Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 09:09 PM GMT

PDB ID	:	4V2R
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	:	2.20 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:

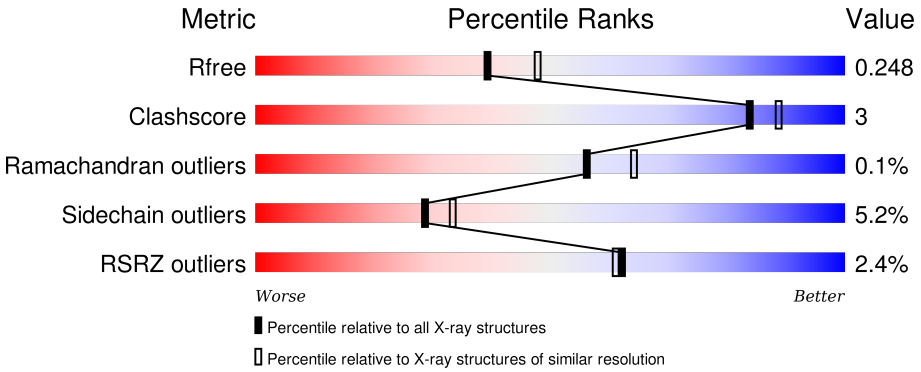
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.20 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	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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	705	% 76% 9% • 13%
1	B	705	3% 79% 8% 12%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 9751 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 AMINOMUTASE (L-BETA-PHENYLALANINE FORMING).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	613	Total	C	N	O	S	0	0	0
			4772	3033	818	899	22			
1	B	618	Total	C	N	O	S	0	0	0
			4799	3050	822	905	22			

There are 48 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	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

Continued on next page...

Continued from previous page...

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	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.

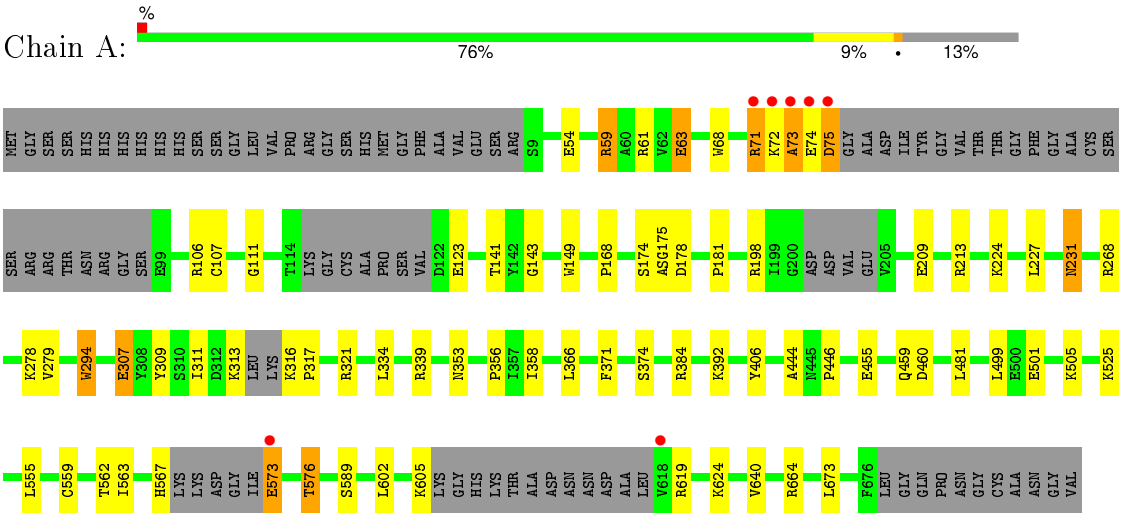
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	109	Total O 109 109	0	0
2	B	71	Total O 71 71	0	0

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.

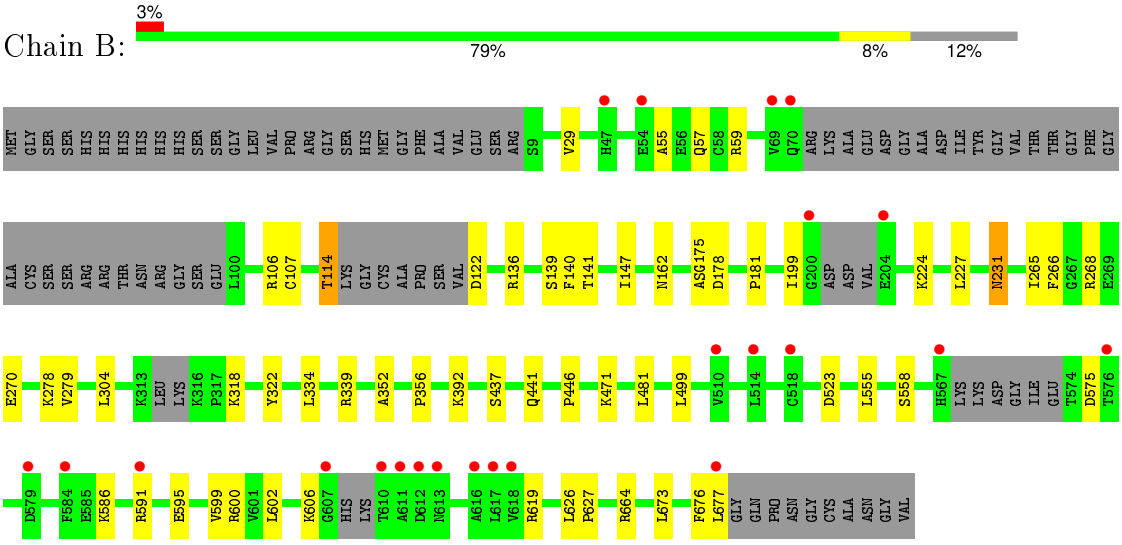
• Molecule 1: PHENYLALANINE AMINOMUTASE (L-BETA-PHENYLALANINE FORMING)

Chain A:



• Molecule 1: PHENYLALANINE AMINOMUTASE (L-BETA-PHENYLALANINE FORMING)

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	181.49Å 76.49Å 120.42Å 90.00° 120.02° 90.00°	Depositor
Resolution (Å)	104.26 – 2.20 47.45 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.3 (104.26-2.20) 99.3 (47.45-2.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	11.26 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.212 , 0.247 0.238 , 0.248	Depositor DCC
R_{free} test set	3644 reflections (5.31%)	DCC
Wilson B-factor (Å^2)	21.1	Xtriage
Anisotropy	0.263	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.65 , 33.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	1 of 72245 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	9751	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 6.43% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.58	1/4839 (0.0%)	0.69	3/6563 (0.0%)
1	B	0.54	0/4866	0.67	2/6602 (0.0%)
All	All	0.56	1/9705 (0.0%)	0.68	5/13165 (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	B	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	294	TRP	CD2-CE2	5.14	1.47	1.41

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	664	ARG	NE-CZ-NH1	6.56	123.58	120.30
1	B	664	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	A	339	ARG	NE-CZ-NH2	-5.51	117.55	120.30
1	A	460	ASP	CB-CG-OD1	5.32	123.09	118.30
1	B	339	ARG	NE-CZ-NH2	-5.02	117.79	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
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	4772	0	4830	42	0
1	B	4799	0	4859	20	0
2	A	109	0	0	0	0
2	B	71	0	0	0	0
All	All	9751	0	9689	56	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 3.

All (56) 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:175:MDO:O	1:A:178:ASP:N	2.05	0.89
1:A:573:GLU:HG2	1:A:576:THR:OG1	1.75	0.85
1:A:279:VAL:HG13	1:B:352:ALA:HB3	1.59	0.85
1:A:59:ARG:HD2	1:A:63:GLU:OE1	1.77	0.84
1:A:573:GLU:CG	1:A:576:THR:OG1	2.29	0.79
1:B:676:PHE:O	1:B:677:LEU:HD13	1.83	0.79
1:B:114:THR:HG22	1:B:122:ASP:HB2	1.71	0.71
1:A:501:GLU:OE1	1:A:619:ARG:HD2	1.90	0.71
1:A:279:VAL:CG1	1:B:352:ALA:HB3	2.19	0.71
1:A:74:GLU:O	1:A:75:ASP:C	2.30	0.66
1:B:227:LEU:O	1:B:231:ASN:HB2	1.97	0.65
1:B:591:ARG:HG2	1:B:595:GLU:OE2	1.97	0.65
1:A:294:TRP:CH2	1:A:624:LYS:HE2	2.33	0.63
1:A:446:PRO:HD3	1:B:446:PRO:HD3	1.80	0.63
1:A:227:LEU:O	1:A:231:ASN:HB2	1.99	0.63
1:A:573:GLU:HG3	1:A:576:THR:OG1	2.03	0.59
1:A:178:ASP:HB3	1:A:181:PRO:HG2	1.85	0.59
1:A:573:GLU:HG2	1:A:573:GLU:O	2.02	0.58
1:A:175:MDO:HA32	1:A:371:PHE:O	2.04	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:ARG:HA	1:A:71:ARG:HE	1.70	0.56
1:A:175:MDO:HB1	1:B:322:TYR:HE2	1.74	0.53
1:A:73:ALA:O	1:A:74:GLU:C	2.46	0.53
1:A:123:GLU:OE1	1:A:198:ARG:NH2	2.42	0.53
1:A:573:GLU:HG2	1:A:576:THR:HG1	1.70	0.52
1:B:437:SER:O	1:B:441:GLN:HG2	2.10	0.52
1:A:111:GLY:HA3	1:A:168:PRO:HG2	1.93	0.50
1:A:175:MDO:O	1:A:178:ASP:CA	2.61	0.48
1:B:55:ALA:O	1:B:59:ARG:HB3	2.13	0.48
1:B:29:VAL:HG12	1:B:141:THR:HG21	1.96	0.47
1:A:209:GLU:O	1:A:213:ARG:HG3	2.15	0.46
1:A:366:LEU:HA	1:B:270:GLU:OE2	2.17	0.45
1:A:174:SER:HA	1:A:175:MDO:C	2.47	0.45
1:A:384:ARG:HG2	1:A:444:ALA:HA	1.98	0.44
1:A:459:GLN:HG2	1:B:322:TYR:CZ	2.52	0.44
1:A:68:TRP:CZ2	1:A:72:LYS:HE3	2.52	0.43
1:B:140:PHE:CG	1:B:147:ILE:HG21	2.53	0.43
1:A:61:ARG:HG3	1:A:143:GLY:HA3	2.01	0.43
1:B:224:LYS:HE2	1:B:356:PRO:HD2	2.00	0.43
1:A:61:ARG:NH1	1:A:141:THR:O	2.52	0.42
1:A:68:TRP:CZ3	1:A:358:ILE:HD12	2.55	0.42
1:A:559:CYS:O	1:A:562:THR:HG22	2.18	0.42
1:A:316:LYS:HA	1:A:317:PRO:HD3	1.96	0.42
1:B:178:ASP:HB3	1:B:181:PRO:HG2	2.01	0.42
1:B:626:LEU:HB3	1:B:627:PRO:HD3	2.02	0.42
1:A:71:ARG:HA	1:A:71:ARG:NE	2.35	0.41
1:B:265:ILE:O	1:B:266:PHE:HB2	2.21	0.41
1:A:563:ILE:O	1:A:567:HIS:HB2	2.21	0.41
1:A:307:GLU:HA	1:A:307:GLU:OE1	2.19	0.41
1:A:605:LYS:HE2	1:A:605:LYS:HB3	1.88	0.41
1:B:471:LYS:HD3	1:B:471:LYS:HA	1.88	0.41
1:A:321:ARG:CZ	1:A:406:TYR:HD1	2.35	0.40
1:A:224:LYS:HE2	1:A:356:PRO:HD2	2.03	0.40
1:B:499:LEU:HD11	1:B:600:ARG:HA	2.04	0.40
1:A:309:TYR:O	1:A:313:LYS:HD3	2.22	0.40
1:A:59:ARG:HD3	1:A:149:TRP:CG	2.56	0.40
1:A:54:GLU:HA	1:A:54:GLU:OE1	2.22	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	597/705 (85%)	578 (97%)	18 (3%)	1 (0%)	52 59
1	B	603/705 (86%)	584 (97%)	19 (3%)	0	100 100
All	All	1200/1410 (85%)	1162 (97%)	37 (3%)	1 (0%)	56 64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	73	ALA

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	521/591 (88%)	494 (95%)	27 (5%)	29 33
1	B	524/591 (89%)	497 (95%)	27 (5%)	29 33
All	All	1045/1182 (88%)	991 (95%)	54 (5%)	29 33

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	ARG
1	A	63	GLU
1	A	71	ARG
1	A	75	ASP
1	A	106	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	107	CYS
1	A	231	ASN
1	A	268	ARG
1	A	278	LYS
1	A	307	GLU
1	A	311	ILE
1	A	334	LEU
1	A	353	ASN
1	A	374	SER
1	A	392	LYS
1	A	455	GLU
1	A	481	LEU
1	A	499	LEU
1	A	505	LYS
1	A	525	LYS
1	A	555	LEU
1	A	573	GLU
1	A	576	THR
1	A	589	SER
1	A	602	LEU
1	A	640	VAL
1	A	673	LEU
1	B	57	GLN
1	B	106	ARG
1	B	107	CYS
1	B	114	THR
1	B	136	ARG
1	B	139	SER
1	B	162	ASN
1	B	199	ILE
1	B	231	ASN
1	B	268	ARG
1	B	278	LYS
1	B	279	VAL
1	B	304	LEU
1	B	318	LYS
1	B	334	LEU
1	B	392	LYS
1	B	481	LEU
1	B	523	ASP
1	B	555	LEU
1	B	558	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	575	ASP
1	B	586	LYS
1	B	599	VAL
1	B	602	LEU
1	B	606	LYS
1	B	619	ARG
1	B	673	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	231	ASN
1	B	231	ASN

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	175	1	11,13,14	3.61	4 (36%)	13,18,20	6.42	6 (46%)
1	MDO	B	175	1	11,13,14	2.90	5 (45%)	13,18,20	2.33	2 (15%)

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	-	0/4/23/24	0/1/1/1
1	MDO	B	175	1	-	0/4/23/24	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	175	MDO	C2-N3	-4.71	1.29	1.39
1	B	175	MDO	C2-N3	-3.46	1.32	1.39
1	A	175	MDO	CA2-N2	-2.62	1.33	1.39
1	B	175	MDO	CA2-N2	-2.52	1.33	1.39
1	A	175	MDO	CA3-N3	-2.28	1.43	1.47
1	B	175	MDO	CA-C1	3.11	1.55	1.51
1	B	175	MDO	O-C	3.70	1.43	1.19
1	B	175	MDO	O2-C2	6.60	1.37	1.23
1	A	175	MDO	O2-C2	9.91	1.44	1.23

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	175	MDO	C2-CA2-N2	-10.63	100.43	108.91
1	A	175	MDO	O2-C2-CA2	-8.26	126.49	130.95
1	B	175	MDO	N3-C1-N2	-2.34	109.75	111.56
1	A	175	MDO	N3-C1-N2	-2.11	109.92	111.56
1	A	175	MDO	CA3-N3-C2	2.16	127.51	123.99
1	A	175	MDO	CA2-N2-C1	5.41	111.62	105.35
1	B	175	MDO	CA2-C2-N3	7.11	107.11	103.39
1	A	175	MDO	CA2-C2-N3	17.53	112.54	103.39

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	175	MDO	5	0

5.5 Carbohydrates (i)

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	612/705 (86%)	-0.21	7 (1%)	82	82	15, 26, 44, 61	0
1	B	617/705 (87%)	-0.00	23 (3%)	45	44	15, 27, 50, 70	0
All	All	1229/1410 (87%)	-0.10	30 (2%)	62	61	15, 26, 48, 70	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	607	GLY	6.5
1	B	610	THR	5.2
1	A	75	ASP	4.7
1	B	611	ALA	4.3
1	B	616	ALA	4.1
1	B	204	GLU	3.7
1	B	617	LEU	3.5
1	A	573	GLU	3.5
1	A	72	LYS	3.5
1	A	73	ALA	3.4
1	B	613	ASN	3.4
1	B	69	VAL	3.3
1	B	677	LEU	3.2
1	B	612	ASP	3.2
1	B	584	PHE	2.9
1	A	74	GLU	2.8
1	B	200	GLY	2.8
1	B	591	ARG	2.7
1	A	618	VAL	2.6
1	B	47	HIS	2.5
1	B	618	VAL	2.4
1	B	54	GLU	2.4
1	B	70	GLN	2.4
1	B	576	THR	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	579	ASP	2.3
1	B	514	LEU	2.2
1	A	71	ARG	2.2
1	B	567	HIS	2.2
1	B	510	VAL	2.1
1	B	518	CYS	2.1

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
1	MDO	B	175	13/14	0.92	0.14	-	22,23,24,24	0
1	MDO	A	175	13/14	0.84	0.15	-	20,23,24,24	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.