



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 02:36 PM EDT

PDB ID : 4BAA / pdb_00004baa
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 : 2.50 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
Mogul : 2022.3.0, CSD as543be (2022)
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

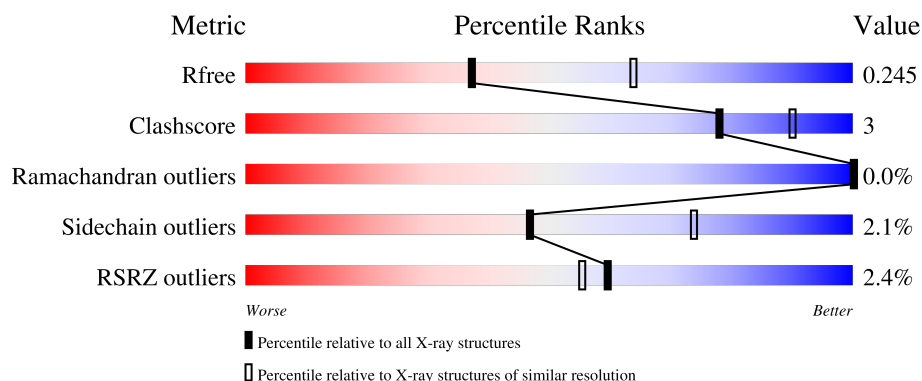
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	705	
1	B	705	
1	C	705	
1	D	705	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 19964 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	636	Total	C	N	O	S	0	0	0
			4933	3129	847	934	23			
1	B	644	Total	C	N	O	S	0	0	0
			4998	3171	857	947	23			
1	C	618	Total	C	N	O	S	0	0	0
			4812	3062	825	903	22			
1	D	642	Total	C	N	O	S	0	0	0
			4981	3160	855	943	23			

There are 96 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	92	SER	ARG	engineered mutation	UNP Q68G84

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Chain	Residue	Modelled	Actual	Comment	Reference
A	175	MDO	ALA	chromophore	UNP Q68G84
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	92	SER	ARG	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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	PRO	-	expression tag	UNP Q68G84
C	-3	ARG	-	expression tag	UNP Q68G84
C	-2	GLY	-	expression tag	UNP Q68G84
C	-1	SER	-	expression tag	UNP Q68G84
C	0	HIS	-	expression tag	UNP Q68G84
C	92	SER	ARG	engineered mutation	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	92	SER	ARG	engineered mutation	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	67	Total O 67 67	0	0
2	B	59	Total O 59 59	0	0
2	C	61	Total O 61 61	0	0

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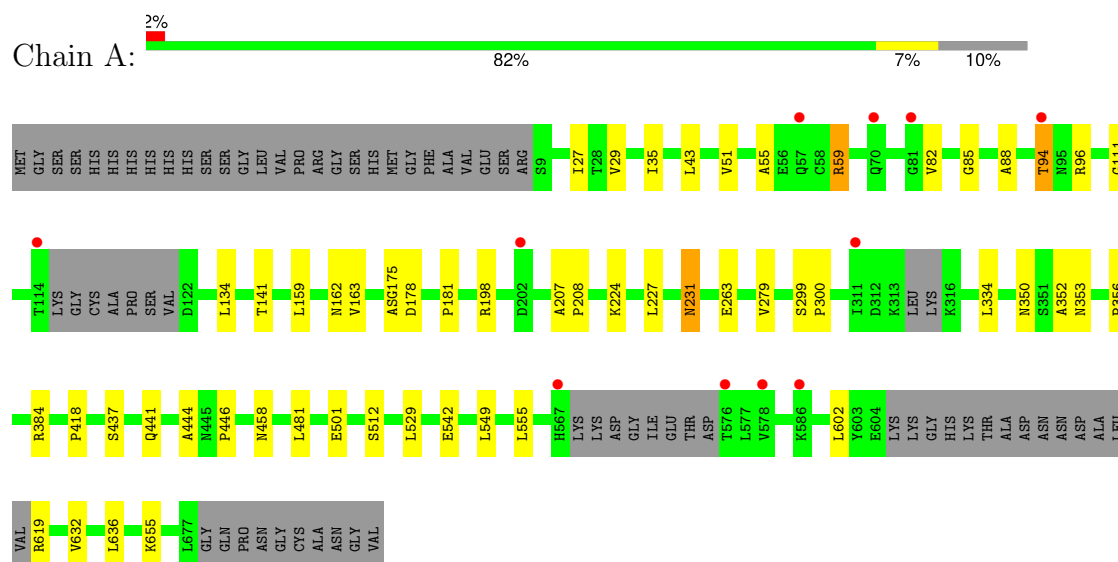
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	53	Total	O	0	0
			53	53		

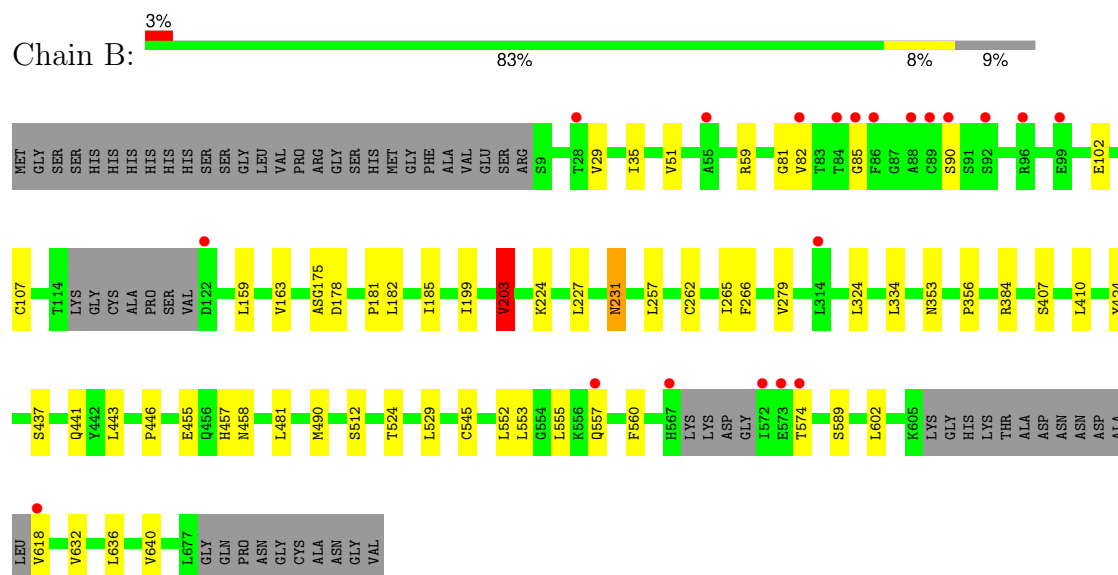
3 Residue-property plots [i](#)

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



• Molecule 1: PHENYLALANINE AMMONIA-LYASE



• Molecule 1: PHENYLALANINE AMMONIA-LYASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	99.30Å 145.84Å 99.41Å 90.00° 99.96° 90.00°	Depositor
Resolution (Å)	48.90 – 2.50 48.90 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.0 (48.90-2.50) 98.0 (48.90-2.50)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.39 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.209 , 0.246 0.208 , 0.245	Depositor DCC
R_{free} test set	4821 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	31.5	Xtriage
Anisotropy	0.023	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 18.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.022 for l,-k,h	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	19964	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.81% 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 [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	0.56	0/5004	0.82	2/6790 (0.0%)
1	B	0.58	3/5070 (0.1%)	0.82	1/6880 (0.0%)
1	C	0.58	2/4880 (0.0%)	0.81	0/6618
1	D	0.63	2/5053 (0.0%)	0.83	0/6857
All	All	0.59	7/20007 (0.0%)	0.82	3/27145 (0.0%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	457	HIS	CG-ND1	-7.98	1.29	1.38
1	C	457	HIS	CG-ND1	-7.65	1.29	1.38
1	C	457	HIS	CD2-NE2	-6.82	1.30	1.37
1	B	457	HIS	CD2-NE2	-6.63	1.30	1.37
1	D	458	ASN	C-O	-5.76	1.17	1.24
1	B	458	ASN	C-O	-5.24	1.17	1.24
1	D	460	ASP	C-O	-5.02	1.17	1.24

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	203	VAL	N-CA-C	6.29	117.19	108.89
1	A	549	LEU	CA-C-N	5.28	125.34	119.32
1	A	549	LEU	C-N-CA	5.28	125.34	119.32

There are no chirality outliers.

There are no planarity outliers.

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	4933	0	4974	28	0
1	B	4998	0	5049	25	0
1	C	4812	0	4885	33	0
1	D	4981	0	5032	35	0
2	A	67	0	0	0	0
2	B	59	0	0	1	0
2	C	61	0	0	0	0
2	D	53	0	0	0	0
All	All	19964	0	19940	110	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 (110) 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:D:83:THR:HG23	1:D:94:THR:O	1.63	0.96
1:D:145:SER:O	1:D:224:LYS:HE3	1.70	0.92
1:D:320:ASP:O	1:D:325:ARG:NH1	2.03	0.89
1:D:83:THR:CG2	1:D:94:THR:O	2.20	0.88
1:A:35:ILE:H	1:A:350:ASN:HD21	1.26	0.81
1:D:506:VAL:HG21	1:D:599:VAL:HG21	1.71	0.72
1:D:29:VAL:O	1:D:29:VAL:HG23	1.87	0.71
1:A:224:LYS:HE2	1:A:356:PRO:HD2	1.71	0.71
1:B:407:SER:HB3	1:B:410:LEU:HB2	1.74	0.69
1:B:224:LYS:HE2	1:B:356:PRO:HD2	1.76	0.66
1:A:352:ALA:HB3	1:B:279:VAL:CG1	2.27	0.64
1:D:29:VAL:O	1:D:29:VAL:CG2	2.46	0.63
1:C:506:VAL:HG21	1:C:599:VAL:HG21	1.80	0.62
1:D:227:LEU:O	1:D:231:ASN:HB2	2.02	0.59
1:B:29:VAL:HG12	1:B:35:ILE:HD11	1.83	0.59
1:D:544:PRO:HB3	1:D:596:MET:HE1	1.84	0.59
1:B:424:TYR:OH	1:D:85:GLY:HA2	2.02	0.58
1:A:29:VAL:HG12	1:A:141:THR:HG21	1.85	0.58
1:A:35:ILE:H	1:A:350:ASN:ND2	2.00	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:446:PRO:HD3	1:D:446:PRO:HD3	1.86	0.58
1:C:257:LEU:HB3	1:C:490:MET:HE1	1.85	0.57
1:B:512:SER:HB2	1:B:529:LEU:HD21	1.87	0.57
1:D:224:LYS:HG3	1:D:224:LYS:O	2.04	0.57
1:D:437:SER:O	1:D:441:GLN:HG2	2.05	0.57
1:D:80:TYR:HA	1:D:84:THR:HG23	1.87	0.56
1:A:227:LEU:O	1:A:231:ASN:HB2	2.07	0.55
1:C:43:LEU:HD13	1:C:134:LEU:HD22	1.89	0.54
1:B:632:VAL:HA	1:B:636:LEU:HD12	1.89	0.53
1:A:446:PRO:HD3	1:B:446:PRO:HD3	1.90	0.52
1:B:384:ARG:HD2	1:B:443:LEU:O	2.10	0.52
1:A:352:ALA:HB3	1:B:279:VAL:HG12	1.92	0.51
1:C:632:VAL:HA	1:C:636:LEU:HD12	1.93	0.50
1:C:384:ARG:HG2	1:C:444:ALA:HA	1.93	0.50
1:D:531:VAL:O	1:D:535:VAL:HG22	2.12	0.50
1:C:51:VAL:HG21	1:C:159:LEU:HD13	1.94	0.50
1:B:178:ASP:HB3	1:B:181:PRO:HG2	1.93	0.49
1:D:632:VAL:HA	1:D:636:LEU:HD12	1.93	0.49
1:B:227:LEU:O	1:B:231:ASN:HB2	2.12	0.49
1:D:257:LEU:HB3	1:D:490:MET:HE1	1.95	0.48
1:A:111:GLY:O	1:C:650:GLN:HG3	2.13	0.48
1:C:300:PRO:HB2	1:C:619:ARG:HG3	1.94	0.48
1:A:94:THR:HG22	1:A:96:ARG:H	1.79	0.48
1:A:384:ARG:HG2	1:A:444:ALA:HA	1.96	0.48
1:A:632:VAL:HA	1:A:636:LEU:HD12	1.96	0.48
1:A:85:GLY:HA2	1:C:424:TYR:OH	2.14	0.48
1:D:80:TYR:HA	1:D:84:THR:CG2	2.43	0.47
1:B:437:SER:O	1:B:441:GLN:HG2	2.14	0.47
1:C:182:LEU:HD23	1:C:185:ILE:HD12	1.96	0.47
1:B:85:GLY:HA2	1:D:424:TYR:OH	2.14	0.47
1:C:506:VAL:CG2	1:C:599:VAL:HG21	2.43	0.47
1:B:51:VAL:HG21	1:B:159:LEU:HD13	1.95	0.47
1:A:178:ASP:HB3	1:A:181:PRO:HG2	1.96	0.46
1:B:257:LEU:HB3	1:B:490:MET:HE1	1.96	0.46
1:C:291:LEU:HD11	1:C:673:LEU:HD22	1.98	0.46
1:B:182:LEU:HD23	1:B:185:ILE:HD12	1.98	0.46
1:C:387:VAL:HG13	1:C:479:LEU:HD22	1.97	0.46
1:A:299:SER:HA	1:A:300:PRO:HD3	1.81	0.46
1:C:136:ARG:HD3	1:C:182:LEU:HD22	1.97	0.46
1:D:255:GLU:HG2	1:D:331:LEU:HD13	1.98	0.46
1:A:43:LEU:HD22	1:A:134:LEU:HD22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:265:ILE:O	1:B:266:PHE:HB2	2.14	0.45
1:D:384:ARG:HG2	1:D:444:ALA:HA	1.98	0.45
1:A:88:ALA:HB2	1:A:458:ASN:HB2	1.98	0.45
1:B:557:GLN:HB3	2:B:2054:HOH:O	2.17	0.45
1:C:380:MET:HA	1:C:380:MET:HE2	1.98	0.45
1:C:537:VAL:HA	1:C:540:TYR:CE2	2.51	0.45
1:A:207:ALA:N	1:A:208:PRO:HD2	2.32	0.45
1:A:636:LEU:HD22	1:A:655:LYS:HB3	1.98	0.45
1:C:437:SER:O	1:C:441:GLN:HG2	2.17	0.45
1:A:418:PRO:O	1:A:542:GLU:HG3	2.17	0.45
1:D:182:LEU:HD21	1:D:234:SER:HB2	1.99	0.45
1:D:88:ALA:HB2	1:D:458:ASN:HB2	1.99	0.44
1:D:567:HIS:HA	1:D:574:THR:HG21	1.98	0.44
1:A:55:ALA:O	1:A:59:ARG:HB3	2.17	0.44
1:B:81:GLY:HA3	1:B:227:LEU:HD22	1.99	0.44
1:C:224:LYS:HE3	1:C:356:PRO:HD2	1.98	0.44
1:A:512:SER:HB2	1:A:529:LEU:HD21	1.99	0.44
1:A:51:VAL:HG21	1:A:159:LEU:HD13	1.99	0.44
1:A:263:GLU:OE2	1:A:299:SER:OG	2.28	0.44
1:B:560:PHE:HB2	1:C:560:PHE:HB2	1.99	0.44
1:C:123:GLU:HG3	1:C:198:ARG:HH22	1.83	0.43
1:D:43:LEU:HD22	1:D:134:LEU:HD22	2.00	0.43
1:C:348:GLU:OE1	1:D:280:LYS:HE3	2.18	0.43
1:D:537:VAL:HA	1:D:540:TYR:CE2	2.53	0.43
1:A:27:ILE:CD1	1:A:43:LEU:HB2	2.49	0.42
1:D:80:TYR:CD1	1:D:80:TYR:C	2.97	0.42
1:C:531:VAL:O	1:C:535:VAL:HG22	2.19	0.42
1:C:322:TYR:CZ	1:D:459:GLN:HG2	2.54	0.42
1:D:82:VAL:HG23	1:D:83:THR:OG1	2.18	0.42
1:A:437:SER:O	1:A:441:GLN:HG2	2.20	0.42
1:C:165:PRO:HA	1:C:197:ALA:HA	2.01	0.42
1:B:199:ILE:HB	1:B:203:VAL:HG22	2.01	0.42
1:D:180:ILE:HB	1:D:181:PRO:HD3	2.02	0.41
1:B:545:CYS:SG	1:B:589:SER:HA	2.61	0.41
1:C:43:LEU:HD11	1:C:51:VAL:HG22	2.02	0.41
1:D:83:THR:HG22	1:D:83:THR:O	2.20	0.41
1:C:102:GLU:HG3	1:C:221:LEU:HD12	2.03	0.41
1:C:379:TYR:O	1:C:383:VAL:HG23	2.20	0.41
1:D:79:ILE:O	1:D:84:THR:HG23	2.20	0.41
1:B:163:VAL:HG22	1:B:199:ILE:HG12	2.03	0.41
1:D:84:THR:HA	1:D:92:SER:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:524:THR:HG23	1:D:562:THR:HG21	2.01	0.41
1:A:501:GLU:OE2	1:A:619:ARG:NH1	2.51	0.41
1:C:262:CYS:HB2	1:C:324:LEU:HD11	2.03	0.41
1:C:295:LEU:HA	1:C:624:LYS:HD2	2.02	0.41
1:B:262:CYS:HB2	1:B:324:LEU:HD11	2.03	0.41
1:C:299:SER:HA	1:C:300:PRO:HD3	1.91	0.41
1:C:136:ARG:HH22	1:C:354:ASP:HB3	1.86	0.40
1:C:37:VAL:HG13	1:C:346:GLU:HG3	2.02	0.40
1:A:163:VAL:HA	1:A:198:ARG:O	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	623/705 (88%)	609 (98%)	14 (2%)	0	100	100
1	B	633/705 (90%)	619 (98%)	13 (2%)	1 (0%)	43	63
1	C	603/705 (86%)	593 (98%)	10 (2%)	0	100	100
1	D	631/705 (90%)	616 (98%)	15 (2%)	0	100	100
All	All	2490/2820 (88%)	2437 (98%)	52 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	90	SER

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	538/592 (91%)	527 (98%)	11 (2%)	48	75
1	B	546/592 (92%)	528 (97%)	18 (3%)	33	61
1	C	526/592 (89%)	522 (99%)	4 (1%)	73	88
1	D	544/592 (92%)	531 (98%)	13 (2%)	43	70
All	All	2154/2368 (91%)	2108 (98%)	46 (2%)	47	74

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	ARG
1	A	82	VAL
1	A	94	THR
1	A	162	ASN
1	A	231	ASN
1	A	279	VAL
1	A	334	LEU
1	A	353	ASN
1	A	481	LEU
1	A	555	LEU
1	A	602	LEU
1	B	59	ARG
1	B	82	VAL
1	B	102	GLU
1	B	107	CYS
1	B	203	VAL
1	B	231	ASN
1	B	334	LEU
1	B	353	ASN
1	B	455	GLU
1	B	481	LEU
1	B	524	THR
1	B	552	LEU
1	B	553	LEU
1	B	555	LEU
1	B	574	THR
1	B	602	LEU
1	B	618	VAL

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Mol	Chain	Res	Type
1	B	640	VAL
1	C	279	VAL
1	C	552	LEU
1	C	555	LEU
1	C	640	VAL
1	D	29	VAL
1	D	82	VAL
1	D	84	THR
1	D	224	LYS
1	D	231	ASN
1	D	279	VAL
1	D	324	LEU
1	D	325	ARG
1	D	353	ASN
1	D	481	LEU
1	D	555	LEU
1	D	576	THR
1	D	602	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	231	ASN
1	A	350	ASN
1	A	360	HIS
1	A	413	ASN
1	A	459	GLN
1	A	462	ASN
1	A	509	ASN
1	A	522	ASN
1	B	222	GLN
1	B	231	ASN
1	C	19	ASN
1	C	162	ASN
1	C	231	ASN
1	C	273	HIS
1	C	353	ASN
1	C	621	GLN
1	D	22	ASN
1	D	222	GLN
1	D	231	ASN
1	D	462	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	D	175	1	11,13,14	2.88	5 (45%)	15,18,20	2.39	4 (26%)
1	MDO	B	175	1	11,13,14	2.85	5 (45%)	15,18,20	2.50	4 (26%)
1	MDO	C	175	1	11,13,14	2.90	5 (45%)	15,18,20	2.36	4 (26%)
1	MDO	A	175	1	11,13,14	2.88	5 (45%)	15,18,20	2.61	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	D	175	1	-	0/4/23/24	0/1/1/1
1	MDO	B	175	1	-	1/4/23/24	0/1/1/1
1	MDO	C	175	1	-	2/4/23/24	0/1/1/1
1	MDO	A	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	O2-C2	6.59	1.36	1.23
1	D	175	MDO	O2-C2	6.58	1.36	1.23
1	A	175	MDO	O2-C2	6.50	1.36	1.23
1	B	175	MDO	O2-C2	6.42	1.36	1.23
1	D	175	MDO	O3-C3	4.22	1.44	1.20
1	C	175	MDO	O3-C3	4.19	1.43	1.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	175	MDO	O3-C3	4.16	1.43	1.20
1	B	175	MDO	O3-C3	4.13	1.43	1.20
1	C	175	MDO	C2-N3	-3.15	1.32	1.40
1	D	175	MDO	CA2-N2	-3.11	1.33	1.39
1	B	175	MDO	CA2-N2	-3.11	1.33	1.39
1	A	175	MDO	CA2-N2	-3.10	1.33	1.39
1	C	175	MDO	CA2-N2	-3.07	1.33	1.39
1	B	175	MDO	C2-N3	-3.07	1.32	1.40
1	A	175	MDO	C2-N3	-3.04	1.33	1.40
1	D	175	MDO	C2-N3	-3.00	1.33	1.40
1	A	175	MDO	CA2-C2	-2.28	1.38	1.43
1	B	175	MDO	CA2-C2	-2.26	1.38	1.43
1	C	175	MDO	CA2-C2	-2.15	1.38	1.43
1	D	175	MDO	CA2-C2	-2.01	1.39	1.43

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	175	MDO	O2-C2-CA2	-7.28	126.38	131.02
1	B	175	MDO	O2-C2-CA2	-6.84	126.66	131.02
1	C	175	MDO	O2-C2-CA2	-6.53	126.85	131.02
1	D	175	MDO	O2-C2-CA2	-6.40	126.93	131.02
1	A	175	MDO	CA2-C2-N3	4.71	107.46	103.50
1	B	175	MDO	CA2-C2-N3	4.52	107.29	103.50
1	D	175	MDO	CA2-C2-N3	4.48	107.26	103.50
1	C	175	MDO	CA2-C2-N3	4.32	107.13	103.50
1	A	175	MDO	O3-C3-CA3	-3.48	109.83	125.47
1	B	175	MDO	O3-C3-CA3	-3.35	110.40	125.47
1	D	175	MDO	O3-C3-CA3	-3.25	110.85	125.47
1	C	175	MDO	O3-C3-CA3	-3.25	110.85	125.47
1	B	175	MDO	N3-C1-N2	-2.52	109.50	111.48
1	D	175	MDO	N3-C1-N2	-2.45	109.56	111.48
1	A	175	MDO	N3-C1-N2	-2.44	109.56	111.48
1	C	175	MDO	N3-C1-N2	-2.38	109.61	111.48

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	175	MDO	N2-C1-CA1-CB
1	C	175	MDO	N2-C1-CA1-CB
1	C	175	MDO	N3-C1-CA1-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

There are no oligosaccharides 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, 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	635/705 (90%)	0.13	11 (1%) 69 65	21, 38, 60, 72	0
1	B	643/705 (91%)	0.21	20 (3%) 51 47	20, 37, 63, 84	0
1	C	617/705 (87%)	0.10	11 (1%) 67 64	20, 36, 54, 76	0
1	D	641/705 (90%)	0.24	18 (2%) 55 50	21, 37, 63, 77	0
All	All	2536/2820 (89%)	0.17	60 (2%) 59 55	20, 37, 61, 84	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	572	ILE	7.3
1	D	314	LEU	4.7
1	C	73	ALA	3.8
1	B	82	VAL	3.7
1	A	576	THR	3.6
1	D	574	THR	3.5
1	D	567	HIS	3.3
1	C	568	LYS	3.1
1	B	314	LEU	3.1
1	C	55	ALA	3.1
1	C	314	LEU	2.9
1	B	88	ALA	2.8
1	D	96	ARG	2.8
1	D	554	GLY	2.7
1	D	92	SER	2.7
1	B	89	CYS	2.6
1	C	100	LEU	2.6
1	B	84	THR	2.6
1	D	618	VAL	2.6
1	A	114	THR	2.6
1	B	85	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	574	THR	2.5
1	A	94	THR	2.5
1	A	578	VAL	2.5
1	C	576	THR	2.4
1	B	90	SER	2.4
1	A	81	GLY	2.4
1	B	99	GLU	2.4
1	D	75	ASP	2.3
1	B	96	ARG	2.3
1	B	618	VAL	2.3
1	A	57	GLN	2.3
1	D	361	ALA	2.3
1	A	70	GLN	2.3
1	D	90	SER	2.3
1	A	311	ILE	2.3
1	D	577	LEU	2.3
1	D	71	ARG	2.3
1	B	55	ALA	2.2
1	B	557	GLN	2.2
1	C	122	ASP	2.2
1	C	99	GLU	2.2
1	A	567	HIS	2.2
1	B	573	GLU	2.2
1	D	526	ALA	2.2
1	A	586	LYS	2.2
1	B	567	HIS	2.1
1	C	671	HIS	2.1
1	C	581	LEU	2.1
1	D	86	PHE	2.1
1	C	573	GLU	2.1
1	B	92	SER	2.1
1	B	122	ASP	2.1
1	B	86	PHE	2.1
1	B	28	THR	2.1
1	A	202	ASP	2.1
1	D	77	ALA	2.0
1	D	122	ASP	2.0
1	D	76	GLY	2.0
1	D	95	ASN	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($\text{\AA}^2$)	Q<0.9
1	MDO	D	175	13/14	0.84	0.12	31,32,33,33	0
1	MDO	B	175	13/14	0.88	0.11	31,32,33,33	0
1	MDO	C	175	13/14	0.92	0.09	30,32,32,32	0
1	MDO	A	175	13/14	0.92	0.08	28,29,29,30	0

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.