSE:HE2	1.92	0.51
1:C:399:VAL:O	1:C:403:ILE:HG12	2.11	0.50
1:A:441:LEU:HD22	1:A:448:TRP:CD1	2.46	0.50
1:C:461:THR:O	1:C:461:THR:HG22	2.11	0.50
1:B:461:THR:O	1:B:461:THR:HG22	2.11	0.50
1:C:294:MSE:O	1:C:384:GLU:HA	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:335:ARG:HG3	1:D:335:ARG:NH1	2.27	0.49
1:A:363:ASP:OD2	1:A:455:ARG:HG2	2.12	0.49
1:B:399:VAL:O	1:B:403:ILE:HG12	2.12	0.49
1:A:335:ARG:HG3	1:A:335:ARG:NH1	2.28	0.48
1:D:342:ASN:HB2	1:D:395:ASP:OD1	2.12	0.48
1:A:321:LEU:HD12	1:A:321:LEU:O	2.13	0.48
1:A:308:GLN:HE21	1:A:308:GLN:HA	1.79	0.47
1:A:344:ALA:HB1	1:B:395:ASP:HB3	1.96	0.47
1:B:380:ILE:HG22	1:B:422:VAL:HG21	1.94	0.47
1:B:301:THR:OG1	1:B:348:PHE:HB2	2.15	0.47
1:A:396:VAL:HG12	1:A:401:VAL:CG2	2.45	0.47
1:A:447:ARG:HB3	1:A:447:ARG:CZ	2.44	0.47
1:C:301:THR:OG1	1:C:348:PHE:HB2	2.15	0.46
1:C:440:GLU:HG2	1:C:440:GLU:O	2.14	0.46
1:B:461:THR:O	1:B:462:ARG:CB	2.63	0.46
1:A:438:GLU:HG2	1:A:447:ARG:HH12	1.78	0.46
1:B:411:ALA:HA	1:B:417:LEU:HD22	1.97	0.46
1:B:390:ALA:HB3	1:B:392:HIS:ND1	2.31	0.46
1:B:369:VAL:CG1	1:B:374:ILE:HG13	2.45	0.46
1:D:293:ARG:HH11	1:D:293:ARG:CG	2.29	0.45
1:B:406:ARG:HH12	1:B:441:LEU:HA	1.78	0.45
1:C:461:THR:O	1:C:462:ARG:CB	2.64	0.45
1:D:355:PRO:HG2	1:D:425:ILE:CG2	2.46	0.45
1:A:344:ALA:CB	1:B:395:ASP:OD2	2.62	0.45
1:A:380:ILE:HB	1:A:418:VAL:HG22	1.98	0.45
1:D:300:PHE:CE1	1:D:404:GLY:HA3	2.51	0.45
1:D:321:LEU:HD12	1:D:321:LEU:O	2.17	0.45
1:A:293:ARG:HH11	1:A:293:ARG:CG	2.27	0.45
1:C:438:GLU:HG3	1:C:448:TRP:O	2.17	0.44
1:D:438:GLU:HG2	1:D:447:ARG:HH12	1.80	0.44
1:B:339:ARG:NH2	1:B:394:THR:HG21	2.32	0.44
1:B:369:VAL:HG13	1:B:374:ILE:HG13	2.00	0.44
1:B:438:GLU:HG3	1:B:448:TRP:O	2.17	0.44
1:B:339:ARG:HH11	1:B:339:ARG:HG3	1.81	0.44
1:A:355:PRO:HG2	1:A:425:ILE:CG2	2.47	0.44
1:C:369:VAL:HG13	1:C:374:ILE:HG13	2.00	0.44
1:A:418:VAL:HG13	1:A:422:VAL:HB	2.00	0.43
1:C:385:VAL:HG12	1:C:400:ALA:HB3	1.99	0.43
1:B:298:ILE:HD12	1:B:351:THR:HG22	2.00	0.43
1:A:454:MSE:HE2	1:A:454:MSE:HA	2.00	0.43
1:A:300:PHE:CE1	1:A:404:GLY:HA3	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:ASN:HB3	2:B:109:HOH:O	2.17	0.43
1:C:436:ARG:O	1:C:436:ARG:CG	2.66	0.43
1:A:294:MSE:O	1:A:384:GLU:HA	2.19	0.42
1:C:298:ILE:HD12	1:C:351:THR:HG22	2.02	0.42
1:D:343:THR:HG21	1:D:349:VAL:CG2	2.49	0.42
1:D:447:ARG:HB3	1:D:447:ARG:CZ	2.49	0.42
1:A:316:ASP:HB2	2:A:150:HOH:O	2.19	0.42
1:B:385:VAL:HG12	1:B:400:ALA:HB3	2.00	0.42
1:B:436:ARG:O	1:B:436:ARG:CG	2.67	0.42
1:D:342:ASN:O	1:D:343:THR:HG23	2.20	0.42
1:D:380:ILE:HB	1:D:418:VAL:HG22	2.02	0.42
1:D:308:GLN:CD	1:D:308:GLN:H	2.22	0.42
1:D:396:VAL:HG12	1:D:401:VAL:CG2	2.50	0.41
1:A:308:GLN:NE2	1:A:308:GLN:CA	2.82	0.41
1:D:294:MSE:O	1:D:384:GLU:HA	2.20	0.41
1:A:293:ARG:NH2	1:B:315:ASP:OD1	2.53	0.41
1:C:406:ARG:HH12	1:C:441:LEU:HA	1.79	0.41
1:D:380:ILE:HG22	1:D:422:VAL:HG21	2.03	0.41
1:A:308:GLN:HA	1:A:308:GLN:NE2	2.35	0.41
1:D:343:THR:HG21	1:D:349:VAL:HG21	2.03	0.41
1:C:380:ILE:HG22	1:C:422:VAL:HG21	2.03	0.40
1:C:462:ARG:HG3	1:C:462:ARG:HH11	1.85	0.40
1:D:433:PHE:HB3	1:D:451:CYS:HB3	2.03	0.40
1:A:433:PHE:HB3	1:A:451:CYS:HB3	2.04	0.40
1:D:379:GLY:HA2	1:D:417:LEU: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	165/184 (90%)	160 (97%)	4 (2%)	1 (1%)	25 30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	170/184 (92%)	161 (95%)	8 (5%)	1 (1%)	25	30
1	C	170/184 (92%)	161 (95%)	8 (5%)	1 (1%)	25	30
1	D	165/184 (90%)	159 (96%)	5 (3%)	1 (1%)	25	30
All	All	670/736 (91%)	641 (96%)	25 (4%)	4 (1%)	25	30

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	346	ASP
1	D	346	ASP
1	B	343	THR
1	C	343	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	127/137 (93%)	116 (91%)	11 (9%)	10	12
1	B	131/137 (96%)	118 (90%)	13 (10%)	8	9
1	C	131/137 (96%)	121 (92%)	10 (8%)	13	16
1	D	127/137 (93%)	117 (92%)	10 (8%)	12	15
All	All	516/548 (94%)	472 (92%)	44 (8%)	10	12

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	293	ARG
1	A	295	LEU
1	A	308	GLN
1	A	364	ASP
1	A	376	VAL
1	A	399	VAL
1	A	406	ARG

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Mol	Chain	Res	Type
1	A	441	LEU
1	A	447	ARG
1	A	453	LEU
1	A	456	ASP
1	B	293	ARG
1	B	295	LEU
1	B	313	LEU
1	B	316	ASP
1	B	317	ARG
1	B	332	GLU
1	B	339	ARG
1	B	353	THR
1	B	364	ASP
1	B	389	ASP
1	B	406	ARG
1	B	430	ARG
1	B	445	PRO
1	C	293	ARG
1	C	295	LEU
1	C	313	LEU
1	C	316	ASP
1	C	317	ARG
1	C	332	GLU
1	C	353	THR
1	C	364	ASP
1	C	406	ARG
1	C	445	PRO
1	D	293	ARG
1	D	295	LEU
1	D	364	ASP
1	D	376	VAL
1	D	399	VAL
1	D	406	ARG
1	D	441	LEU
1	D	447	ARG
1	D	453	LEU
1	D	456	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	308	GLN

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Mol	Chain	Res	Type
1	B	324	ASN
1	B	439	GLN
1	C	308	GLN
1	C	324	ASN
1	C	439	GLN

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 (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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, 95th 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	164/184 (89%)	-0.13	3 (1%)	68	75	23, 42, 99, 131	0
1	B	169/184 (91%)	0.23	21 (12%)	4	6	26, 44, 125, 143	1 (0%)
1	C	169/184 (91%)	0.29	19 (11%)	5	7	23, 44, 123, 145	1 (0%)
1	D	164/184 (89%)	-0.16	4 (2%)	59	66	23, 41, 97, 127	0
All	All	666/736 (90%)	0.06	47 (7%)	16	21	23, 43, 113, 145	2 (0%)

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	391	SER	14.1
1	C	390	ALA	13.0
1	A	457	ASP	7.0
1	B	392	HIS	5.9
1	C	460	ARG	5.6
1	C	462	ARG	5.2
1	B	460	ARG	4.5
1	B	390	ALA	4.5
1	B	444	VAL	4.4
1	C	445	PRO	4.2
1	B	445	PRO	4.1
1	C	444	VAL	4.1
1	B	461	THR	3.9
1	D	457	ASP	3.8
1	B	462	ARG	3.7
1	C	389	ASP	3.6
1	B	442	LYS	3.5
1	B	391	SER	3.5
1	C	461	THR	3.5
1	C	441	LEU	3.4
1	B	446	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	457	ASP	3.3
1	A	346	ASP	3.3
1	C	393	GLY	3.2
1	C	392	HIS	3.2
1	B	440	GLU	3.1
1	D	346	ASP	3.1
1	B	447	ARG	3.1
1	C	442	LYS	3.0
1	C	443	GLY	2.9
1	B	393	GLY	2.9
1	B	441	LEU	2.9
1	D	444	VAL	2.9
1	C	447	ARG	2.8
1	C	457	ASP	2.8
1	A	444	VAL	2.7
1	C	440	GLU	2.6
1	B	389	ASP	2.6
1	B	443	GLY	2.5
1	C	448	TRP	2.5
1	B	386	GLU	2.2
1	C	438	GLU	2.1
1	D	292	GLU	2.1
1	B	291	ALA	2.1
1	B	346	ASP	2.1
1	B	458	ALA	2.1
1	C	346	ASP	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 monosaccharides 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.