Full wwPDB X-ray Structure Validation Report (i)

Nov 6, 2023 – 02:08 pm GMT

PDB ID	:	6H2O
Title	:	APO structure of Phenylalanine ammonia-lyase from Petroselinum crispum
Authors	:	Molnar, B.; Bata, Z.; Leveles, I.; Poppe, L.; Vertessy, G.B.
Deposited on	:	2018-07-14
Resolution	:	1.90 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:

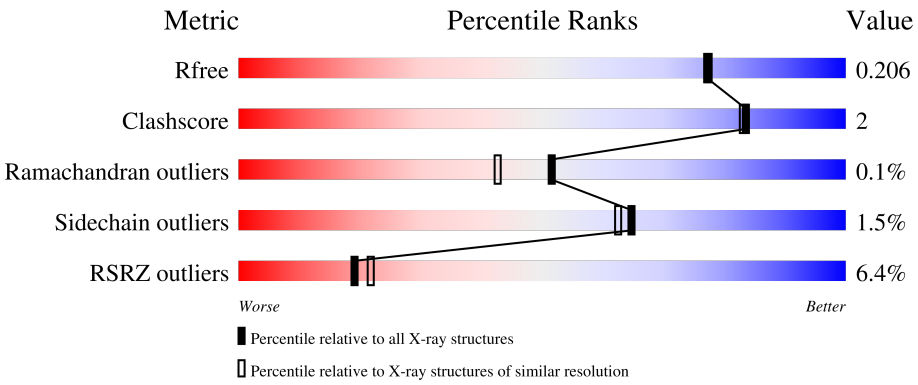
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	714	7%, 85%, 5%, 10%
1	B	714	4%, 84%, 6%, 10%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 10341 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 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	643	4858	3078	820	937	23	0	2	1
1	B	646	4899	3106	829	940	24	0	4	1

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	203	MDO	ALA	modified residue	UNP P24481
A	203	MDO	SER	modified residue	UNP P24481
A	203	MDO	GLY	modified residue	UNP P24481
A	704	SER	CYS	engineered mutation	UNP P24481
A	716	SER	CYS	engineered mutation	UNP P24481
B	203	MDO	ALA	modified residue	UNP P24481
B	203	MDO	SER	modified residue	UNP P24481
B	203	MDO	GLY	modified residue	UNP P24481
B	704	SER	CYS	engineered mutation	UNP P24481
B	716	SER	CYS	engineered mutation	UNP P24481

- Molecule 2 is water.

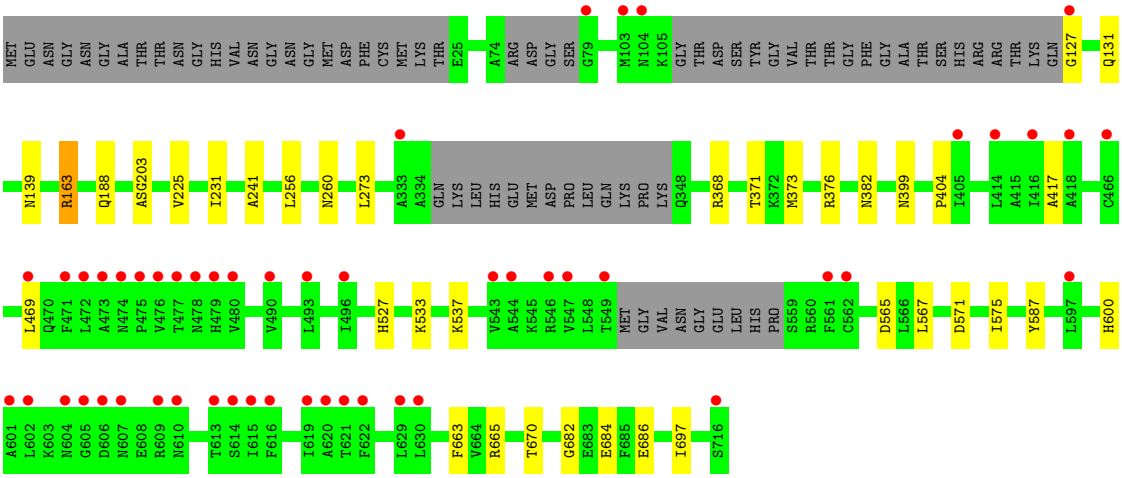
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	300	321	321	0	21
2	B	249	263	263	0	14

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.

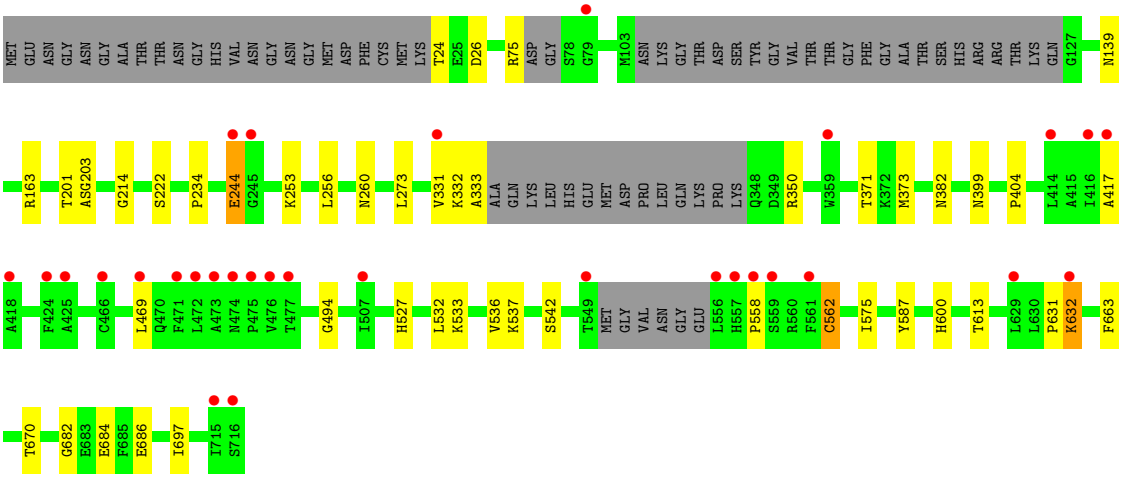
• Molecule 1: Phenylalanine ammonia-lyase 1

Chain A:



• Molecule 1: Phenylalanine ammonia-lyase 1

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	119.89Å 161.12Å 141.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.10 – 1.90 48.09 – 1.90	Depositor EDS
% Data completeness (in resolution range)	97.5 (48.10-1.90) 97.5 (48.09-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.49 (at 1.90Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.170 , 0.206 0.170 , 0.206	Depositor DCC
R_{free} test set	5261 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	28.0	Xtriage
Anisotropy	0.373	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 52.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	10341	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% 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)

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	0.37	0/4932	0.50	0/6681
1	B	0.36	0/4981	0.51	0/6744
All	All	0.36	0/9913	0.50	0/13425

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (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	4858	0	4808	19	0
1	B	4899	0	4867	27	0
2	A	321	0	0	3	0
2	B	263	0	0	6	0
All	All	10341	0	9675	46	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 (46) 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:376:ARG:NH1	2:A:803:HOH:O	2.30	0.64
1:A:127:GLY:N	2:A:804:HOH:O	2.31	0.63
1:B:350:ARG:NE	2:B:802:HOH:O	2.24	0.59
1:B:533:LYS:HG2	1:B:537:LYS:HE2	1.84	0.58
1:A:537:LYS:HG3	1:A:567:LEU:HD22	1.89	0.54
1:A:682:GLY:O	1:A:686:GLU:HG2	2.08	0.53
1:B:670:THR:HG23	1:B:684:GLU:HB3	1.90	0.53
1:A:163:ARG:NH1	1:A:260:ASN:O	2.37	0.52
1:A:382:ASN:HA	1:A:399:ASN:HB3	1.90	0.52
1:B:682:GLY:O	1:B:686:GLU:HG2	2.11	0.51
1:A:670:THR:HG23	1:A:684:GLU:HB3	1.93	0.51
1:B:527:HIS:HD2	2:B:965:HOH:O	1.94	0.49
1:A:663:PHE:CE2	1:A:697:ILE:HD13	2.48	0.49
1:A:225:VAL:HG22	1:A:231:ILE:HD13	1.96	0.48
1:B:562:CYS:HB3	1:B:600:HIS:CD2	2.50	0.47
1:B:256:LEU:O	1:B:260:ASN:HB2	2.15	0.46
1:A:273:LEU:HD13	1:A:371:THR:HA	1.97	0.46
1:B:417:ALA:HA	1:B:469:LEU:HG	1.98	0.46
1:B:562:CYS:HA	2:B:808:HOH:O	2.16	0.45
1:A:373:MET:HG2	1:A:404:PRO:HB3	1.98	0.45
1:B:214:GLY:HA3	2:B:881:HOH:O	2.17	0.45
1:B:373[B]:MET:HG2	1:B:404:PRO:HB3	1.98	0.45
1:A:665:ARG:HD3	1:A:670:THR:O	2.16	0.44
1:A:565:ASP:OD2	1:A:600:HIS:NE2	2.39	0.44
1:B:26:ASP:N	2:B:803:HOH:O	2.36	0.43
1:B:382:ASN:HA	1:B:399:ASN:HB3	2.00	0.43
1:B:558:PRO:HG2	1:B:613:THR:HB	2.01	0.43
1:B:244:GLU:H	1:B:244:GLU:HG3	1.66	0.43
1:B:201:THR:HB	1:B:494:GLY:H	1.83	0.42
1:B:331:VAL:O	1:B:333:ALA:N	2.52	0.42
1:B:562:CYS:HB3	1:B:600:HIS:CG	2.54	0.42
1:B:24:THR:O	2:B:801:HOH:O	2.21	0.42
1:A:417:ALA:HA	1:A:469:LEU:HG	2.01	0.42
1:A:537:LYS:HE3	1:A:567:LEU:HB3	2.01	0.42
1:B:532:LEU:O	1:B:536:VAL:HG23	2.20	0.42
1:B:632:LYS:HE2	1:B:632:LYS:HB2	1.66	0.42
1:A:188:GLN:HG3	1:A:241:ALA:HA	2.02	0.42
1:B:663:PHE:CE2	1:B:697:ILE:HD13	2.55	0.41
1:B:273:LEU:HD13	1:B:371:THR:HA	2.02	0.41
1:A:527:HIS:HD2	2:A:941:HOH:O	2.04	0.41
1:B:631:PRO:HD2	1:B:632:LYS:HZ3	1.86	0.41
1:A:127:GLY:O	1:A:131:GLN:HG2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:663:PHE:HE2	1:B:697:ILE:HD13	1.86	0.40
1:B:253:LYS:HA	1:B:253:LYS:HD2	1.90	0.40
1:B:222:SER:HB3	1:B:234:PRO:HG3	2.03	0.40
1:A:533:LYS:HE2	1:A:571:ASP:HA	2.03	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	632/714 (88%)	621 (98%)	11 (2%)	0	100	100
1	B	637/714 (89%)	628 (99%)	8 (1%)	1 (0%)	47	38
All	All	1269/1428 (89%)	1249 (98%)	19 (2%)	1 (0%)	51	42

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	332	LYS

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	513/591 (87%)	507 (99%)	6 (1%)	71	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	519/591 (88%)	510 (98%)	9 (2%)	60	57
All	All	1032/1182 (87%)	1017 (98%)	15 (2%)	65	62

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	139	ASN
1	A	163	ARG
1	A	256	LEU
1	A	368	ARG
1	A	575	ILE
1	A	587	TYR
1	B	75	ARG
1	B	139	ASN
1	B	163	ARG
1	B	244	GLU
1	B	542	SER
1	B	562	CYS
1	B	575	ILE
1	B	587	TYR
1	B	632	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	260	ASN
1	A	527	HIS
1	B	527	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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	203	1	12,13,14	0.78	0	15,18,20	1.59	3 (20%)
1	MDO	B	203	1	12,13,14	0.86	0	15,18,20	1.47	4 (26%)

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	203	1	-	0/4/23/24	0/1/1/1
1	MDO	B	203	1	-	0/4/23/24	0/1/1/1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	203	MDO	CA2-C2-N3	3.16	104.86	103.37
1	A	203	MDO	O2-C2-CA2	-2.84	129.36	130.96
1	B	203	MDO	CA2-C2-N3	2.79	104.69	103.37
1	B	203	MDO	CA2-N2-C1	2.65	107.80	105.40
1	A	203	MDO	CA2-N2-C1	2.60	107.75	105.40
1	B	203	MDO	C2-CA2-N2	-2.43	107.23	108.93
1	B	203	MDO	O2-C2-CA2	-2.14	129.76	130.96

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	642/714 (89%)	0.24	51 (7%)	12	14	19, 31, 59, 87	0
1	B	645/714 (90%)	0.11	31 (4%)	30	33	19, 30, 57, 86	0
All	All	1287/1428 (90%)	0.17	82 (6%)	19	22	19, 31, 59, 87	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	559	SER	7.1
1	B	558	PRO	5.8
1	B	414	LEU	4.3
1	A	561	PHE	4.2
1	A	615	ILE	4.1
1	A	606	ASP	3.8
1	A	629	LEU	3.7
1	A	414	LEU	3.6
1	B	716	SER	3.6
1	A	602	LEU	3.6
1	B	473	ALA	3.5
1	A	562	CYS	3.5
1	A	127	GLY	3.5
1	B	471	PHE	3.3
1	A	476	VAL	3.2
1	B	469	LEU	3.2
1	A	103	MET	3.2
1	B	472	LEU	3.2
1	A	547	VAL	3.2
1	A	604	ASN	3.2
1	B	549	THR	3.1
1	A	543	VAL	3.1
1	A	549	THR	3.0
1	A	605	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	493	LEU	3.0
1	B	466	CYS	3.0
1	A	480	VAL	2.9
1	A	616	PHE	2.9
1	B	79	GLY	2.8
1	B	359	TRP	2.8
1	A	496	ILE	2.8
1	A	469	LEU	2.8
1	B	417	ALA	2.7
1	A	622	PHE	2.7
1	A	477	THR	2.7
1	A	473	ALA	2.7
1	B	418	ALA	2.7
1	B	561	PHE	2.6
1	A	472	LEU	2.6
1	A	475	PRO	2.6
1	A	416	ILE	2.6
1	A	609	ARG	2.6
1	B	476	VAL	2.6
1	B	556	LEU	2.6
1	A	601	ALA	2.5
1	A	613	THR	2.5
1	A	478	ASN	2.5
1	A	614	SER	2.5
1	B	244	GLU	2.5
1	A	479	HIS	2.4
1	A	405	ILE	2.4
1	A	716	SER	2.4
1	A	597	LEU	2.3
1	B	632	LYS	2.3
1	A	471	PHE	2.3
1	A	333	ALA	2.3
1	A	104	ASN	2.3
1	A	607	ASN	2.3
1	B	557	HIS	2.3
1	A	619	ILE	2.3
1	B	425	ALA	2.3
1	A	474	ASN	2.3
1	A	79	GLY	2.2
1	B	245	GLY	2.2
1	B	424	PHE	2.2
1	A	621	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	507	ILE	2.2
1	A	630	LEU	2.2
1	A	610	ASN	2.2
1	A	546	ARG	2.2
1	B	715	ILE	2.2
1	A	490	VAL	2.1
1	B	331	VAL	2.1
1	B	474	ASN	2.1
1	B	416	ILE	2.1
1	A	466	CYS	2.1
1	B	475	PRO	2.1
1	A	418	ALA	2.1
1	A	544	ALA	2.1
1	A	620	ALA	2.1
1	B	629	LEU	2.0
1	B	477	THR	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	203	13/14	0.93	0.13	21,26,29,35	0
1	MDO	B	203	13/14	0.93	0.12	20,23,26,27	0

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.