



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 01:59 PM UTC

PDB ID : 3DDM / pdb_00003ddm
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

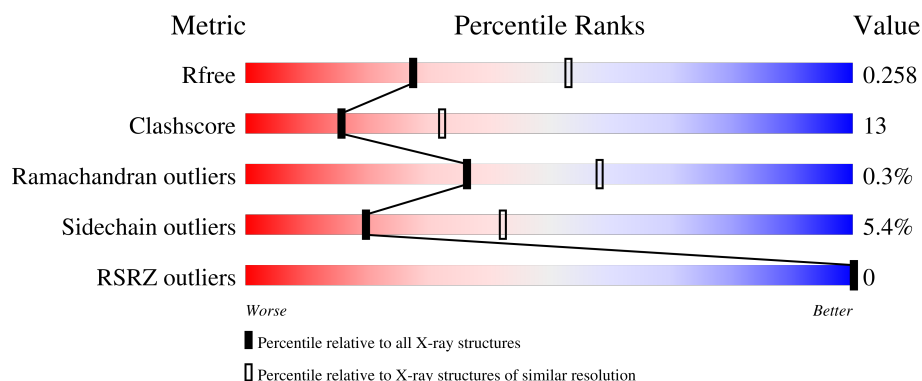
1 Overall quality at a glance

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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (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 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 $\leq 5\%$. 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	 65% 26% • 7%
1	B	392	 64% 27% • 7%
1	C	392	 65% 26% • 7%
1	D	392	 66% 24% • 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 mutation	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

Continued on next page...

Continued from previous page...

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 mutation	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 mutation	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

Continued on next page...

Continued from previous page...

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 mutation	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

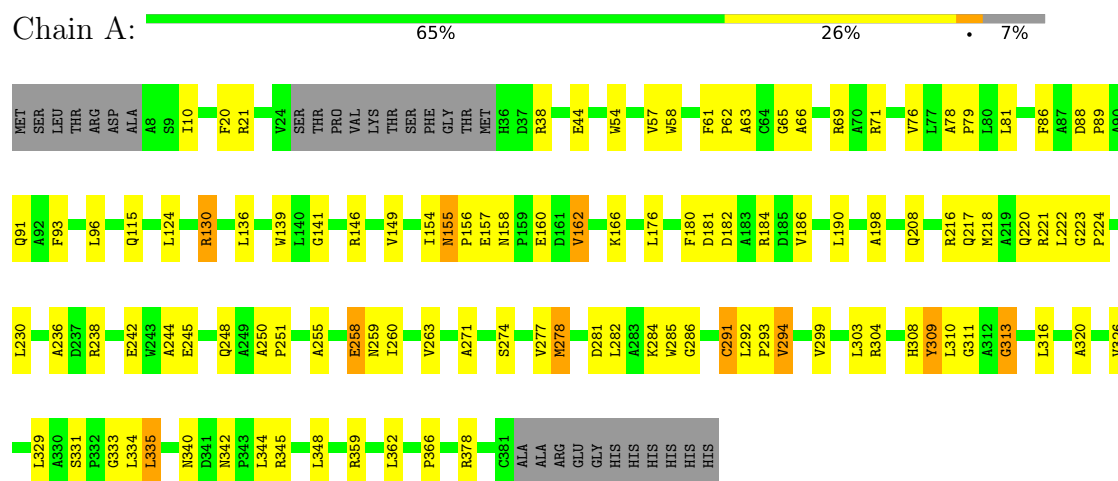
- Molecule 2 is water.

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

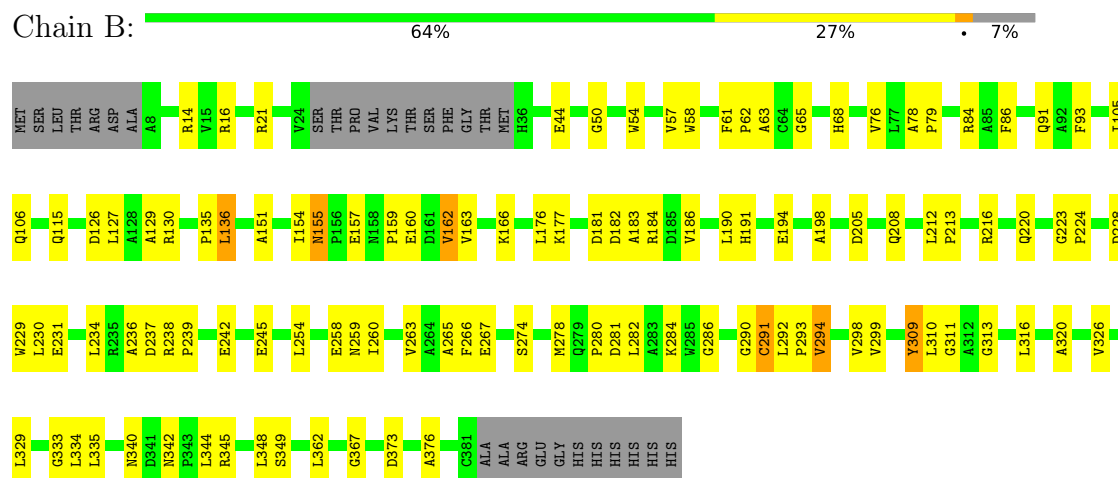
3 Residue-property plots

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: Putative mandelate racemase/muconate lactonizing enzyme

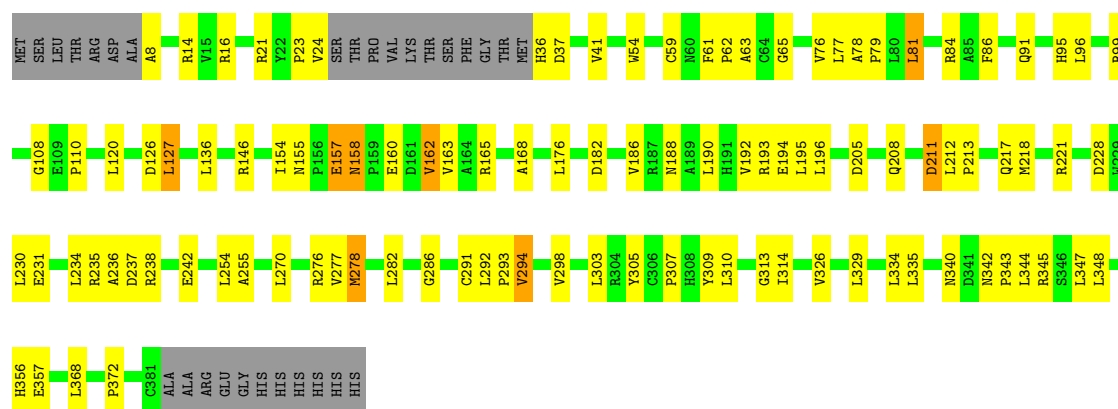


- Molecule 1: Putative mandelate racemase/muconate lactonizing enzyme



- Molecule 1: Putative mandelate racemase/muconate lactonizing enzyme





4 Data and refinement statistics

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 24.58 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.9 (24.58-2.60) 99.9 (24.58-2.60)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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	4732 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	51.8	Xtriage
Anisotropy	0.210	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 24.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.480 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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	0.45	0/2734	0.99	14/3735 (0.4%)
1	B	0.46	0/2734	0.99	13/3735 (0.3%)
1	C	0.45	0/2734	0.92	6/3735 (0.2%)
1	D	0.46	0/2734	0.94	11/3735 (0.3%)
All	All	0.46	0/10936	0.96	44/14940 (0.3%)

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 (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	155	ASN	CA-C-N	8.94	128.68	119.56
1	D	155	ASN	C-N-CA	8.94	128.68	119.56
1	B	326	VAL	CA-C-N	8.63	128.22	119.24
1	B	326	VAL	C-N-CA	8.63	128.22	119.24
1	A	155	ASN	CA-C-N	8.40	128.05	119.56
1	A	155	ASN	C-N-CA	8.40	128.05	119.56
1	C	155	ASN	CA-C-N	8.17	127.90	119.56
1	C	155	ASN	C-N-CA	8.17	127.90	119.56
1	B	155	ASN	CA-C-N	8.16	127.88	119.56
1	B	155	ASN	C-N-CA	8.16	127.88	119.56
1	A	326	VAL	CA-C-N	8.10	128.56	119.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	326	VAL	C-N-CA	8.10	128.56	119.32
1	A	65	GLY	N-CA-C	7.66	123.10	114.67
1	D	76	VAL	CB-CA-C	-6.86	105.88	111.71
1	B	76	VAL	N-CA-C	6.71	116.92	111.62
1	C	76	VAL	CB-CA-C	-6.54	106.15	111.71
1	A	274	SER	N-CA-C	-6.34	103.89	111.69
1	D	211	ASP	N-CA-C	-6.25	101.20	110.46
1	D	313	GLY	N-CA-C	5.92	119.83	112.73
1	A	158	ASN	CA-C-N	5.78	125.25	119.24
1	A	158	ASN	C-N-CA	5.78	125.25	119.24
1	A	313	GLY	N-CA-C	5.77	119.65	112.73
1	D	158	ASN	CA-C-N	5.51	126.73	119.84
1	D	158	ASN	C-N-CA	5.51	126.73	119.84
1	A	66	ALA	N-CA-C	5.51	116.97	111.07
1	B	274	SER	N-CA-C	-5.49	105.31	112.23
1	A	76	VAL	N-CA-C	5.48	115.95	111.62
1	A	260	ILE	N-CA-C	-5.45	100.49	108.11
1	D	326	VAL	CA-C-N	5.43	125.52	119.87
1	D	326	VAL	C-N-CA	5.43	125.52	119.87
1	A	291	CYS	N-CA-C	5.43	119.07	112.23
1	B	135	PRO	N-CA-C	-5.42	102.05	111.32
1	C	200	THR	N-CA-C	5.41	116.22	109.57
1	C	199	ALA	N-CA-C	5.38	117.58	111.02
1	C	291	CYS	N-CA-C	5.33	118.00	111.82
1	B	291	CYS	N-CA-C	5.25	118.85	112.23
1	B	126	ASP	N-CA-C	-5.23	105.58	111.28
1	D	65	GLY	N-CA-C	5.19	120.38	114.67
1	B	151	ALA	N-CA-C	-5.18	102.19	109.96
1	B	65	GLY	N-CA-C	5.17	123.97	115.34
1	B	349	SER	CA-C-N	5.08	124.86	119.28
1	B	349	SER	C-N-CA	5.08	124.86	119.28
1	D	291	CYS	N-CA-C	5.03	117.66	111.82
1	A	182	ASP	N-CA-C	5.01	117.13	111.02

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 ⓘ

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	71	0
1	B	2672	0	2665	78	0
1	C	2672	0	2665	84	0
1	D	2672	0	2665	64	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	284	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 (284) 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:D:270:LEU:HA	1:D:278:MET:HE1	1.70	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:211:ASP:OD2	1:C:213:PRO:HD2	1.92	0.68
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:A:278:MET:HE1	1:A:303:LEU:HD13	1.76	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:86:PHE:HA	1:C:91:GLN:NE2	2.14	0.63
1:C:291:CYS:HA	1:C:294:VAL:CG1	2.29	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:160:GLU:CD	1:B:160:GLU:H	2.06	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:D:270:LEU:CA	1:D:278:MET:HE1	2.30	0.61
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:O	1:C:127:LEU:HD12	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:B:320:ALA:HB1	1:B:362:LEU:HD21	1.83	0.59
1:D:238:ARG:HD3	1:D:242:GLU:OE2	2.03	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:A:291:CYS:HA	1:A:294:VAL:HG13	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:ASN:HD21	1:A:344:LEU:HB2	1.67	0.58
1:C:61:PHE:HA	1:C:62:PRO:C	2.29	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
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:B:299:VAL:CG1	1:B:329:LEU:HG	2.35	0.56
1:D:14:ARG:NH2	1:D:16:ARG:HD3	2.20	0.56
1:A:259:ASN:ND2	1:A:284:LYS:HZ3	2.04	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:127:LEU:HD12	1:C:127:LEU:C	2.33	0.53
1:C:179:GLY:HA2	1:C:210:TRP:NE1	2.24	0.53
1:A:160:GLU:CD	1:A:160:GLU:H	2.16	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:195:LEU:HD12	1:C:195:LEU:O	2.09	0.52
1:C:294:VAL:O	1:C:298:VAL:HG23	2.09	0.52
1:D:61:PHE:HA	1:D:62:PRO:C	2.34	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:C:342:ASN:HD22	1:C:342:ASN:C	2.18	0.52
1:B:162:VAL:O	1:B:166:LYS:HG2	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:61:PHE:HA	1:B:62:PRO:C	2.35	0.51
1:D:211:ASP:CG	1:D:213:PRO:HD2	2.35	0.51
1:C:147:ILE:O	1:C:359:ARG:HB2	2.11	0.51
1:C:160:GLU:CD	1:C:160:GLU:H	2.19	0.50
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:A:130:ARG:HH11	1:A:130:ARG:CG	2.25	0.50
1:A:259:ASN:ND2	1:A:284:LYS:NZ	2.59	0.50
1:B:345:ARG:NH1	2:B:399:HOH:O	2.45	0.50
1:C:165:ARG:O	1:C:168:ALA:HB3	2.12	0.50
1:A:342:ASN:C	1:A:342:ASN:HD22	2.19	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:A:238:ARG:HD3	1:A:242:GLU:OE2	2.13	0.49
1:B:191:HIS:O	1:B:194:GLU:HB3	2.12	0.49
1:A:304:ARG:HG2	1:A:331:SER:HB2	1.92	0.49
1:D:342:ASN:C	1:D:342:ASN:HD22	2.20	0.49
1:A:244:ALA:O	1:A:248:GLN:HG3	2.12	0.49
1:A:333:GLY:O	1:A:334:LEU:HD23	2.13	0.49
1:B:184:ARG:HH11	1:B:184:ARG:HG2	1.77	0.49
1:C:118:ALA:HB1	1:C:282:LEU:O	2.12	0.49
1:A:58:TRP:CG	1:A:284:LYS:HG3	2.47	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:44:GLU:HB3	1:A:54:TRP:CZ3	2.48	0.49
1:B:223:GLY:N	1:B:224:PRO:HD2	2.28	0.49
1:C:205:ASP:HA	1:C:231:GLU:HB3	1.95	0.49
1:A:130:ARG:NH1	1:A:366:PRO:O	2.46	0.48
1:D:357:GLU:CG	1:D:357:GLU:O	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: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:A:57:VAL:HG13	1:A:115:GLN:C	2.38	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:77:LEU:HD13	1:D:120:LEU:HD12	1.94	0.48
1:B:259:ASN:ND2	1:C:106:GLN:HA	2.28	0.47
1:D:86:PHE:HA	1:D:91:GLN:HE21	1.79	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:C:235:ARG:C	1:C:237:ASP:N	2.72	0.47
1:A:186:VAL:HG13	1:A:218:MET:HE1	1.97	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:D:342:ASN:C	1:D:342:ASN:ND2	2.72	0.47
1:A:184:ARG:HG2	1:A:184:ARG:HH11	1.80	0.47
1:C:235:ARG:C	1:C:237:ASP:H	2.22	0.47
1:D:126:ASP:OD1	1:D:368:LEU:N	2.48	0.47
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:B:154:ILE:N	1:B:154:ILE:HD12	2.31	0.46
1:C:217:GLN:O	1:C:221:ARG:HG3	2.15	0.46
1:D:108:GLY:C	1:D:110:PRO:HD2	2.41	0.46
1:B:129:ALA:HB2	1:B:136:LEU:HD13	1.98	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:C:190:LEU:O	1:C:194:GLU:HG3	2.15	0.46
1:D:276:ARG:HA	1:D:303:LEU:HD22	1.98	0.46
1:B:105:ILE:CD1	1:C:237:ASP:HB2	2.45	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:B:68:HIS:HB2	1:C:68:HIS:HB2	1.97	0.46
1:D:95:HIS:O	1:D:99:ARG:HG2	2.16	0.46
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:A:255:ALA:HB2	1:A:277:VAL:HB	1.99	0.45
1:C:179:GLY:HA2	1:C:210:TRP:HE1	1.81	0.45
1:B:259:ASN:HD21	1:C:106:GLN:HA	1.81	0.45
1:A:217:GLN:HE21	1:A:221:ARG:HH11	1.65	0.45
1:D:41:VAL:HG23	1:D:59:CYS:SG	2.57	0.45
1:A:313:GLY:HA3	1:A:348:LEU:HB2	1.99	0.45
1:C:158:ASN:HD22	1:C:158:ASN:HA	1.57	0.45
1:C:193:ARG:HD3	1:C:193:ARG:O	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:GLU:O	1:A:44:GLU:HG3	2.17	0.44
1:A:146:ARG:NH1	1:A:359:ARG:NH2	2.65	0.44
1:A:271:ALA:HA	1:B:50:GLY:O	2.17	0.44
1:B:294:VAL:O	1:B:298:VAL:HG23	2.17	0.44
1:C:226:GLN:OE1	1:C:226:GLN:HA	2.17	0.44
1:D:356:HIS:O	1:D:357:GLU:HB3	2.17	0.44
1:A:146:ARG:NH1	1:A:359:ARG:HH21	2.15	0.44
1:A:208:GLN:HE21	1:A:236:ALA:N	1.95	0.44
1:A:309:TYR:CE2	1:A:311:GLY:HA3	2.51	0.44
1:B:260:ILE:HG23	1:B:265:ALA:HB1	1.99	0.44
1:B:183:ALA:O	1:B:186:VAL:HG22	2.17	0.44
1:C:88:ASP:HB2	1:C:89:PRO:HD2	1.99	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:D:127:LEU:HD12	1:D:127:LEU:C	2.43	0.44
1:B:57:VAL:HG13	1:B:115:GLN:C	2.42	0.44
1:C:188:ASN:O	1:C:192:VAL:HG23	2.18	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:A:61:PHE:HA	1:A:62:PRO:C	2.43	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:211:ASP:CG	1:C:213:PRO:HD2	2.43	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:C:282:LEU:HD11	1:C:318:ALA:HB1	1.99	0.43
1:A:156:PRO:HG3	1:A:180:PHE:CE2	2.53	0.43
1:A:223:GLY:N	1:A:224:PRO:HD2	2.33	0.43
1:B:342:ASN:C	1:B:342:ASN:HD22	2.26	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:C:342:ASN:C	1:C:342:ASN:ND2	2.76	0.43
1:D:54:TRP:CE3	1:D:372:PRO:HG3	2.54	0.43
1:B:154:ILE:HD12	1:B:154:ILE:H	1.83	0.43
1:C:329:LEU:CD1	1:D:329:LEU:HD12	2.48	0.43
1:A:216:ARG:HD2	1:A:245:GLU:OE2	2.19	0.43
1:A:342:ASN:ND2	1:A:344:LEU:HB2	2.33	0.43
1:B:84:ARG:HG3	1:B:86:PHE:CZ	2.53	0.43
1:B:281:ASP:HB3	1:B:284:LYS:HB2	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:GLU:O	1:B:44:GLU:HG3	2.17	0.42
1:A:149:VAL:HA	1:A:335:LEU:O	2.19	0.42
1:A:238:ARG:HD3	1:A:242:GLU:CD	2.44	0.42
1:B:229:TRP:CD1	1:B:229:TRP:C	2.97	0.42
1:B:239:PRO:HG3	1:D:8:ALA:HA	2.00	0.42
1:A:250:ALA:HA	1:A:251:PRO:HD3	1.79	0.42
1:B:127:LEU:HD12	1:B:127:LEU:O	2.20	0.42
1:C:263:VAL:O	1:C:267:GLU:HB2	2.20	0.42
1:C:290:GLY:O	1:C:294:VAL:HG12	2.19	0.42
1:A:154:ILE:HG23	1:A:162:VAL:CG2	2.49	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:D:120:LEU:HD23	1:D:120:LEU:HA	1.91	0.42
1:C:343:PRO:O	1:C:347:LEU:HG	2.19	0.42
1:B:234:LEU:HB3	1:B:238:ARG:HG3	2.02	0.42
1:B:335:LEU:HD13	1:B:335:LEU:C	2.45	0.42
1:D:182:ASP:O	1:D:186:VAL:HG23	2.19	0.42
1:D:195:LEU:O	1:D:195:LEU:HD12	2.19	0.42
1:D:342:ASN:ND2	1:D:344:LEU:H	2.17	0.42
1:A:71:ARG:HA	1:A:71:ARG:HD2	1.91	0.41
1:A:139:TRP:C	1:A:141:GLY:H	2.28	0.41
1:C:277:VAL:HG22	1:C:304:ARG:HB3	2.02	0.41
1:C:314:ILE:HD11	1:C:348:LEU:HD22	2.00	0.41
1:D:127:LEU:C	1:D:127:LEU:CD1	2.93	0.41
1:A:342:ASN:ND2	1:A:342:ASN:C	2.78	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:HG3	1:A:69:ARG:HH11	1.85	0.41
1:A:285:TRP:CG	1:A:286:GLY:N	2.89	0.41
1:C:44:GLU:HB3	1:C:54:TRP:CZ3	2.56	0.41
1:C:92:ALA:O	1:C:96:LEU:HG	2.20	0.41
1:C:292:LEU:HB3	1:C:293:PRO:CD	2.51	0.41
1:A:81:LEU:HD13	1:A:96:LEU:HD11	2.02	0.41
1:A:222:LEU:O	1:A:223:GLY:C	2.64	0.41
1:B:58:TRP:CG	1:B:284:LYS:HG3	2.56	0.41
1:B:342:ASN:ND2	1:B:342:ASN:C	2.78	0.41
1:B:342:ASN:ND2	1:B:344:LEU:HB2	2.34	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:54:TRP:CE3	1:C:372:PRO:HG3	2.56	0.41
1:C:131:ARG:HG2	1:C:131:ARG:HH11	1.86	0.41
1:C:203:MET:HG2	1:C:229:TRP:CZ2	2.56	0.41
1:C:282:LEU:O	1:C:287:GLY:HA2	2.21	0.41
1:C:308:HIS:ND1	1:C:308:HIS:C	2.79	0.41
1:D:193:ARG:HD3	1:D:193:ARG:O	2.21	0.41
1:A:58:TRP:HB3	1:A:115:GLN:HG2	2.03	0.40
1:B:266:PHE:CZ	1:B:280:PRO:HB3	2.55	0.40
1:C:122:ILE:HD11	1:C:282:LEU:HG	2.02	0.40
1:B:86:PHE:HA	1:B:91:GLN:NE2	2.36	0.40
1:A:38:ARG:HD3	1:A:342:ASN:CG	2.47	0.40
1:A:320:ALA:HB1	1:A:362:LEU:HD21	2.04	0.40
1:C:174:PHE:CD2	1:C:174:PHE:N	2.90	0.40
1:C:342:ASN:ND2	1:C:344:LEU:H	2.19	0.40
1:D:235:ARG:C	1:D:237:ASP:N	2.80	0.40
1:D:357:GLU:O	1:D:357:GLU:HG2	2.20	0.40
1:B:344:LEU:HA	1:B:344:LEU:HD23	1.79	0.40
1:D:36:HIS:ND1	1:D:36:HIS:N	2.70	0.40
1:D:186:VAL:HG23	1:D:218:MET:HE1	2.04	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%)	36	58
1	B	359/392 (92%)	342 (95%)	16 (4%)	1 (0%)	36	58
1	C	359/392 (92%)	336 (94%)	22 (6%)	1 (0%)	36	58
1	D	359/392 (92%)	339 (94%)	18 (5%)	2 (1%)	21	42
All	All	1436/1568 (92%)	1359 (95%)	72 (5%)	5 (0%)	36	58

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%)	241 (95%)	13 (5%)	21	45
1	B	254/278 (91%)	243 (96%)	11 (4%)	26	51
1	C	254/278 (91%)	240 (94%)	14 (6%)	19	41
1	D	254/278 (91%)	237 (93%)	17 (7%)	15	33
All	All	1016/1112 (91%)	961 (95%)	55 (5%)	20	42

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	130	ARG
1	A	136	LEU
1	A	162	VAL
1	A	176	LEU
1	A	220	GLN
1	A	230	LEU
1	A	258	GLU
1	A	263	VAL
1	A	278	MET
1	A	282	LEU
1	A	294	VAL
1	A	310	LEU
1	A	335	LEU
1	B	136	LEU
1	B	162	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	176	LEU
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	310	LEU
1	C	24	VAL
1	C	81	LEU
1	C	127	LEU
1	C	136	LEU
1	C	158	ASN
1	C	220	GLN
1	C	228	ASP
1	C	230	LEU
1	C	254	LEU
1	C	263	VAL
1	C	278	MET
1	C	294	VAL
1	C	310	LEU
1	C	335	LEU
1	D	24	VAL
1	D	81	LEU
1	D	127	LEU
1	D	136	LEU
1	D	157	GLU
1	D	158	ASN
1	D	162	VAL
1	D	176	LEU
1	D	228	ASP
1	D	230	LEU
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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) 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	308	HIS
1	A	342	ASN
1	B	18	HIS
1	B	91	GLN
1	B	106	GLN
1	B	158	ASN
1	B	191	HIS
1	B	207	ASN
1	B	208	GLN
1	B	259	ASN
1	B	342	ASN
1	C	91	GLN
1	C	106	GLN
1	C	155	ASN
1	C	158	ASN
1	C	208	GLN
1	C	248	GLN
1	C	259	ASN
1	C	279	GLN
1	C	340	ASN
1	C	342	ASN
1	D	18	HIS
1	D	91	GLN
1	D	208	GLN
1	D	217	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 [i](#)

There are no oligosaccharides 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	363/392 (92%)	-1.52	0 100 100	31, 46, 68, 78	0
1	B	363/392 (92%)	-1.52	0 100 100	32, 46, 68, 79	0
1	C	363/392 (92%)	-1.52	0 100 100	30, 46, 73, 84	0
1	D	363/392 (92%)	-1.51	0 100 100	29, 47, 73, 85	0
All	All	1452/1568 (92%)	-1.52	0 100 100	29, 46, 70, 85	0

There are no RSRZ outliers to report.

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 oligosaccharides 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.