



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 05:18 am BST

PDB ID : 4V2Q
Title : Ironing out their differences: Dissecting the structural determinants of a phenylalanine aminomutase and ammonia lyase
Authors : Heberling, M.; Masman, M.; Bartsch, S.; Wybenga, G.G.; Dijkstra, B.W.; Marrink, S.; Janssen, D.
Deposited on : 2014-10-14
Resolution : 1.95 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

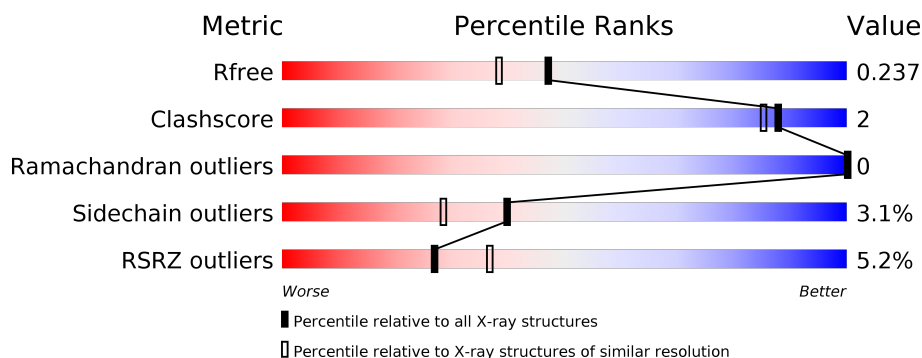
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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 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	705	<div> <div>3%</div> <div> <div></div> <div>81%</div> <div>6%</div> <div>13%</div> </div> </div>
1	B	705	<div> <div>7%</div> <div> <div></div> <div>81%</div> <div>6%</div> <div>12%</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9878 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 PHENYLALANINE AMMONIA-LYASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	613	Total	C	N	O	S	0	0	0
			4770	3031	816	901	22			
1	B	621	Total	C	N	O	S	0	0	0
			4829	3068	826	913	22			

There are 50 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP Q68G84
A	-18	GLY	-	expression tag	UNP Q68G84
A	-17	SER	-	expression tag	UNP Q68G84
A	-16	SER	-	expression tag	UNP Q68G84
A	-15	HIS	-	expression tag	UNP Q68G84
A	-14	HIS	-	expression tag	UNP Q68G84
A	-13	HIS	-	expression tag	UNP Q68G84
A	-12	HIS	-	expression tag	UNP Q68G84
A	-11	HIS	-	expression tag	UNP Q68G84
A	-10	HIS	-	expression tag	UNP Q68G84
A	-9	SER	-	expression tag	UNP Q68G84
A	-8	SER	-	expression tag	UNP Q68G84
A	-7	GLY	-	expression tag	UNP Q68G84
A	-6	LEU	-	expression tag	UNP Q68G84
A	-5	VAL	-	expression tag	UNP Q68G84
A	-4	PRO	-	expression tag	UNP Q68G84
A	-3	ARG	-	expression tag	UNP Q68G84
A	-2	GLY	-	expression tag	UNP Q68G84
A	-1	SER	-	expression tag	UNP Q68G84
A	0	HIS	-	expression tag	UNP Q68G84
A	89	THR	CYS	engineered mutation	UNP Q68G84
A	97	GLY	LEU	engineered mutation	UNP Q68G84
A	175	MDO	ALA	chromophore	UNP Q68G84
A	175	MDO	SER	chromophore	UNP Q68G84
A	175	MDO	GLY	chromophore	UNP Q68G84

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	MET	-	expression tag	UNP Q68G84
B	-18	GLY	-	expression tag	UNP Q68G84
B	-17	SER	-	expression tag	UNP Q68G84
B	-16	SER	-	expression tag	UNP Q68G84
B	-15	HIS	-	expression tag	UNP Q68G84
B	-14	HIS	-	expression tag	UNP Q68G84
B	-13	HIS	-	expression tag	UNP Q68G84
B	-12	HIS	-	expression tag	UNP Q68G84
B	-11	HIS	-	expression tag	UNP Q68G84
B	-10	HIS	-	expression tag	UNP Q68G84
B	-9	SER	-	expression tag	UNP Q68G84
B	-8	SER	-	expression tag	UNP Q68G84
B	-7	GLY	-	expression tag	UNP Q68G84
B	-6	LEU	-	expression tag	UNP Q68G84
B	-5	VAL	-	expression tag	UNP Q68G84
B	-4	PRO	-	expression tag	UNP Q68G84
B	-3	ARG	-	expression tag	UNP Q68G84
B	-2	GLY	-	expression tag	UNP Q68G84
B	-1	SER	-	expression tag	UNP Q68G84
B	0	HIS	-	expression tag	UNP Q68G84
B	89	THR	CYS	engineered mutation	UNP Q68G84
B	97	GLY	LEU	engineered mutation	UNP Q68G84
B	175	MDO	ALA	chromophore	UNP Q68G84
B	175	MDO	SER	chromophore	UNP Q68G84
B	175	MDO	GLY	chromophore	UNP Q68G84

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	154	Total O 154 154	0	0
2	B	125	Total O 125 125	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	181.53Å 76.17Å 120.45Å 90.00° 120.42° 90.00°	Depositor
Resolution (Å)	103.87 – 1.95 47.38 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.7 (103.87-1.95) 99.7 (47.38-1.95)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.39 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.190 , 0.216 0.227 , 0.237	Depositor DCC
R_{free} test set	5159 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	26.0	Xtriage
Anisotropy	0.084	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.73 , 44.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9878	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.28% 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

Bond lengths and bond angles in the following residue types are not validated in this section: MDO

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	1/4837 (0.0%)	0.58	1/6563 (0.0%)
1	B	0.46	1/4895 (0.0%)	0.58	2/6640 (0.0%)
All	All	0.46	2/9732 (0.0%)	0.58	3/13203 (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	2
1	B	0	2
All	All	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	294	TRP	CD2-CE2	5.07	1.47	1.41
1	A	68	TRP	CD2-CE2	5.01	1.47	1.41

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	381	ASP	CB-CG-OD1	5.58	123.33	118.30
1	B	481	LEU	CA-CB-CG	5.42	127.75	115.30
1	A	481	LEU	CA-CB-CG	5.39	127.69	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	175	MDO	Mainchain,Peptide
1	B	175	MDO	Mainchain,Peptide

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	4770	0	4821	22	0
1	B	4829	0	4893	22	0
2	A	154	0	0	0	0
2	B	125	0	0	0	0
All	All	9878	0	9714	37	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 2.

All (37) 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:352:ALA:HB3	1:B:279:VAL:HG13	1.66	0.75
1:B:501:GLU:OE1	1:B:619:ARG:HD2	1.91	0.70
1:A:446:PRO:HD3	1:B:446:PRO:HD3	1.76	0.67
1:A:322:TYR:HE2	1:B:175:MDO:HB1	1.60	0.66
1:B:227:LEU:O	1:B:231:ASN:HB2	1.97	0.64
1:A:294:TRP:CH2	1:A:624:LYS:HE2	2.35	0.62
1:A:227:LEU:O	1:A:231:ASN:HB2	2.04	0.58
1:A:437:SER:O	1:A:441:GLN:HG2	2.06	0.55
1:A:174:SER:C	1:A:175:MDO:CA	2.72	0.55
1:B:55:ALA:O	1:B:59:ARG:HB3	2.11	0.51
1:A:27:ILE:CD1	1:A:43:LEU:HB2	2.40	0.51
1:B:31:GLY:HA3	1:B:61:ARG:HH12	1.78	0.48
1:A:175:MDO:HB1	1:B:322:TYR:HE2	1.77	0.48
1:A:352:ALA:HB3	1:B:279:VAL:CG1	2.39	0.48
1:B:178:ASP:HB3	1:B:181:PRO:HG2	1.96	0.47
1:B:437:SER:O	1:B:441:GLN:HG2	2.14	0.47
1:B:545:CYS:SG	1:B:589:SER:HA	2.56	0.45
1:B:552:LEU:O	1:B:556:LYS:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:460:ASP:OD2	1:B:400:GLU:OE2	2.34	0.45
1:B:114:THR:HG22	1:B:122:ASP:HB2	1.98	0.45
1:A:51:VAL:HG21	1:A:159:LEU:HD13	1.98	0.45
1:B:175:MDO:HA32	1:B:175:MDO:N	2.32	0.45
1:B:224:LYS:HE2	1:B:356:PRO:HD2	2.01	0.43
1:A:131:SER:HB2	1:A:238:ALA:HB1	2.00	0.43
1:A:384:ARG:HG2	1:A:444:ALA:HA	2.00	0.42
1:A:175:MDO:O2	1:A:231:ASN:ND2	2.48	0.42
1:A:111:GLY:HA3	1:A:168:PRO:HG2	2.02	0.42
1:B:209:GLU:O	1:B:213:ARG:HG3	2.19	0.42
1:B:500:GLU:HG3	1:B:537:VAL:HG12	2.01	0.42
1:A:330:TRP:O	1:A:333:PRO:HD2	2.20	0.42
1:B:51:VAL:HG21	1:B:159:LEU:HD13	2.01	0.41
1:A:322:TYR:CE2	1:B:175:MDO:HB1	2.48	0.41
1:A:43:LEU:HD22	1:A:134:LEU:HD22	2.03	0.41
1:B:537:VAL:HA	1:B:540:TYR:CE2	2.56	0.41
1:A:59:ARG:HD3	1:A:149:TRP:CG	2.56	0.40
1:A:182:LEU:HD21	1:A:234:SER:HB2	2.03	0.40
1:A:559:CYS:O	1:A:562:THR:HG22	2.20	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	598/705 (85%)	587 (98%)	11 (2%)	0	100	100
1	B	606/705 (86%)	594 (98%)	12 (2%)	0	100	100
All	All	1204/1410 (85%)	1181 (98%)	23 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	521/591 (88%)	507 (97%)	14 (3%)	44	34
1	B	528/591 (89%)	510 (97%)	18 (3%)	37	25
All	All	1049/1182 (89%)	1017 (97%)	32 (3%)	40	28

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	ARG
1	A	107	CYS
1	A	231	ASN
1	A	268	ARG
1	A	334	LEU
1	A	353	ASN
1	A	392	LYS
1	A	455	GLU
1	A	481	LEU
1	A	555	LEU
1	A	591	ARG
1	A	602	LEU
1	A	619	ARG
1	A	671	HIS
1	B	43	LEU
1	B	59	ARG
1	B	107	CYS
1	B	114	THR
1	B	123	GLU
1	B	147	ILE
1	B	231	ASN
1	B	268	ARG
1	B	278	LYS
1	B	279	VAL
1	B	304	LEU
1	B	334	LEU
1	B	392	LYS

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Mol	Chain	Res	Type
1	B	481	LEU
1	B	555	LEU
1	B	589	SER
1	B	602	LEU
1	B	673	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	GLN
1	A	231	ASN
1	B	231	ASN
1	B	413	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MDO	A	175	1	12,13,14	2.75	4 (33%)	15,18,20	2.64	8 (53%)
1	MDO	B	175	1	12,13,14	2.82	5 (41%)	15,18,20	2.51	7 (46%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MDO	A	175	1	-	3/4/23/24	0/1/1/1
1	MDO	B	175	1	-	1/4/23/24	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	175	MDO	O2-C2	6.98	1.37	1.23
1	A	175	MDO	O2-C2	6.67	1.37	1.23
1	A	175	MDO	O-C	4.22	1.43	1.19
1	B	175	MDO	O-C	4.04	1.42	1.19
1	A	175	MDO	C2-N3	-3.16	1.32	1.39
1	B	175	MDO	C2-N3	-3.02	1.32	1.39
1	B	175	MDO	CA-C1	2.73	1.55	1.51
1	A	175	MDO	CA2-N2	-2.46	1.34	1.39
1	B	175	MDO	CA2-N2	-2.42	1.34	1.39

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	175	MDO	CA2-C2-N3	6.76	106.57	103.37
1	B	175	MDO	CA2-C2-N3	5.49	105.97	103.37
1	B	175	MDO	O-C-CA3	-3.55	115.66	126.39
1	A	175	MDO	CB2-CA2-C2	3.49	129.15	122.76
1	A	175	MDO	O-C-CA3	-3.24	116.59	126.39
1	B	175	MDO	N3-C1-N2	-3.23	109.22	111.45
1	B	175	MDO	CA-C1-N2	3.20	128.15	124.05
1	B	175	MDO	CB2-CA2-C2	3.08	128.40	122.76
1	A	175	MDO	CA-C1-N2	2.92	127.78	124.05
1	B	175	MDO	C2-N3-C1	2.86	109.42	107.97
1	A	175	MDO	N3-C1-N2	-2.83	109.49	111.45
1	A	175	MDO	CA2-N2-C1	2.22	107.40	105.40
1	B	175	MDO	CA2-N2-C1	2.19	107.38	105.40
1	A	175	MDO	C2-N3-C1	2.11	109.03	107.97
1	A	175	MDO	C2-CA2-N2	-2.05	107.50	108.93

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	175	MDO	C-CA3-N3-C2
1	A	175	MDO	C-CA3-N3-C2
1	A	175	MDO	N2-C1-CA-CB

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Mol	Chain	Res	Type	Atoms
1	A	175	MDO	N3-C1-CA-CB

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	175	MDO	3	0
1	B	175	MDO	3	0

5.5 Carbohydrates [i](#)

There are no carbohydrates 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	2
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	174:SER	C	175:MDO	N	1.71
1	B	174:SER	C	175:MDO	N	1.70
1	B	175:MDO	C	178:ASP	N	1.65
1	A	175:MDO	C	178:ASP	N	1.63

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, 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	612/705 (86%)	0.19	18 (2%)	51 60	17, 26, 43, 57	0
1	B	620/705 (87%)	0.41	46 (7%)	14 22	17, 28, 49, 66	0
All	All	1232/1410 (87%)	0.30	64 (5%)	27 37	17, 27, 46, 66	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	314	LEU	7.2
1	B	610	THR	5.9
1	A	75	ASP	5.6
1	B	617	LEU	5.5
1	B	313	LYS	5.3
1	B	611	ALA	5.0
1	B	616	ALA	4.8
1	B	606	LYS	4.3
1	A	73	ALA	4.2
1	B	315	LYS	4.1
1	B	201	ASP	3.9
1	A	567	HIS	3.8
1	B	69	VAL	3.8
1	B	61	ARG	3.7
1	B	518	CYS	3.7
1	B	589	SER	3.4
1	A	566	LEU	3.4
1	B	613	ASN	3.3
1	B	70	GLN	3.2
1	A	100	LEU	3.2
1	A	74	GLU	3.2
1	B	582	ALA	3.1
1	A	424	TYR	3.1
1	B	590	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	590	ASP	2.9
1	B	361	ALA	2.9
1	B	579	ASP	2.8
1	B	360	HIS	2.8
1	B	591	ARG	2.8
1	B	586	LYS	2.7
1	A	618	VAL	2.7
1	B	618	VAL	2.7
1	B	217	ARG	2.7
1	B	584	PHE	2.7
1	A	57	GLN	2.6
1	B	62	VAL	2.6
1	B	68	TRP	2.6
1	B	100	LEU	2.6
1	B	514	LEU	2.6
1	B	64	THR	2.6
1	B	362	ASN	2.5
1	B	67	SER	2.4
1	B	53	LEU	2.4
1	B	59	ARG	2.4
1	A	565	ALA	2.4
1	B	58	CYS	2.4
1	B	32	THR	2.4
1	B	199	ILE	2.4
1	A	576	THR	2.4
1	A	47	HIS	2.3
1	B	614	ASN	2.3
1	A	591	ARG	2.3
1	B	65	CYS	2.2
1	A	564	LEU	2.2
1	B	612	ASP	2.2
1	B	424	TYR	2.2
1	B	562	THR	2.2
1	A	560	PHE	2.2
1	A	573	GLU	2.2
1	B	566	LEU	2.2
1	B	223	ALA	2.1
1	B	520	LEU	2.1
1	B	573	GLU	2.0
1	A	586	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	MDO	A	175	13/14	0.81	0.14	23,25,26,28	0
1	MDO	B	175	13/14	0.82	0.18	25,28,29,31	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.