Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:06 AM GMT

PDB ID	:	3DDM
Title	:	CRYSTAL STRUCTURE OF MANDELATE RACEMASE/MUCONATE LACTONIZING ENZYME FROM Bordetella bronchiseptica RB50
Authors	:	Fedorov, A.A.; Fedorov, E.V.; Toro, R.; Gerlt, J.A.; Burley, S.K.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on	:	2008-06-05
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:

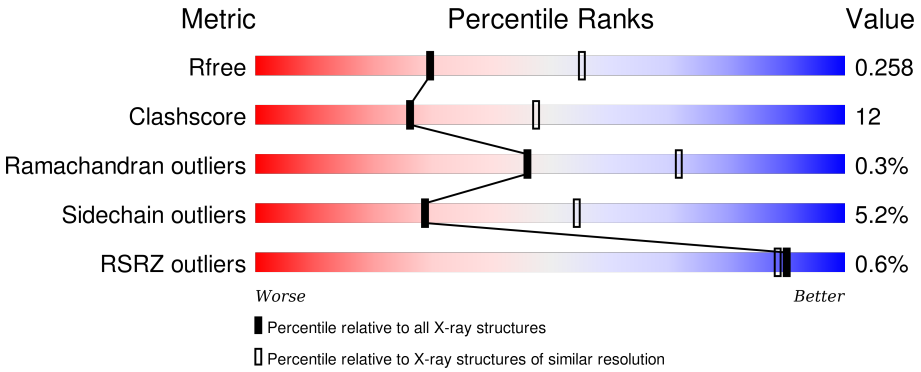
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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	392	% 69% 22% • 7%
1	B	392	% 67% 25% • 7%
1	C	392	% 66% 25% • 7%
1	D	392	% 69% 23% • 7%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10762 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 Putative mandelate racemase/muconate lactonizing enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	363	Total	C	N	O	S	0	0	0
			2672	1687	494	481	10			
1	B	363	Total	C	N	O	S	0	0	0
			2672	1687	494	481	10			
1	C	363	Total	C	N	O	S	0	0	0
			2672	1687	494	481	10			
1	D	363	Total	C	N	O	S	0	0	0
			2672	1687	494	481	10			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP Q7WJN4
A	2	SER	-	expression tag	UNP Q7WJN4
A	3	LEU	-	expression tag	UNP Q7WJN4
A	336	GLY	GLU	engineered	UNP Q7WJN4
A	374	LEU	-	expression tag	UNP Q7WJN4
A	375	ALA	-	expression tag	UNP Q7WJN4
A	376	ALA	-	expression tag	UNP Q7WJN4
A	377	LEU	-	expression tag	UNP Q7WJN4
A	378	ARG	-	expression tag	UNP Q7WJN4
A	379	ALA	-	expression tag	UNP Q7WJN4
A	380	ALA	-	expression tag	UNP Q7WJN4
A	381	CYS	-	expression tag	UNP Q7WJN4
A	382	ALA	-	expression tag	UNP Q7WJN4
A	383	ALA	-	expression tag	UNP Q7WJN4
A	384	ARG	-	expression tag	UNP Q7WJN4
A	385	GLU	-	expression tag	UNP Q7WJN4
A	386	GLY	-	expression tag	UNP Q7WJN4
A	387	HIS	-	expression tag	UNP Q7WJN4
A	388	HIS	-	expression tag	UNP Q7WJN4
A	389	HIS	-	expression tag	UNP Q7WJN4
A	390	HIS	-	expression tag	UNP Q7WJN4

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Chain	Residue	Modelled	Actual	Comment	Reference
A	391	HIS	-	expression tag	UNP Q7WJN4
A	392	HIS	-	expression tag	UNP Q7WJN4
B	1	MET	-	expression tag	UNP Q7WJN4
B	2	SER	-	expression tag	UNP Q7WJN4
B	3	LEU	-	expression tag	UNP Q7WJN4
B	336	GLY	GLU	engineered	UNP Q7WJN4
B	374	LEU	-	expression tag	UNP Q7WJN4
B	375	ALA	-	expression tag	UNP Q7WJN4
B	376	ALA	-	expression tag	UNP Q7WJN4
B	377	LEU	-	expression tag	UNP Q7WJN4
B	378	ARG	-	expression tag	UNP Q7WJN4
B	379	ALA	-	expression tag	UNP Q7WJN4
B	380	ALA	-	expression tag	UNP Q7WJN4
B	381	CYS	-	expression tag	UNP Q7WJN4
B	382	ALA	-	expression tag	UNP Q7WJN4
B	383	ALA	-	expression tag	UNP Q7WJN4
B	384	ARG	-	expression tag	UNP Q7WJN4
B	385	GLU	-	expression tag	UNP Q7WJN4
B	386	GLY	-	expression tag	UNP Q7WJN4
B	387	HIS	-	expression tag	UNP Q7WJN4
B	388	HIS	-	expression tag	UNP Q7WJN4
B	389	HIS	-	expression tag	UNP Q7WJN4
B	390	HIS	-	expression tag	UNP Q7WJN4
B	391	HIS	-	expression tag	UNP Q7WJN4
B	392	HIS	-	expression tag	UNP Q7WJN4
C	1	MET	-	expression tag	UNP Q7WJN4
C	2	SER	-	expression tag	UNP Q7WJN4
C	3	LEU	-	expression tag	UNP Q7WJN4
C	336	GLY	GLU	engineered	UNP Q7WJN4
C	374	LEU	-	expression tag	UNP Q7WJN4
C	375	ALA	-	expression tag	UNP Q7WJN4
C	376	ALA	-	expression tag	UNP Q7WJN4
C	377	LEU	-	expression tag	UNP Q7WJN4
C	378	ARG	-	expression tag	UNP Q7WJN4
C	379	ALA	-	expression tag	UNP Q7WJN4
C	380	ALA	-	expression tag	UNP Q7WJN4
C	381	CYS	-	expression tag	UNP Q7WJN4
C	382	ALA	-	expression tag	UNP Q7WJN4
C	383	ALA	-	expression tag	UNP Q7WJN4
C	384	ARG	-	expression tag	UNP Q7WJN4
C	385	GLU	-	expression tag	UNP Q7WJN4
C	386	GLY	-	expression tag	UNP Q7WJN4

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Chain	Residue	Modelled	Actual	Comment	Reference
C	387	HIS	-	expression tag	UNP Q7WJN4
C	388	HIS	-	expression tag	UNP Q7WJN4
C	389	HIS	-	expression tag	UNP Q7WJN4
C	390	HIS	-	expression tag	UNP Q7WJN4
C	391	HIS	-	expression tag	UNP Q7WJN4
C	392	HIS	-	expression tag	UNP Q7WJN4
D	1	MET	-	expression tag	UNP Q7WJN4
D	2	SER	-	expression tag	UNP Q7WJN4
D	3	LEU	-	expression tag	UNP Q7WJN4
D	336	GLY	GLU	engineered	UNP Q7WJN4
D	374	LEU	-	expression tag	UNP Q7WJN4
D	375	ALA	-	expression tag	UNP Q7WJN4
D	376	ALA	-	expression tag	UNP Q7WJN4
D	377	LEU	-	expression tag	UNP Q7WJN4
D	378	ARG	-	expression tag	UNP Q7WJN4
D	379	ALA	-	expression tag	UNP Q7WJN4
D	380	ALA	-	expression tag	UNP Q7WJN4
D	381	CYS	-	expression tag	UNP Q7WJN4
D	382	ALA	-	expression tag	UNP Q7WJN4
D	383	ALA	-	expression tag	UNP Q7WJN4
D	384	ARG	-	expression tag	UNP Q7WJN4
D	385	GLU	-	expression tag	UNP Q7WJN4
D	386	GLY	-	expression tag	UNP Q7WJN4
D	387	HIS	-	expression tag	UNP Q7WJN4
D	388	HIS	-	expression tag	UNP Q7WJN4
D	389	HIS	-	expression tag	UNP Q7WJN4
D	390	HIS	-	expression tag	UNP Q7WJN4
D	391	HIS	-	expression tag	UNP Q7WJN4
D	392	HIS	-	expression tag	UNP Q7WJN4

- Molecule 2 is water.

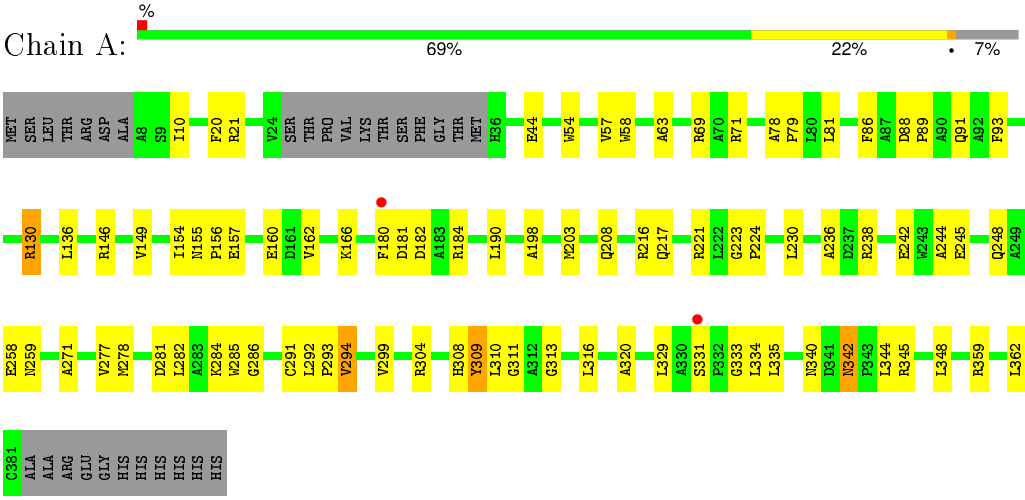
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	20	Total O 20 20	0	0
2	B	23	Total O 23 23	0	0
2	C	18	Total O 18 18	0	0
2	D	13	Total O 13 13	0	0

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.

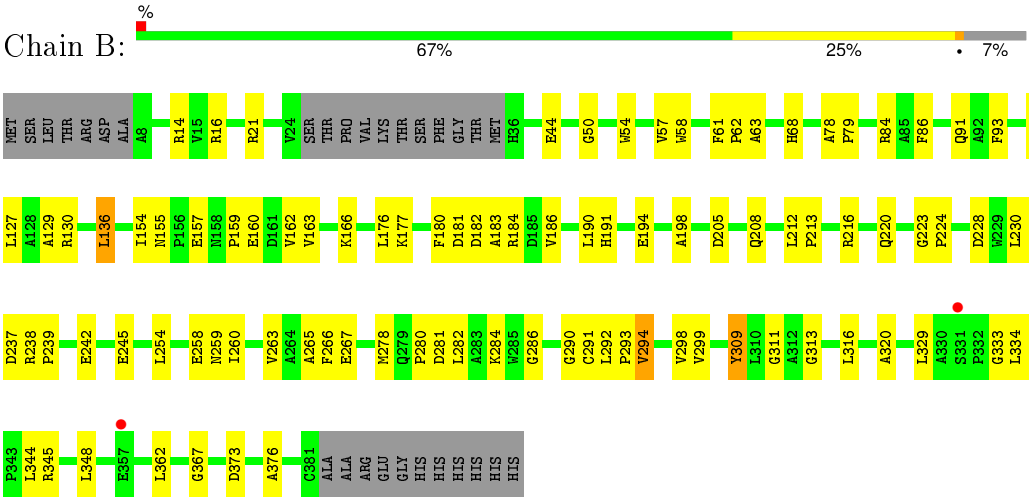
- Molecule 1: Putative mandelate racemase/muconate lactonizing enzyme

Chain A:



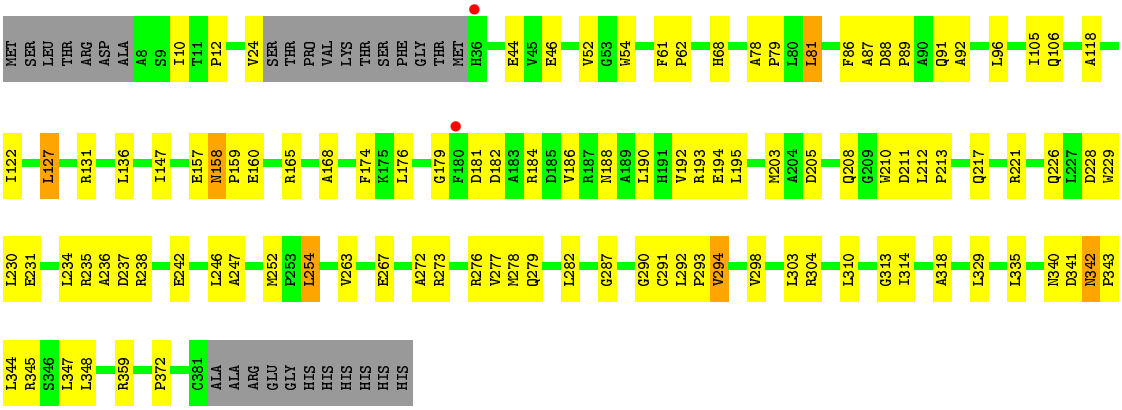
- Molecule 1: Putative mandelate racemase/muconate lactonizing enzyme

Chain B:



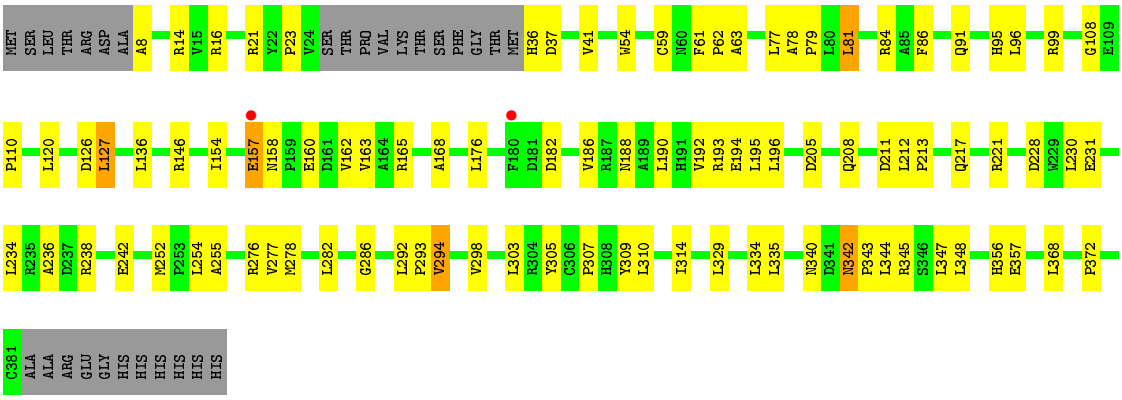
- Molecule 1: Putative mandelate racemase/muconate lactonizing enzyme

Chain C:



• Molecule 1: Putative mandelate racemase/muconate lactonizing enzyme

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	122.60Å 122.64Å 164.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.58 – 2.60 28.90 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (24.58-2.60) 97.1 (28.90-2.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.17 (at 2.39Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.224 , 0.258 0.224 , 0.258	Depositor DCC
R_{free} test set	3855 reflections (5.03%)	DCC
Wilson B-factor (Å^2)	51.8	Xtriage
Anisotropy	0.210	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 26.8	EDS
Estimated twinning fraction	0.480 for k,h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Outliers	6 of 94362 reflections (0.006%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	10762	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.80% 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	0/2734	0.60	0/3735
1	B	0.36	0/2734	0.61	0/3735
1	C	0.36	0/2734	0.58	0/3735
1	D	0.37	0/2734	0.59	1/3735 (0.0%)
All	All	0.36	0/10936	0.60	1/14940 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	D	0	1
All	All	0	3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	127	LEU	CA-CB-CG	5.36	127.62	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	309	TYR	Sidechain
1	B	309	TYR	Sidechain
1	D	309	TYR	Sidechain

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	2672	0	2665	63	0
1	B	2672	0	2665	74	0
1	C	2672	0	2665	81	0
1	D	2672	0	2665	58	0
2	A	20	0	0	1	0
2	B	23	0	0	3	0
2	C	18	0	0	1	0
2	D	13	0	0	0	0
All	All	10762	0	10660	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 12.

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:C:208:GLN:HE21	1:C:236:ALA:H	1.07	0.95
1:D:208:GLN:HE21	1:D:236:ALA:H	1.13	0.95
1:B:208:GLN:HE21	1:B:236:ALA:H	1.15	0.94
1:A:208:GLN:HE21	1:A:236:ALA:H	1.11	0.94
1:B:14:ARG:HH21	1:B:16:ARG:HH11	1.23	0.84
1:C:208:GLN:HE21	1:C:236:ALA:N	1.82	0.77
1:C:81:LEU:HD13	1:C:96:LEU:HD21	1.65	0.77
1:C:208:GLN:NE2	1:C:236:ALA:H	1.82	0.77
1:B:316:LEU:HD11	1:B:335:LEU:HD11	1.68	0.75
1:C:231:GLU:HG3	1:C:279:GLN:HE22	1.53	0.73
1:B:14:ARG:NH2	1:B:16:ARG:HH11	1.86	0.73
1:B:208:GLN:NE2	1:B:236:ALA:H	1.86	0.73
1:A:292:LEU:HB3	1:A:293:PRO:HD3	1.72	0.72
1:D:208:GLN:NE2	1:D:236:ALA:H	1.86	0.71
1:B:78:ALA:HB3	1:B:79:PRO:HD3	1.71	0.71
1:B:340:ASN:O	1:B:345:ARG:NH2	2.25	0.70
1:A:340:ASN:O	1:A:345:ARG:NH2	2.24	0.69
1:A:78:ALA:HB3	1:A:79:PRO:HD3	1.73	0.69
1:C:211:ASP:OD2	1:C:213:PRO:HD2	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:81:LEU:HD13	1:D:96:LEU:HD21	1.75	0.68
1:D:342:ASN:HD21	1:D:344:LEU:HB2	1.58	0.67
1:A:316:LEU:HD11	1:A:335:LEU:HD11	1.76	0.67
1:B:208:GLN:HE22	1:C:105:ILE:HG21	1.59	0.66
1:B:292:LEU:HB3	1:B:293:PRO:HD3	1.77	0.66
1:D:211:ASP:OD2	1:D:213:PRO:HD2	1.95	0.66
1:D:208:GLN:HE21	1:D:236:ALA:N	1.90	0.66
1:A:162:VAL:O	1:A:166:LYS:HG2	1.96	0.66
1:C:340:ASN:O	1:C:345:ARG:NH2	2.29	0.65
1:C:181:ASP:OD2	1:C:184:ARG:HB2	1.96	0.65
1:B:313:GLY:HA3	1:B:348:LEU:HB2	1.79	0.65
1:C:329:LEU:HD12	1:D:329:LEU:HD12	1.78	0.65
1:C:176:LEU:HD21	1:C:192:VAL:HG21	1.80	0.64
1:D:154:ILE:HG23	1:D:162:VAL:HG11	1.79	0.64
1:C:291:CYS:HA	1:C:294:VAL:CG1	2.29	0.63
1:C:86:PHE:HA	1:C:91:GLN:NE2	2.14	0.63
1:B:105:ILE:HG21	1:C:208:GLN:HE22	1.63	0.63
1:B:238:ARG:HD3	1:B:242:GLU:OE2	1.98	0.63
1:B:106:GLN:HG3	2:B:411:HOH:O	1.98	0.63
1:B:190:LEU:HD21	1:B:224:PRO:HG2	1.81	0.62
1:B:208:GLN:HE21	1:B:236:ALA:N	1.93	0.62
1:A:190:LEU:HD21	1:A:224:PRO:HG2	1.82	0.62
1:C:87:ALA:H	1:C:91:GLN:NE2	1.97	0.61
1:A:20:PHE:HE2	1:A:378:ARG:HG3	1.65	0.61
1:C:127:LEU:HD12	1:C:127:LEU:O	2.01	0.61
1:D:212:LEU:HB3	1:D:213:PRO:HD3	1.82	0.61
1:C:238:ARG:HD3	1:C:242:GLU:OE2	2.01	0.60
1:D:340:ASN:O	1:D:345:ARG:NH2	2.35	0.60
1:C:184:ARG:HG2	1:C:184:ARG:HH11	1.67	0.59
1:B:21:ARG:NH2	1:B:63:ALA:O	2.32	0.59
1:B:291:CYS:HA	1:B:294:VAL:HG13	1.84	0.59
1:D:238:ARG:HD3	1:D:242:GLU:OE2	2.03	0.59
1:B:320:ALA:HB1	1:B:362:LEU:HD21	1.83	0.59
1:C:342:ASN:HD21	1:C:344:LEU:HB2	1.68	0.58
1:B:155:ASN:HB3	1:B:157:GLU:OE1	2.03	0.58
1:B:14:ARG:HH21	1:B:16:ARG:NH1	1.98	0.58
1:B:160:GLU:H	1:B:160:GLU:CD	2.06	0.58
1:A:291:CYS:HA	1:A:294:VAL:HG13	1.85	0.58
1:A:342:ASN:HD21	1:A:344:LEU:HB2	1.67	0.58
1:B:373:ASP:OD2	1:B:376:ALA:HB2	2.03	0.58
1:D:78:ALA:HB3	1:D:79:PRO:HD3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:ILE:HG21	1:A:124:LEU:HD22	1.86	0.57
1:C:86:PHE:HA	1:C:91:GLN:HE21	1.68	0.57
1:B:342:ASN:HD21	1:B:344:LEU:HB2	1.67	0.57
1:A:208:GLN:NE2	1:A:236:ALA:H	1.92	0.57
1:B:237:ASP:OD2	1:C:105:ILE:HD11	2.04	0.57
1:D:14:ARG:NH2	1:D:16:ARG:HD3	2.20	0.56
1:B:299:VAL:CG1	1:B:329:LEU:HG	2.35	0.56
1:A:281:ASP:HB3	1:A:284:LYS:HB2	1.87	0.56
1:D:146:ARG:HG2	1:D:146:ARG:HH11	1.70	0.56
1:D:21:ARG:NH2	1:D:63:ALA:O	2.33	0.56
1:A:21:ARG:NH2	1:A:63:ALA:O	2.30	0.56
1:D:86:PHE:HA	1:D:91:GLN:NE2	2.21	0.56
1:A:130:ARG:HG3	1:A:130:ARG:HH11	1.71	0.55
1:A:155:ASN:HB3	1:A:157:GLU:OE1	2.07	0.55
1:B:44:GLU:HB3	1:B:54:TRP:CZ3	2.41	0.55
1:D:154:ILE:HG23	1:D:162:VAL:CG1	2.37	0.54
1:A:258:GLU:HB2	2:A:395:HOH:O	2.06	0.54
1:A:342:ASN:ND2	1:A:344:LEU:H	2.06	0.54
1:D:314:ILE:HD11	1:D:348:LEU:HD22	1.90	0.54
1:D:343:PRO:O	1:D:347:LEU:HB2	2.08	0.53
1:D:160:GLU:HB2	1:D:195:LEU:HD22	1.90	0.53
1:A:299:VAL:CG1	1:A:329:LEU:HG	2.38	0.53
1:C:61:PHE:HA	1:C:62:PRO:C	2.29	0.53
1:C:179:GLY:HA2	1:C:210:TRP:NE1	2.24	0.53
1:C:78:ALA:N	1:C:79:PRO:HD2	2.23	0.52
1:B:159:PRO:O	1:B:163:VAL:HG23	2.09	0.52
1:B:258:GLU:HB3	2:B:395:HOH:O	2.10	0.52
1:C:294:VAL:O	1:C:298:VAL:HG23	2.09	0.52
1:C:195:LEU:O	1:C:195:LEU:HD12	2.09	0.52
1:D:190:LEU:O	1:D:194:GLU:HG3	2.09	0.52
1:C:159:PRO:HG2	1:C:160:GLU:OE2	2.09	0.52
1:A:93:PHE:CZ	1:A:286:GLY:HA2	2.45	0.52
1:B:313:GLY:N	1:B:345:ARG:HA	2.25	0.51
1:C:212:LEU:HB3	1:C:213:PRO:HD3	1.91	0.51
1:B:162:VAL:O	1:B:166:LYS:HG2	2.10	0.51
1:A:181:ASP:OD2	1:A:184:ARG:HB2	2.10	0.51
1:C:247:ALA:HA	1:C:254:LEU:HD22	1.92	0.51
1:C:147:ILE:O	1:C:359:ARG:HB2	2.11	0.51
1:B:105:ILE:HD11	1:C:237:ASP:HB2	1.92	0.50
1:D:23:PRO:HA	1:D:37:ASP:HB3	1.92	0.50
1:B:345:ARG:NH1	2:B:399:HOH:O	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:ASN:ND2	1:A:284:LYS:NZ	2.59	0.50
1:A:130:ARG:CG	1:A:130:ARG:HH11	2.25	0.50
1:C:165:ARG:O	1:C:168:ALA:HB3	2.12	0.50
1:A:86:PHE:HA	1:A:91:GLN:NE2	2.27	0.50
1:B:342:ASN:ND2	1:B:344:LEU:H	2.10	0.50
1:D:294:VAL:O	1:D:298:VAL:HG23	2.12	0.50
1:C:313:GLY:N	1:C:345:ARG:HA	2.27	0.49
1:D:205:ASP:HA	1:D:231:GLU:HB3	1.94	0.49
1:B:191:HIS:O	1:B:194:GLU:HB3	2.12	0.49
1:A:238:ARG:HD3	1:A:242:GLU:OE2	2.13	0.49
1:A:304:ARG:HG2	1:A:331:SER:HB2	1.92	0.49
1:B:184:ARG:HH11	1:B:184:ARG:HG2	1.77	0.49
1:A:333:GLY:O	1:A:334:LEU:HD23	2.13	0.49
1:A:244:ALA:O	1:A:248:GLN:HG3	2.12	0.49
1:C:118:ALA:HB1	1:C:282:LEU:O	2.12	0.49
1:A:313:GLY:N	1:A:345:ARG:HA	2.28	0.49
1:D:234:LEU:HB3	1:D:238:ARG:HG3	1.95	0.49
1:A:58:TRP:CG	1:A:284:LYS:HG3	2.47	0.49
1:C:205:ASP:HA	1:C:231:GLU:HB3	1.95	0.49
1:B:223:GLY:N	1:B:224:PRO:HD2	2.28	0.49
1:A:44:GLU:HB3	1:A:54:TRP:CZ3	2.48	0.49
1:A:130:ARG:NH1	1:A:366:PRO:O	2.46	0.48
1:D:357:GLU:O	1:D:357:GLU:CG	2.60	0.48
1:C:246:LEU:HG	1:C:254:LEU:HD21	1.95	0.48
1:D:108:GLY:O	1:D:110:PRO:HD2	2.13	0.48
1:C:127:LEU:C	1:C:127:LEU:HD12	2.33	0.48
1:D:84:ARG:NH2	1:D:91:GLN:NE2	2.62	0.48
1:B:130:ARG:HH11	1:B:367:GLY:HA3	1.77	0.48
1:B:212:LEU:HB3	1:B:213:PRO:HD3	1.95	0.48
1:D:165:ARG:O	1:D:168:ALA:HB3	2.14	0.48
1:A:160:GLU:H	1:A:160:GLU:CD	2.16	0.48
1:D:77:LEU:HD13	1:D:120:LEU:HD12	1.94	0.48
1:D:86:PHE:HA	1:D:91:GLN:HE21	1.79	0.47
1:D:61:PHE:HA	1:D:62:PRO:C	2.34	0.47
1:B:259:ASN:ND2	1:C:106:GLN:HA	2.28	0.47
1:C:182:ASP:O	1:C:186:VAL:HG23	2.15	0.47
1:C:46:GLU:HG3	1:C:52:VAL:HG22	1.96	0.47
1:B:181:ASP:OD2	1:B:184:ARG:HB2	2.15	0.47
1:D:217:GLN:HE21	1:D:221:ARG:HD2	1.79	0.47
1:A:184:ARG:HH11	1:A:184:ARG:HG2	1.80	0.47
1:D:126:ASP:OD1	1:D:368:LEU:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:58:TRP:HB3	1:B:115:GLN:HG2	1.97	0.46
1:C:88:ASP:HB2	1:C:89:PRO:CD	2.45	0.46
1:C:342:ASN:C	1:C:342:ASN:HD22	2.18	0.46
1:C:217:GLN:O	1:C:221:ARG:HG3	2.15	0.46
1:B:154:ILE:HD12	1:B:154:ILE:N	2.31	0.46
1:B:154:ILE:O	1:B:177:LYS:HG3	2.15	0.46
1:C:10:ILE:HG22	1:C:12:PRO:HD3	1.96	0.46
1:D:276:ARG:HA	1:D:303:LEU:HD22	1.98	0.46
1:B:129:ALA:HB2	1:B:136:LEU:HD13	1.98	0.46
1:C:190:LEU:O	1:C:194:GLU:HG3	2.15	0.46
1:B:105:ILE:CD1	1:C:237:ASP:HB2	2.45	0.46
1:D:211:ASP:CG	1:D:213:PRO:HD2	2.35	0.46
1:B:61:PHE:HA	1:B:62:PRO:C	2.35	0.46
1:B:216:ARG:HD2	1:B:245:GLU:OE2	2.16	0.46
1:B:93:PHE:CZ	1:B:286:GLY:HA2	2.51	0.46
1:C:160:GLU:CD	1:C:160:GLU:H	2.19	0.46
1:D:95:HIS:O	1:D:99:ARG:HG2	2.16	0.46
1:B:68:HIS:HB2	1:C:68:HIS:HB2	1.97	0.46
1:A:342:ASN:C	1:A:342:ASN:HD22	2.19	0.45
1:D:292:LEU:HB3	1:D:293:PRO:CD	2.46	0.45
1:A:258:GLU:HG2	1:A:308:HIS:CE1	2.52	0.45
1:B:263:VAL:O	1:B:267:GLU:HG3	2.16	0.45
1:C:179:GLY:HA2	1:C:210:TRP:HE1	1.81	0.45
1:A:255:ALA:HB2	1:A:277:VAL:HB	1.99	0.45
1:B:259:ASN:HD21	1:C:106:GLN:HA	1.81	0.45
1:D:41:VAL:HG23	1:D:59:CYS:SG	2.57	0.45
1:A:217:GLN:HE21	1:A:221:ARG:HH11	1.65	0.45
1:A:313:GLY:HA3	1:A:348:LEU:HB2	1.99	0.45
1:B:44:GLU:HG3	1:B:44:GLU:O	2.17	0.45
1:C:193:ARG:HD3	1:C:193:ARG:O	2.17	0.45
1:C:158:ASN:HD22	1:C:158:ASN:HA	1.57	0.45
1:B:294:VAL:O	1:B:298:VAL:HG23	2.17	0.44
1:A:44:GLU:HG3	1:A:44:GLU:O	2.17	0.44
1:D:356:HIS:O	1:D:357:GLU:HB3	2.17	0.44
1:A:271:ALA:HA	1:B:50:GLY:O	2.17	0.44
1:C:226:GLN:OE1	1:C:226:GLN:HA	2.17	0.44
1:A:146:ARG:NH1	1:A:359:ARG:NH2	2.65	0.44
1:A:208:GLN:HE21	1:A:236:ALA:N	1.95	0.44
1:A:146:ARG:NH1	1:A:359:ARG:HH21	2.15	0.44
1:A:309:TYR:CE2	1:A:311:GLY:HA3	2.51	0.44
1:D:342:ASN:C	1:D:342:ASN:HD22	2.20	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:260:ILE:HG23	1:B:265:ALA:HB1	1.99	0.44
1:C:88:ASP:HB2	1:C:89:PRO:HD2	1.99	0.44
1:B:183:ALA:O	1:B:186:VAL:HG22	2.17	0.44
1:D:163:VAL:HG11	1:D:196:LEU:HD21	2.00	0.44
1:A:88:ASP:HB2	1:A:89:PRO:CD	2.48	0.44
1:C:208:GLN:HG2	1:C:235:ARG:HA	2.00	0.44
1:C:329:LEU:HD12	1:D:329:LEU:CD1	2.46	0.44
1:C:188:ASN:O	1:C:192:VAL:HG23	2.18	0.44
1:B:205:ASP:HA	1:B:231:GLU:HB3	2.00	0.44
1:B:290:GLY:O	1:B:294:VAL:HG12	2.17	0.43
1:B:299:VAL:HG12	1:B:329:LEU:HG	2.00	0.43
1:C:282:LEU:HD11	1:C:318:ALA:HB1	1.99	0.43
1:C:272:ALA:O	1:C:273:ARG:HB2	2.17	0.43
1:C:276:ARG:HA	1:C:303:LEU:HD22	1.98	0.43
1:A:223:GLY:N	1:A:224:PRO:HD2	2.33	0.43
1:A:57:VAL:HG13	1:A:115:GLN:C	2.38	0.43
1:A:156:PRO:HG3	1:A:180:PHE:CE2	2.53	0.43
1:C:267:GLU:HG3	2:C:400:HOH:O	2.19	0.43
1:D:255:ALA:HB2	1:D:277:VAL:HB	1.98	0.43
1:C:234:LEU:HB3	1:C:238:ARG:HG3	1.99	0.43
1:D:54:TRP:CE3	1:D:372:PRO:HG3	2.54	0.43
1:C:329:LEU:CD1	1:D:329:LEU:HD12	2.48	0.43
1:B:154:ILE:HD12	1:B:154:ILE:H	1.83	0.43
1:C:235:ARG:C	1:C:237:ASP:N	2.72	0.43
1:A:342:ASN:ND2	1:A:344:LEU:HB2	2.33	0.43
1:B:281:ASP:HB3	1:B:284:LYS:HB2	2.00	0.43
1:B:84:ARG:HG3	1:B:86:PHE:CZ	2.53	0.43
1:A:216:ARG:HD2	1:A:245:GLU:OE2	2.19	0.43
1:A:149:VAL:HA	1:A:335:LEU:O	2.19	0.42
1:D:342:ASN:ND2	1:D:342:ASN:C	2.72	0.42
1:B:239:PRO:HG3	1:D:8:ALA:HA	2.00	0.42
1:C:235:ARG:C	1:C:237:ASP:H	2.22	0.42
1:C:290:GLY:O	1:C:294:VAL:HG12	2.19	0.42
1:C:263:VAL:O	1:C:267:GLU:HB2	2.20	0.42
1:B:127:LEU:HD12	1:B:127:LEU:O	2.20	0.42
1:A:250:ALA:HA	1:A:251:PRO:HD3	1.79	0.42
1:A:154:ILE:HG23	1:A:162:VAL:CG2	2.49	0.42
1:D:120:LEU:HD23	1:D:120:LEU:HA	1.91	0.42
1:A:217:GLN:NE2	1:A:221:ARG:HH11	2.18	0.42
1:B:309:TYR:CE2	1:B:311:GLY:HA3	2.54	0.42
1:C:343:PRO:O	1:C:347:LEU:HG	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:234:LEU:HB3	1:B:238:ARG:HG3	2.02	0.42
1:A:259:ASN:HD21	1:A:284:LYS:HZ1	1.67	0.42
1:D:182:ASP:O	1:D:186:VAL:HG23	2.19	0.42
1:D:342:ASN:ND2	1:D:344:LEU:H	2.17	0.42
1:D:195:LEU:HD12	1:D:195:LEU:O	2.19	0.42
1:D:108:GLY:C	1:D:110:PRO:HD2	2.41	0.42
1:C:277:VAL:HG22	1:C:304:ARG:HB3	2.02	0.41
1:A:71:ARG:HA	1:A:71:ARG:HD2	1.91	0.41
1:C:314:ILE:HD11	1:C:348:LEU:HD22	2.00	0.41
1:C:342:ASN:ND2	1:C:344:LEU:HB2	2.33	0.41
1:D:188:ASN:O	1:D:192:VAL:HG23	2.20	0.41
1:A:130:ARG:CG	1:A:130:ARG:NH1	2.83	0.41
1:B:182:ASP:O	1:B:186:VAL:HG13	2.20	0.41
1:B:333:GLY:O	1:B:334:LEU:HD23	2.21	0.41
1:D:305:TYR:CZ	1:D:307:PRO:HD3	2.55	0.41
1:A:69:ARG:HH11	1:A:69:ARG:HG3	1.85	0.41
1:C:92:ALA:O	1:C:96:LEU:HG	2.20	0.41
1:A:285:TRP:CG	1:A:286:GLY:N	2.89	0.41
1:C:292:LEU:HB3	1:C:293:PRO:CD	2.51	0.41
1:C:44:GLU:HB3	1:C:54:TRP:CZ3	2.56	0.41
1:B:342:ASN:ND2	1:B:344:LEU:HB2	2.34	0.41
1:C:282:LEU:O	1:C:287:GLY:HA2	2.21	0.41
1:B:58:TRP:CG	1:B:284:LYS:HG3	2.56	0.41
1:C:54:TRP:CE3	1:C:372:PRO:HG3	2.56	0.41
1:D:193:ARG:HD3	1:D:193:ARG:O	2.21	0.41
1:C:131:ARG:HG2	1:C:131:ARG:HH11	1.86	0.41
1:A:81:LEU:HD13	1:A:96:LEU:HD11	2.02	0.41
1:C:203:MET:HG2	1:C:229:TRP:CZ2	2.56	0.41
1:A:58:TRP:HB3	1:A:115:GLN:HG2	2.03	0.40
1:B:57:VAL:HG13	1:B:115:GLN:C	2.42	0.40
1:C:122:ILE:HD11	1:C:282:LEU:HG	2.02	0.40
1:B:266:PHE:CZ	1:B:280:PRO:HB3	2.55	0.40
1:B:86:PHE:HA	1:B:91:GLN:NE2	2.36	0.40
1:C:342:ASN:ND2	1:C:344:LEU:H	2.19	0.40
1:D:357:GLU:O	1:D:357:GLU:HG2	2.20	0.40
1:C:174:PHE:CD2	1:C:174:PHE:N	2.90	0.40
1:A:320:ALA:HB1	1:A:362:LEU:HD21	2.04	0.40
1:B:344:LEU:HD23	1:B:344:LEU:HA	1.79	0.40
1:D:36:HIS:ND1	1:D:36:HIS:N	2.70	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	359/392 (92%)	342 (95%)	16 (4%)	1 (0%)	46	72
1	B	359/392 (92%)	342 (95%)	16 (4%)	1 (0%)	46	72
1	C	359/392 (92%)	336 (94%)	22 (6%)	1 (0%)	46	72
1	D	359/392 (92%)	339 (94%)	18 (5%)	2 (1%)	30	56
All	All	1436/1568 (92%)	1359 (95%)	72 (5%)	5 (0%)	46	72

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	157	GLU
1	D	157	GLU
1	A	198	ALA
1	B	198	ALA
1	D	286	GLY

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	254/278 (91%)	244 (96%)	10 (4%)	39	68
1	B	254/278 (91%)	243 (96%)	11 (4%)	35	64
1	C	254/278 (91%)	239 (94%)	15 (6%)	24	47
1	D	254/278 (91%)	237 (93%)	17 (7%)	20	40
All	All	1016/1112 (91%)	963 (95%)	53 (5%)	29	54

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	130	ARG
1	A	136	LEU
1	A	182	ASP
1	A	203	MET
1	A	230	LEU
1	A	278	MET
1	A	282	LEU
1	A	294	VAL
1	A	310	LEU
1	A	342	ASN
1	B	136	LEU
1	B	176	LEU
1	B	180	PHE
1	B	220	GLN
1	B	228	ASP
1	B	230	LEU
1	B	254	LEU
1	B	278	MET
1	B	282	LEU
1	B	294	VAL
1	B	342	ASN
1	C	24	VAL
1	C	81	LEU
1	C	127	LEU
1	C	136	LEU
1	C	158	ASN
1	C	228	ASP
1	C	230	LEU
1	C	252	MET
1	C	254	LEU
1	C	278	MET
1	C	294	VAL
1	C	310	LEU
1	C	335	LEU
1	C	341	ASP
1	C	342	ASN
1	D	81	LEU
1	D	127	LEU
1	D	136	LEU
1	D	157	GLU
1	D	158	ASN
1	D	176	LEU

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Mol	Chain	Res	Type
1	D	228	ASP
1	D	230	LEU
1	D	252	MET
1	D	254	LEU
1	D	278	MET
1	D	282	LEU
1	D	294	VAL
1	D	310	LEU
1	D	334	LEU
1	D	335	LEU
1	D	342	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	HIS
1	A	91	GLN
1	A	158	ASN
1	A	208	GLN
1	A	217	GLN
1	A	259	ASN
1	A	342	ASN
1	B	18	HIS
1	B	91	GLN
1	B	106	GLN
1	B	158	ASN
1	B	208	GLN
1	B	259	ASN
1	B	342	ASN
1	C	18	HIS
1	C	91	GLN
1	C	106	GLN
1	C	155	ASN
1	C	158	ASN
1	C	208	GLN
1	C	259	ASN
1	C	279	GLN
1	C	342	ASN
1	D	18	HIS
1	D	91	GLN
1	D	208	GLN
1	D	217	GLN

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Mol	Chain	Res	Type
1	D	226	GLN
1	D	259	ASN
1	D	342	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	363/392 (92%)	-0.20	2 (0%)	90	88	31, 46, 68, 78	0
1	B	363/392 (92%)	-0.20	2 (0%)	90	88	32, 46, 68, 79	0
1	C	363/392 (92%)	-0.19	2 (0%)	90	88	30, 46, 73, 84	0
1	D	363/392 (92%)	-0.16	2 (0%)	90	88	29, 47, 73, 85	0
All	All	1452/1568 (92%)	-0.19	8 (0%)	90	88	29, 46, 71, 85	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	180	PHE	3.2
1	A	180	PHE	2.9
1	C	180	PHE	2.6
1	A	331	SER	2.5
1	C	36	HIS	2.3
1	B	331	SER	2.2
1	D	157	GLU	2.0
1	B	357	GLU	2.0

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.