Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 03:02 PM GMT

PDB ID	:	4BAB
Title	:	Redesign of a Phenylalanine Aminomutase into a beta-Phenylalanine Ammonia Lyase
Authors	:	Bartsch, S.; Wybenga, G.G.; Jansen, M.; Heberling, M.M.; Wu, B.; Dijkstra, B.W.; Janssen, D.B.
Deposited on	:	2012-09-12
Resolution	:	2.56 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:

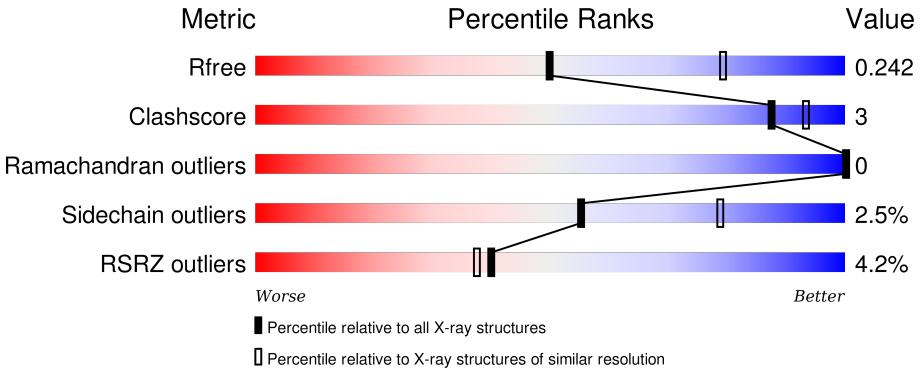
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.56 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	3324 (2.60-2.52)
Clashscore	102246	3729 (2.60-2.52)
Ramachandran outliers	100387	3673 (2.60-2.52)
Sidechain outliers	100360	3673 (2.60-2.52)
RSRZ outliers	91569	3333 (2.60-2.52)

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	3% 79% 7% 13%
1	B	705	3% 80% 8% 12%
1	C	705	3% 79% 8% 13%
1	D	705	6% 81% 6% 12%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 19216 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	612	Total	C	N	O	S	0	0	0
			4760	3029	814	895	22			
1	B	620	Total	C	N	O	S	0	0	0
			4828	3067	828	911	22			
1	C	616	Total	C	N	O	S	0	0	1
			4790	3045	822	901	22			
1	D	617	Total	C	N	O	S	0	0	0
			4802	3054	823	903	22			

There are 92 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	175	MDO	ALA	CHROMOPHORE	UNP Q68G84

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Chain	Residue	Modelled	Actual	Comment	Reference
A	175	MDO	SER	CHROMOPHORE	UNP Q68G84
A	175	MDO	GLY	CHROMOPHORE	UNP Q68G84
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	175	MDO	ALA	CHROMOPHORE	UNP Q68G84
B	175	MDO	SER	CHROMOPHORE	UNP Q68G84
B	175	MDO	GLY	CHROMOPHORE	UNP Q68G84
C	-19	MET	-	EXPRESSION TAG	UNP Q68G84
C	-18	GLY	-	EXPRESSION TAG	UNP Q68G84
C	-17	SER	-	EXPRESSION TAG	UNP Q68G84
C	-16	SER	-	EXPRESSION TAG	UNP Q68G84
C	-15	HIS	-	EXPRESSION TAG	UNP Q68G84
C	-14	HIS	-	EXPRESSION TAG	UNP Q68G84
C	-13	HIS	-	EXPRESSION TAG	UNP Q68G84
C	-12	HIS	-	EXPRESSION TAG	UNP Q68G84
C	-11	HIS	-	EXPRESSION TAG	UNP Q68G84
C	-10	HIS	-	EXPRESSION TAG	UNP Q68G84
C	-9	SER	-	EXPRESSION TAG	UNP Q68G84
C	-8	SER	-	EXPRESSION TAG	UNP Q68G84
C	-7	GLY	-	EXPRESSION TAG	UNP Q68G84
C	-6	LEU	-	EXPRESSION TAG	UNP Q68G84
C	-5	VAL	-	EXPRESSION TAG	UNP Q68G84
C	-4	PRO	-	EXPRESSION TAG	UNP Q68G84
C	-3	ARG	-	EXPRESSION TAG	UNP Q68G84

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	GLY	-	EXPRESSION TAG	UNP Q68G84
C	-1	SER	-	EXPRESSION TAG	UNP Q68G84
C	0	HIS	-	EXPRESSION TAG	UNP Q68G84
C	175	MDO	ALA	CHROMOPHORE	UNP Q68G84
C	175	MDO	SER	CHROMOPHORE	UNP Q68G84
C	175	MDO	GLY	CHROMOPHORE	UNP Q68G84
D	-19	MET	-	EXPRESSION TAG	UNP Q68G84
D	-18	GLY	-	EXPRESSION TAG	UNP Q68G84
D	-17	SER	-	EXPRESSION TAG	UNP Q68G84
D	-16	SER	-	EXPRESSION TAG	UNP Q68G84
D	-15	HIS	-	EXPRESSION TAG	UNP Q68G84
D	-14	HIS	-	EXPRESSION TAG	UNP Q68G84
D	-13	HIS	-	EXPRESSION TAG	UNP Q68G84
D	-12	HIS	-	EXPRESSION TAG	UNP Q68G84
D	-11	HIS	-	EXPRESSION TAG	UNP Q68G84
D	-10	HIS	-	EXPRESSION TAG	UNP Q68G84
D	-9	SER	-	EXPRESSION TAG	UNP Q68G84
D	-8	SER	-	EXPRESSION TAG	UNP Q68G84
D	-7	GLY	-	EXPRESSION TAG	UNP Q68G84
D	-6	LEU	-	EXPRESSION TAG	UNP Q68G84
D	-5	VAL	-	EXPRESSION TAG	UNP Q68G84
D	-4	PRO	-	EXPRESSION TAG	UNP Q68G84
D	-3	ARG	-	EXPRESSION TAG	UNP Q68G84
D	-2	GLY	-	EXPRESSION TAG	UNP Q68G84
D	-1	SER	-	EXPRESSION TAG	UNP Q68G84
D	0	HIS	-	EXPRESSION TAG	UNP Q68G84
D	175	MDO	ALA	CHROMOPHORE	UNP Q68G84
D	175	MDO	SER	CHROMOPHORE	UNP Q68G84
D	175	MDO	GLY	CHROMOPHORE	UNP Q68G84

- Molecule 2 is water.

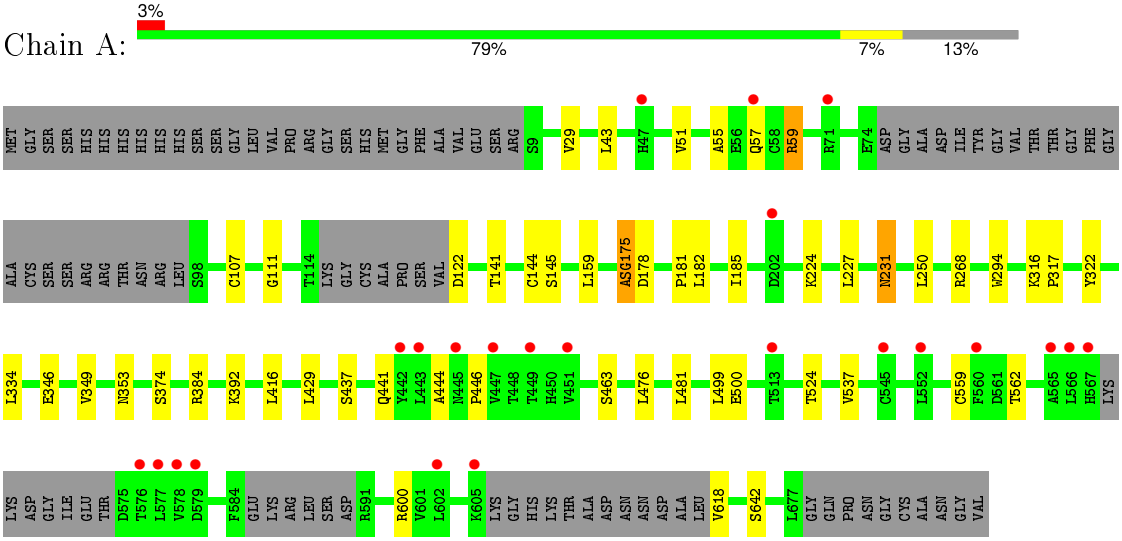
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	10	Total O 10 10	0	0
2	B	17	Total O 17 17	0	0
2	C	5	Total O 5 5	0	0
2	D	4	Total O 4 4	0	0

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.

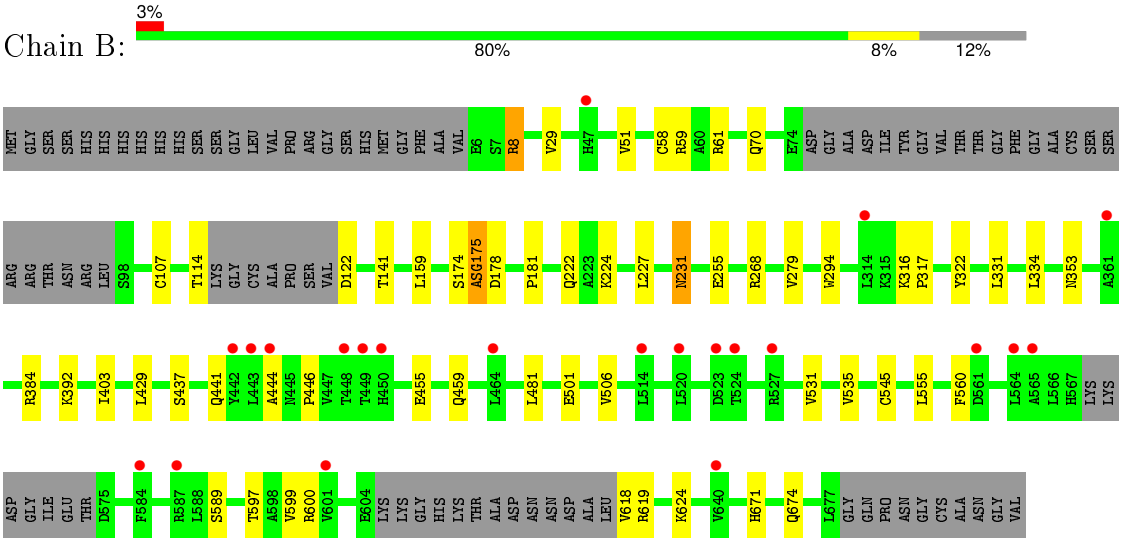
- Molecule 1: PHENYLALANINE AMINOMUTASE

Chain A:



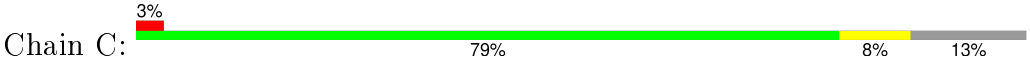
- Molecule 1: PHENYLALANINE AMINOMUTASE

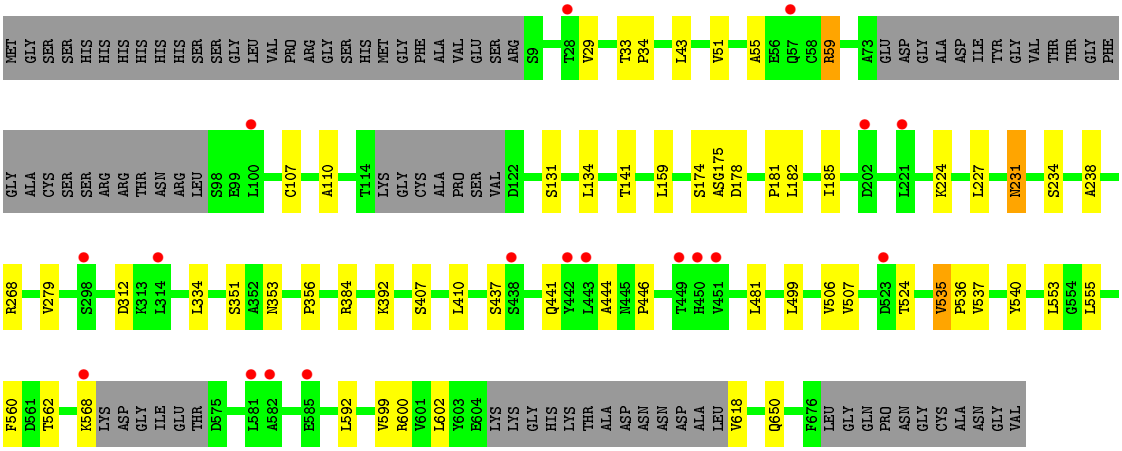
Chain B:



- Molecule 1: PHENYLALANINE AMINOMUTASE

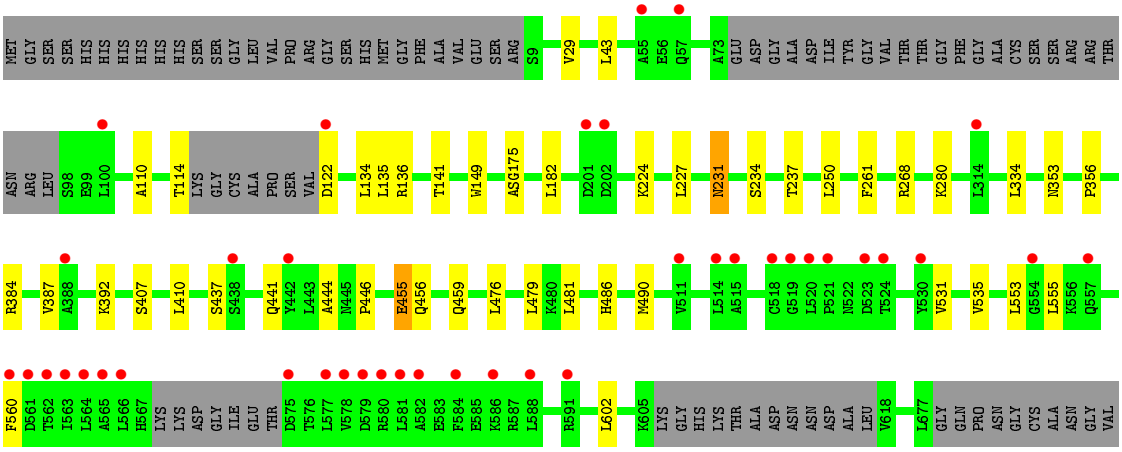
Chain C:





- Molecule 1: PHENYLALANINE AMINOMUTASE

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	94.14Å 132.09Å 110.03Å 90.00° 95.52° 90.00°	Depositor
Resolution (Å)	109.52 – 2.56 49.52 – 2.56	Depositor EDS
% Data completeness (in resolution range)	97.0 (109.52-2.56) 97.2 (49.52-2.56)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.47 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.214 , 0.251 0.208 , 0.242	Depositor DCC
R_{free} test set	4337 reflections (5.48%)	DCC
Wilson B-factor (Å^2)	46.7	Xtriage
Anisotropy	0.217	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 26.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 83391 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	19216	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.75% 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	0.39	1/4828 (0.0%)	0.49	0/6551
1	B	0.40	0/4897	0.49	0/6644
1	C	0.38	0/4859	0.49	0/6593
1	D	0.39	1/4871 (0.0%)	0.49	0/6609
All	All	0.39	2/19455 (0.0%)	0.49	0/26397

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	3
1	C	0	3
1	D	0	2
All	All	0	10

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	294	TRP	CD2-CE2	5.03	1.47	1.41
1	D	149	TRP	CD2-CE2	5.03	1.47	1.41

There are no bond angle outliers.

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	175	MDO	Mainchain,Peptide
1	B	174	SER	Mainchain
1	B	175	MDO	Mainchain,Peptide
1	C	174	SER	Mainchain
1	C	175	MDO	Mainchain,Peptide
1	D	175	MDO	Mainchain,Peptide

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	4760	0	4825	29	0
1	B	4828	0	4889	31	0
1	C	4790	0	4856	26	0
1	D	4802	0	4872	25	0
2	A	10	0	0	0	0
2	B	17	0	0	0	0
2	C	5	0	0	0	0
2	D	4	0	0	0	0
All	All	19216	0	19442	99	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 (99) 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:B:70:GLN:HE22	1:B:222:GLN:NE2	1.44	1.15
1:B:70:GLN:NE2	1:B:222:GLN:NE2	1.99	1.10
1:A:145:SER:O	1:A:224:LYS:HE3	1.55	1.07
1:B:70:GLN:NE2	1:B:222:GLN:HE21	1.64	0.84
1:B:70:GLN:HE22	1:B:222:GLN:HE21	0.84	0.83
1:C:506:VAL:HG21	1:C:599:VAL:HG21	1.59	0.82
1:B:506:VAL:HG21	1:B:599:VAL:HG21	1.61	0.82
1:A:224:LYS:CG	1:A:224:LYS:O	2.30	0.78
1:D:455:GLU:HG2	1:D:459:GLN:HG3	1.66	0.76
1:D:455:GLU:O	1:D:455:GLU:HG3	1.86	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:SER:O	1:A:224:LYS:CE	2.35	0.71
1:B:70:GLN:NE2	1:B:222:GLN:HE22	1.89	0.69
1:D:486:HIS:O	1:D:490:MET:HG2	1.96	0.66
1:A:224:LYS:HG2	1:A:224:LYS:O	1.98	0.62
1:A:429:LEU:HD23	1:C:110:ALA:HB1	1.82	0.62
1:C:227:LEU:O	1:C:231:ASN:HB2	2.00	0.62
1:A:224:LYS:HG3	1:A:224:LYS:O	2.01	0.60
1:D:114:THR:HG1	1:D:122:ASP:N	1.99	0.60
1:D:224:LYS:HE3	1:D:356:PRO:HD2	1.82	0.60
1:B:294:TRP:CH2	1:B:624:LYS:HE2	2.36	0.60
1:A:55:ALA:O	1:A:59:ARG:HB3	2.02	0.59
1:C:446:PRO:HD3	1:D:446:PRO:HD3	1.85	0.58
1:A:446:PRO:HD3	1:B:446:PRO:HD3	1.88	0.56
1:B:403:ILE:HG12	1:D:456:GLN:HG2	1.90	0.54
1:B:227:LEU:O	1:B:231:ASN:HB2	2.08	0.54
1:A:227:LEU:O	1:A:231:ASN:HB2	2.09	0.53
1:D:455:GLU:O	1:D:455:GLU:CG	2.55	0.53
1:B:58:CYS:HA	1:B:61:ARG:HE	1.74	0.52
1:C:43:LEU:HD22	1:C:134:LEU:HD22	1.92	0.52
1:B:560:PHE:HB2	1:C:560:PHE:HB2	1.92	0.52
1:C:178:ASP:HB3	1:C:181:PRO:HG2	1.92	0.51
1:D:437:SER:O	1:D:441:GLN:HG2	2.10	0.51
1:B:29:VAL:HG12	1:B:141:THR:HG21	1.91	0.51
1:B:437:SER:O	1:B:441:GLN:HG2	2.11	0.50
1:D:384:ARG:HG2	1:D:444:ALA:HA	1.94	0.50
1:D:227:LEU:O	1:D:231:ASN:HB2	2.13	0.49
1:B:671:HIS:O	1:B:674:GLN:HG2	2.12	0.49
1:A:384:ARG:HG2	1:A:444:ALA:HA	1.94	0.49
1:C:182:LEU:HD23	1:C:185:ILE:HD12	1.93	0.49
1:A:437:SER:O	1:A:441:GLN:HG2	2.13	0.49
1:A:29:VAL:HG12	1:A:141:THR:HG21	1.94	0.48
1:B:114:THR:HG23	1:B:122:ASP:HB2	1.96	0.48
1:A:111:GLY:O	1:C:650:GLN:HG3	2.13	0.48
1:C:224:LYS:HE2	1:C:356:PRO:HD2	1.95	0.48
1:D:43:LEU:HD22	1:D:134:LEU:HD22	1.96	0.48
1:C:437:SER:O	1:C:441:GLN:HG2	2.14	0.47
1:B:51:VAL:HG21	1:B:159:LEU:HD13	1.95	0.47
1:C:29:VAL:HG12	1:C:141:THR:HG21	1.96	0.47
1:B:545:CYS:SG	1:B:589:SER:HA	2.54	0.47
1:D:182:LEU:HD21	1:D:234:SER:HB2	1.97	0.47
1:A:178:ASP:HB3	1:A:181:PRO:HG2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:MDO:HB1	1:B:322:TYR:HE2	1.80	0.46
1:D:261:PHE:N	1:D:490:MET:HE3	2.31	0.46
1:C:51:VAL:HG21	1:C:159:LEU:HD13	1.97	0.46
1:C:407:SER:HB2	1:C:410:LEU:HB2	1.96	0.46
1:A:51:VAL:HG21	1:A:159:LEU:HD13	1.98	0.46
1:C:506:VAL:CG2	1:C:599:VAL:HG21	2.40	0.46
1:C:384:ARG:HG2	1:C:444:ALA:HA	1.98	0.45
1:B:531:VAL:O	1:B:535:VAL:HG12	2.16	0.45
1:D:407:SER:HB2	1:D:410:LEU:HB2	1.98	0.45
1:C:537:VAL:HA	1:C:540:TYR:CE2	2.52	0.45
1:B:384:ARG:HG2	1:B:444:ALA:HA	1.99	0.45
1:A:322:TYR:CZ	1:B:459:GLN:HG2	2.52	0.45
1:C:182:LEU:HD21	1:C:234:SER:HB2	2.00	0.44
1:A:346:GLU:HA	1:A:349:VAL:HG22	1.99	0.44
1:C:524:THR:HG22	1:C:562:THR:OG1	2.18	0.44
1:B:231:ASN:HA	1:B:231:ASN:HD22	1.67	0.44
1:D:531:VAL:O	1:D:535:VAL:HG22	2.18	0.44
1:A:250:LEU:HD12	1:A:476:LEU:HD22	2.00	0.43
1:B:255:GLU:HG2	1:B:331:LEU:HD13	2.00	0.43
1:B:597:THR:HG23	1:B:600:ARG:HH21	1.83	0.43
1:B:429:LEU:HD23	1:D:110:ALA:HB1	2.01	0.43
1:D:250:LEU:HD12	1:D:476:LEU:HD22	2.00	0.42
1:D:136:ARG:HD3	1:D:182:LEU:HD22	2.01	0.42
1:A:43:LEU:HD21	1:A:159:LEU:HD22	2.00	0.42
1:A:182:LEU:HD23	1:A:185:ILE:HD12	2.01	0.42
1:A:416:LEU:HD23	1:A:642:SER:HB3	2.00	0.42
1:C:131:SER:HB2	1:C:238:ALA:HB1	2.00	0.42
1:A:500:GLU:HG3	1:A:537:VAL:HG12	2.01	0.42
1:D:135:LEU:HD23	1:D:237:THR:HB	2.02	0.41
1:B:178:ASP:HB3	1:B:181:PRO:HG2	2.02	0.41
1:A:499:LEU:HD11	1:A:600:ARG:HA	2.02	0.41
1:D:455:GLU:O	1:D:456:GLN:HB2	2.21	0.41
1:B:316:LYS:HA	1:B:317:PRO:HD3	1.94	0.41
1:B:8:ARG:H	1:B:8:ARG:HG2	1.75	0.41
1:A:316:LYS:HA	1:A:317:PRO:HD3	1.93	0.41
1:C:535:VAL:HA	1:C:536:PRO:HD3	1.85	0.41
1:C:33:THR:HA	1:C:34:PRO:HD3	1.92	0.41
1:A:322:TYR:HE2	1:B:175:MDO:HB1	1.86	0.41
1:C:55:ALA:O	1:C:59:ARG:HB3	2.21	0.41
1:C:499:LEU:HD21	1:C:600:ARG:HG3	2.01	0.41
1:A:524:THR:HG23	1:A:562:THR:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:351:SER:HB2	1:D:280:LYS:HA	2.03	0.41
1:B:501:GLU:OE2	1:B:619:ARG:NH1	2.54	0.41
1:C:507:VAL:HG22	1:C:592:LEU:HD11	2.03	0.40
1:A:374:SER:HA	1:A:463:SER:HB2	2.03	0.40
1:A:559:CYS:HB3	1:D:560:PHE:CE1	2.56	0.40
1:D:29:VAL:HG12	1:D:141:THR:HG21	2.03	0.40
1:D:387:VAL:HG13	1:D:479:LEU:HD22	2.02	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	599/705 (85%)	584 (98%)	15 (2%)	0	100	100
1	B	609/705 (86%)	592 (97%)	17 (3%)	0	100	100
1	C	605/705 (86%)	595 (98%)	10 (2%)	0	100	100
1	D	606/705 (86%)	594 (98%)	12 (2%)	0	100	100
All	All	2419/2820 (86%)	2365 (98%)	54 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	520/592 (88%)	508 (98%)	12 (2%)	58 81
1	B	528/592 (89%)	514 (97%)	14 (3%)	52 77
1	C	524/592 (88%)	508 (97%)	16 (3%)	47 73
1	D	525/592 (89%)	515 (98%)	10 (2%)	65 85
All	All	2097/2368 (89%)	2045 (98%)	52 (2%)	55 79

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	GLN
1	A	59	ARG
1	A	107	CYS
1	A	122	ASP
1	A	144	CYS
1	A	231	ASN
1	A	268	ARG
1	A	334	LEU
1	A	353	ASN
1	A	392	LYS
1	A	481	LEU
1	A	618	VAL
1	B	8	ARG
1	B	59	ARG
1	B	107	CYS
1	B	224	LYS
1	B	231	ASN
1	B	268	ARG
1	B	279	VAL
1	B	334	LEU
1	B	353	ASN
1	B	392	LYS
1	B	455	GLU
1	B	481	LEU
1	B	555	LEU
1	B	618	VAL
1	C	59	ARG
1	C	107	CYS
1	C	231	ASN
1	C	268	ARG
1	C	279	VAL
1	C	312	ASP
1	C	334	LEU

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Mol	Chain	Res	Type
1	C	353	ASN
1	C	392	LYS
1	C	481	LEU
1	C	535	VAL
1	C	553	LEU
1	C	555	LEU
1	C	568	LYS
1	C	602	LEU
1	C	618	VAL
1	D	231	ASN
1	D	268	ARG
1	D	334	LEU
1	D	353	ASN
1	D	392	LYS
1	D	455	GLU
1	D	481	LEU
1	D	553	LEU
1	D	555	LEU
1	D	602	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	231	ASN
1	A	408	ASN
1	B	222	GLN
1	B	231	ASN
1	B	621	GLN
1	C	231	ASN
1	C	362	ASN
1	C	557	GLN
1	D	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)

4 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	2.79	5 (45%)	13,18,20	3.12	3 (23%)
1	MDO	B	175	1	11,13,14	2.81	5 (45%)	13,18,20	3.00	3 (23%)
1	MDO	C	175	1	11,13,14	2.81	5 (45%)	13,18,20	3.07	3 (23%)
1	MDO	D	175	1	11,13,14	2.83	5 (45%)	13,18,20	3.28	3 (23%)

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
1	MDO	C	175	1	-	0/4/23/24	0/1/1/1
1	MDO	D	175	1	-	0/4/23/24	0/1/1/1

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	175	MDO	C2-N3	-3.24	1.32	1.39
1	D	175	MDO	C2-N3	-3.17	1.33	1.39
1	B	175	MDO	C2-N3	-3.12	1.33	1.39
1	A	175	MDO	C2-N3	-3.12	1.33	1.39
1	B	175	MDO	CA2-N2	-2.36	1.33	1.39
1	D	175	MDO	CA2-N2	-2.32	1.33	1.39
1	C	175	MDO	CA2-N2	-2.29	1.34	1.39
1	A	175	MDO	CA2-N2	-2.17	1.34	1.39
1	A	175	MDO	CA-C1	3.16	1.55	1.51
1	B	175	MDO	CA-C1	3.24	1.55	1.51
1	C	175	MDO	CA-C1	3.36	1.55	1.51
1	D	175	MDO	CA-C1	3.46	1.56	1.51
1	B	175	MDO	O-C	3.64	1.43	1.19
1	D	175	MDO	O-C	3.66	1.43	1.19
1	A	175	MDO	O-C	3.67	1.43	1.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	175	MDO	O-C	3.69	1.43	1.19
1	A	175	MDO	O2-C2	6.28	1.36	1.23
1	C	175	MDO	O2-C2	6.30	1.36	1.23
1	B	175	MDO	O2-C2	6.34	1.36	1.23
1	D	175	MDO	O2-C2	6.35	1.36	1.23

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	175	MDO	O2-C2-CA2	-8.49	126.36	130.95
1	A	175	MDO	O2-C2-CA2	-7.54	126.87	130.95
1	C	175	MDO	O2-C2-CA2	-7.49	126.90	130.95
1	B	175	MDO	O2-C2-CA2	-7.12	127.10	130.95
1	D	175	MDO	N3-C1-N2	-3.04	109.21	111.56
1	C	175	MDO	N3-C1-N2	-2.94	109.29	111.56
1	B	175	MDO	N3-C1-N2	-2.61	109.54	111.56
1	A	175	MDO	N3-C1-N2	-2.47	109.65	111.56
1	D	175	MDO	CA2-C2-N3	7.19	107.15	103.39
1	C	175	MDO	CA2-C2-N3	7.26	107.18	103.39
1	B	175	MDO	CA2-C2-N3	7.35	107.23	103.39
1	A	175	MDO	CA2-C2-N3	7.57	107.34	103.39

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

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

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	611/705 (86%)	0.28	23 (3%)	44	41	30, 51, 85, 102	0
1	B	619/705 (87%)	0.27	22 (3%)	46	44	31, 50, 75, 87	0
1	C	615/705 (87%)	0.27	18 (2%)	55	53	33, 52, 78, 102	0
1	D	616/705 (87%)	0.41	40 (6%)	22	20	32, 54, 85, 101	0
All	All	2461/2820 (87%)	0.31	103 (4%)	40	37	30, 51, 81, 102	0

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	515	ALA	5.3
1	D	566	LEU	5.3
1	D	565	ALA	4.8
1	A	566	LEU	4.5
1	A	577	LEU	4.4
1	C	28	THR	4.1
1	D	520	LEU	3.9
1	D	201	ASP	3.6
1	D	554	GLY	3.6
1	D	314	LEU	3.5
1	D	511	VAL	3.5
1	D	100	LEU	3.3
1	D	514	LEU	3.3
1	D	521	PRO	3.3
1	D	577	LEU	3.2
1	A	449	THR	3.2
1	D	562	THR	3.2
1	D	584	PHE	3.2
1	D	561	ASP	3.1
1	C	449	THR	3.1
1	D	524	THR	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	523	ASP	3.1
1	C	100	LEU	3.0
1	C	451	VAL	3.0
1	D	575	ASP	3.0
1	A	579	ASP	3.0
1	B	314	LEU	3.0
1	B	361	ALA	3.0
1	A	451	VAL	2.9
1	A	71	ARG	2.9
1	A	443	LEU	2.9
1	C	298	SER	2.9
1	A	565	ALA	2.9
1	A	605	LYS	2.9
1	D	518	CYS	2.9
1	B	584	PHE	2.8
1	B	587	ARG	2.8
1	D	591	ARG	2.8
1	B	564	LEU	2.8
1	A	545	CYS	2.7
1	A	442	TYR	2.7
1	B	523	ASP	2.7
1	C	581	LEU	2.6
1	C	314	LEU	2.6
1	D	582	ALA	2.6
1	B	565	ALA	2.6
1	D	586	LYS	2.6
1	D	581	LEU	2.6
1	D	388	ALA	2.6
1	C	443	LEU	2.5
1	A	560	PHE	2.5
1	A	202	ASP	2.5
1	D	580	ARG	2.5
1	C	202	ASP	2.5
1	C	438	SER	2.5
1	D	55	ALA	2.5
1	A	57	GLN	2.4
1	C	57	GLN	2.4
1	B	444	ALA	2.4
1	A	445	ASN	2.4
1	B	640	VAL	2.4
1	D	557	GLN	2.4
1	C	582	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	576	THR	2.4
1	D	519	GLY	2.3
1	C	568	LYS	2.3
1	C	523	ASP	2.3
1	D	578	VAL	2.3
1	D	202	ASP	2.3
1	A	602	LEU	2.3
1	B	442	TYR	2.3
1	C	221	LEU	2.3
1	B	514	LEU	2.3
1	B	527	ARG	2.3
1	A	552	LEU	2.3
1	A	567	HIS	2.2
1	B	449	THR	2.2
1	A	47	HIS	2.2
1	D	442	TYR	2.2
1	D	579	ASP	2.2
1	D	564	LEU	2.2
1	D	588	LEU	2.2
1	B	450	HIS	2.2
1	B	561	ASP	2.2
1	C	585	GLU	2.1
1	B	524	THR	2.1
1	D	57	GLN	2.1
1	B	47	HIS	2.1
1	B	520	LEU	2.1
1	D	560	PHE	2.1
1	A	578	VAL	2.1
1	D	438	SER	2.1
1	A	447	VAL	2.1
1	B	443	LEU	2.1
1	B	464	LEU	2.0
1	C	442	TYR	2.0
1	D	530	TYR	2.0
1	B	448	THR	2.0
1	B	601	VAL	2.0
1	D	563	ILE	2.0
1	C	450	HIS	2.0
1	D	122	ASP	2.0
1	A	513	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. 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	D	175	13/14	0.93	0.18	-	47,51,52,52	0
1	MDO	A	175	13/14	0.95	0.16	-	36,38,39,39	0
1	MDO	C	175	13/14	0.90	0.19	-	46,49,51,53	0
1	MDO	B	175	13/14	0.93	0.17	-	36,38,38,38	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.