



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:05 PM UTC

PDB ID : 4C5S / pdb_00004c5s
Title : Structural Investigations into the Stereochemistry and Activity of a Phenylalanine-2,3-Aminomutase from *Taxus chinensis*
Authors : Wybenga, G.G.; Szymanski, W.; Wu, B.; Feringa, B.L.; Janssen, D.B.; Dijkstra, B.W.
Deposited on : 2013-09-16
Resolution : 1.85 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

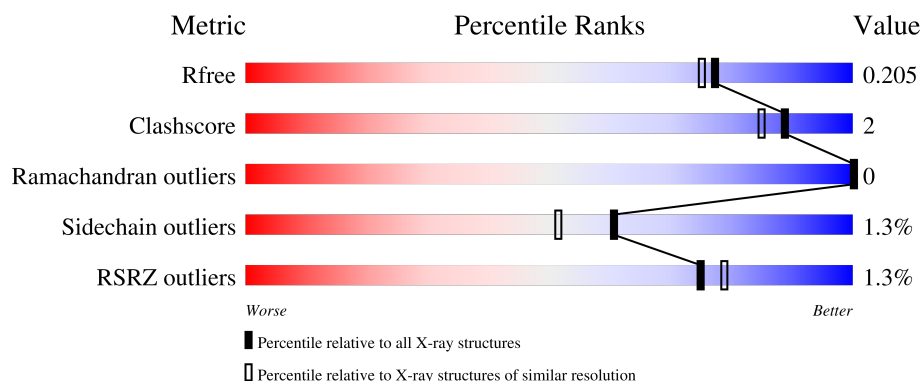
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

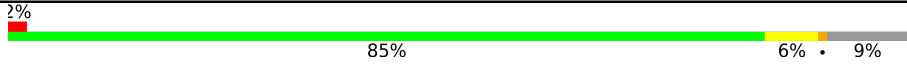
The reported resolution of this entry is 1.85 Å.

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	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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 3 unique types of molecules in this entry. The entry contains 20797 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	639	Total	C	N	O	S	0	0	0
			4955	3143	854	935	23			
1	B	641	Total	C	N	O	S	0	0	0
			4971	3153	857	938	23			
1	C	642	Total	C	N	O	S	0	0	0
			4979	3157	857	942	23			
1	D	641	Total	C	N	O	S	0	0	0
			4971	3153	857	938	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	175	MDO	ALA	chromophore	UNP Q68G84

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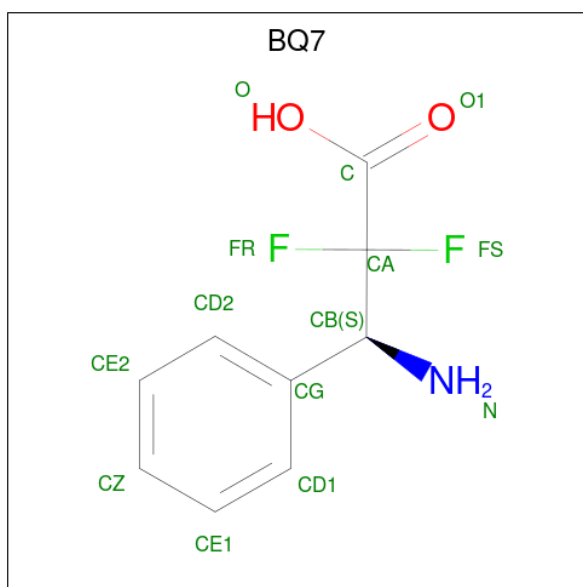
Chain	Residue	Modelled	Actual	Comment	Reference
A	175	MDO	SER	chromophore	UNP Q68G84
A	175	MDO	GLY	chromophore	UNP Q68G84
A	80	ALA	TYR	engineered mutation	UNP P42212
B	-19	MET	-	expression tag	UNP Q68G84
B	-18	GLY	-	expression tag	UNP Q68G84
B	-17	SER	-	expression tag	UNP Q68G84
B	-16	SER	-	expression 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
B	80	ALA	TYR	engineered mutation	UNP P42212
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	175	MDO	ALA	chromophore	UNP Q68G84
C	175	MDO	SER	chromophore	UNP Q68G84
C	175	MDO	GLY	chromophore	UNP Q68G84
C	80	ALA	TYR	engineered mutation	UNP P42212
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
D	80	ALA	TYR	engineered mutation	UNP P42212

- Molecule 2 is (3S)-3-amino-2,2-difluoro-3-phenylpropanoic acid (CCD ID: BQ7) (formula: $C_9H_9F_2NO_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			14	9	2	1	2		
2	B	1	Total	C	F	N	O	0	0
			14	9	2	1	2		
2	C	1	Total	C	F	N	O	0	0
			14	9	2	1	2		
2	D	1	Total	C	F	N	O	0	0
			14	9	2	1	2		

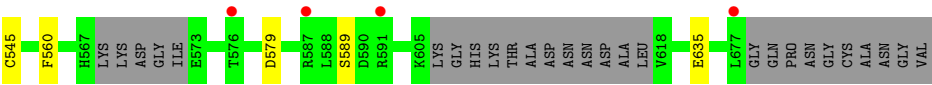
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	246	Total	O	0	0
			246	246		
3	B	226	Total	O	0	0
			226	226		
3	C	202	Total	O	0	0
			202	202		
3	D	191	Total	O	0	0
			191	191		

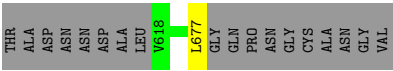
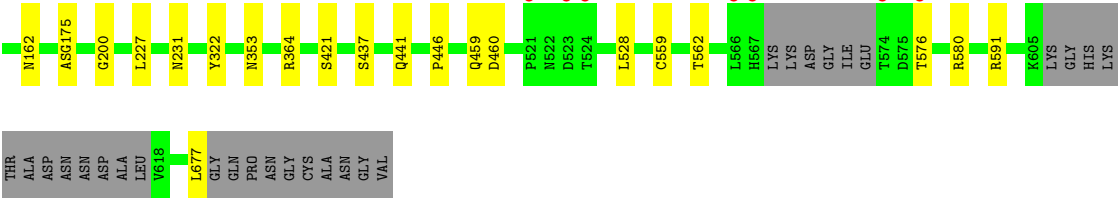
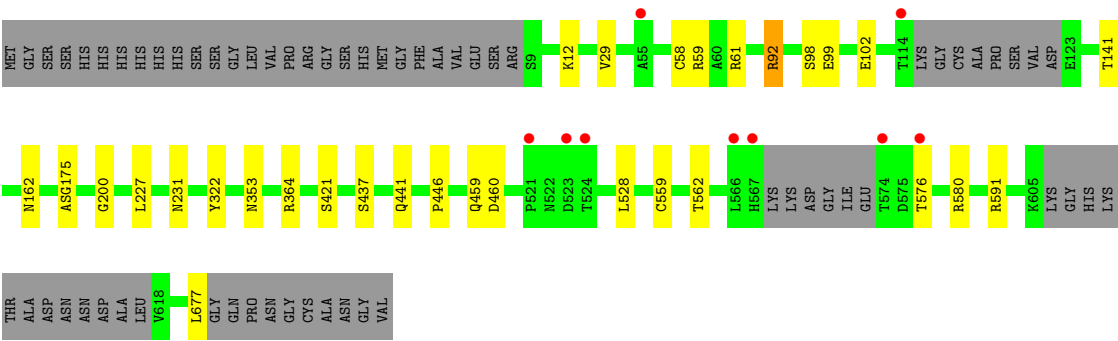
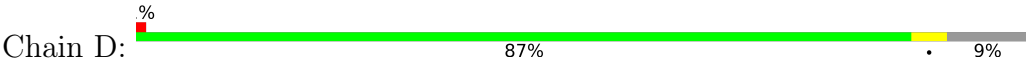
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- Molecule 1: PHENYLALANINE AMMONIA-LYASE





● 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	99.75Å 146.19Å 100.39Å 90.00° 99.31° 90.00°	Depositor
Resolution (Å)	99.07 – 1.85 99.07 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.9 (99.07-1.85) 99.9 (99.07-1.85)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.27 (at 1.86Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.178 , 0.205 0.178 , 0.205	Depositor DCC
R_{free} test set	12073 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	18.3	Xtriage
Anisotropy	0.006	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 29.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.016 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	20797	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.02% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MDO, BQ7

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	0.74	0/5026	0.83	0/6820
1	B	0.74	0/5042	0.83	2/6841 (0.0%)
1	C	0.74	0/5049	0.83	1/6849 (0.0%)
1	D	0.74	0/5042	0.82	0/6841
All	All	0.74	0/20159	0.83	3/27351 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	297	ARG	CA-C-N	-6.74	112.54	122.86
1	B	297	ARG	C-N-CA	-6.74	112.54	122.86
1	C	234	SER	N-CA-C	5.52	117.30	111.28

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	4955	0	5010	25	0
1	B	4971	0	5030	18	0
1	C	4979	0	5031	30	0
1	D	4971	0	5030	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	14	0	7	0	0
2	B	14	0	7	0	0
2	C	14	0	7	0	0
2	D	14	0	7	0	0
3	A	246	0	0	0	0
3	B	226	0	0	0	0
3	C	202	0	0	0	0
3	D	191	0	0	0	0
All	All	20797	0	20129	75	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 (75) 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:174:SER:C	1:A:175:MDO:CA1	2.60	0.73
1:D:92:ARG:HB3	1:D:92:ARG:CZ	2.19	0.72
1:A:47:HIS:CE1	1:A:162:ASN:HD21	2.07	0.71
1:A:98:SER:O	1:A:102:GLU:HG2	1.97	0.65
1:A:446:PRO:HD3	1:B:446:PRO:HD3	1.83	0.60
1:A:92:ARG:HH22	1:C:542:GLU:CD	2.11	0.59
1:A:27:ILE:CD1	1:A:43:LEU:HB2	2.34	0.58
1:A:422:VAL:HG11	1:C:99:GLU:HG3	1.87	0.56
1:B:422:VAL:HG11	1:D:99:GLU:HG3	1.86	0.55
1:B:662:ASP:OD1	1:B:664:ARG:HD3	2.06	0.55
1:B:12:LYS:HE3	1:B:677:LEU:HB2	1.87	0.54
1:A:29:VAL:HG12	1:A:141:THR:HG21	1.89	0.53
1:C:446:PRO:HD3	1:D:446:PRO:HD3	1.91	0.53
1:B:98:SER:O	1:B:102:GLU:HG2	2.08	0.53
1:C:114:THR:OG1	1:C:122:ASP:HB2	2.09	0.53
1:D:437:SER:O	1:D:441:GLN:HG2	2.10	0.52
1:A:99:GLU:HG3	1:C:422:VAL:HG11	1.92	0.51
1:C:55:ALA:O	1:C:56:GLU:C	2.54	0.50
1:B:12:LYS:HE3	1:B:677:LEU:CB	2.41	0.50
1:A:437:SER:O	1:A:441:GLN:HG2	2.11	0.50
1:D:12:LYS:HE3	1:D:677:LEU:HB2	1.93	0.49
1:C:88:ALA:HB2	1:C:458:ASN:HB2	1.93	0.49
1:A:174:SER:CA	1:A:175:MDO:N1	2.71	0.49
1:B:94:THR:HB	1:D:421:SER:HB2	1.95	0.49
1:A:59:ARG:HD2	1:A:63:GLU:CD	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:THR:HB	1:C:421:SER:HB2	1.94	0.48
1:B:162:ASN:ND2	1:B:200:GLY:HA2	2.29	0.47
1:B:567:HIS:NE2	1:C:579:ASP:OD1	2.39	0.47
1:B:163:VAL:HG22	1:B:199:ILE:HG12	1.97	0.47
1:D:227:LEU:O	1:D:231:ASN:HB2	2.15	0.47
1:C:51:VAL:HG21	1:C:159:LEU:HD13	1.97	0.47
1:C:255:GLU:HG2	1:C:331:LEU:HD13	1.96	0.47
1:C:437:SER:O	1:C:441:GLN:HG2	2.15	0.46
1:A:227:LEU:O	1:A:231:ASN:HB2	2.14	0.46
1:D:559:CYS:O	1:D:562:THR:HG22	2.16	0.46
1:B:27:ILE:CD1	1:B:43:LEU:HB2	2.46	0.46
1:D:576:THR:O	1:D:580:ARG:HG3	2.16	0.46
1:A:92:ARG:NH2	1:C:542:GLU:OE1	2.49	0.46
1:C:459:GLN:HG2	1:D:322:TYR:CE2	2.51	0.45
1:A:545:CYS:SG	1:A:589:SER:HA	2.57	0.45
1:C:322:TYR:CZ	1:D:459:GLN:HG2	2.52	0.45
1:C:545:CYS:SG	1:C:589:SER:HA	2.57	0.45
1:D:58:CYS:HB2	1:D:61:ARG:NH1	2.31	0.45
1:B:131:SER:HB2	1:B:238:ALA:HB1	1.98	0.45
1:C:388:ALA:HA	1:C:440:LEU:HG	1.99	0.44
1:C:459:GLN:HG2	1:D:322:TYR:CZ	2.52	0.44
1:D:92:ARG:CZ	1:D:92:ARG:CB	2.94	0.44
1:B:51:VAL:HG21	1:B:159:LEU:HD13	2.00	0.44
1:C:29:VAL:HG12	1:C:141:THR:HG21	2.00	0.43
1:C:174:SER:HB2	1:C:465:ALA:H	1.83	0.43
1:C:227:LEU:O	1:C:231:ASN:HB2	2.18	0.43
1:C:322:TYR:CE2	1:D:459:GLN:HG2	2.54	0.43
1:A:576:THR:O	1:A:580:ARG:HG3	2.19	0.42
1:A:25:LYS:HA	1:A:25:LYS:HE2	2.01	0.42
1:A:174:SER:HB2	1:A:465:ALA:H	1.83	0.42
1:B:61:ARG:NH1	1:B:141:THR:O	2.53	0.42
1:A:563:ILE:O	1:A:567:HIS:HB2	2.20	0.42
1:B:437:SER:O	1:B:441:GLN:HG2	2.19	0.42
1:C:27:ILE:CD1	1:C:43:LEU:HB2	2.49	0.42
1:C:150:GLU:CD	1:C:150:GLU:H	2.28	0.42
1:D:162:ASN:ND2	1:D:200:GLY:HA2	2.34	0.42
1:A:257:LEU:HB3	1:A:490:MET:HE1	2.02	0.41
1:A:419:ASP:OD2	1:C:96:ARG:NH1	2.53	0.41
1:D:29:VAL:HG12	1:D:141:THR:HG21	2.02	0.41
1:C:509:ASN:O	1:C:513:THR:HG23	2.20	0.41
1:A:178:ASP:HB3	1:A:181:PRO:HG2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:299:SER:HA	1:B:300:PRO:HD3	1.95	0.41
1:D:98:SER:O	1:D:102:GLU:HG2	2.21	0.41
1:C:400:GLU:OE2	1:D:460:ASP:OD2	2.38	0.41
1:C:257:LEU:HB3	1:C:490:MET:HE1	2.03	0.40
1:B:387:VAL:HG12	1:B:440:LEU:HD11	2.02	0.40
1:A:255:GLU:HG2	1:A:331:LEU:HD13	2.04	0.40
1:A:207:ALA:N	1:A:208:PRO:HD2	2.37	0.40
1:B:560:PHE:HB2	1:C:560:PHE:HB2	2.04	0.40
1:C:387:VAL:HG12	1:C:440:LEU:HD11	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	628/705 (89%)	616 (98%)	12 (2%)	0	100	100
1	B	630/705 (89%)	619 (98%)	11 (2%)	0	100	100
1	C	629/705 (89%)	618 (98%)	11 (2%)	0	100	100
1	D	630/705 (89%)	617 (98%)	13 (2%)	0	100	100
All	All	2517/2820 (89%)	2470 (98%)	47 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	540/591 (91%)	532 (98%)	8 (2%)	57	47
1	B	542/591 (92%)	535 (99%)	7 (1%)	61	51
1	C	543/591 (92%)	536 (99%)	7 (1%)	61	51
1	D	542/591 (92%)	536 (99%)	6 (1%)	65	57
All	All	2167/2364 (92%)	2139 (99%)	28 (1%)	61	51

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	ARG
1	A	84	THR
1	A	102	GLU
1	A	107	CYS
1	A	162	ASN
1	A	353	ASN
1	A	528	LEU
1	A	562	THR
1	B	43	LEU
1	B	107	CYS
1	B	209	GLU
1	B	353	ASN
1	B	364	ARG
1	B	562	THR
1	B	673	LEU
1	C	43	LEU
1	C	92	ARG
1	C	102	GLU
1	C	209	GLU
1	C	353	ASN
1	C	528	LEU
1	C	635	GLU
1	D	59	ARG
1	D	92	ARG
1	D	353	ASN
1	D	364	ARG
1	D	528	LEU
1	D	591	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	162	ASN
1	A	302	GLN
1	A	362	ASN
1	A	372	GLN
1	A	462	ASN
1	A	674	GLN
1	B	47	HIS
1	B	57	GLN
1	B	302	GLN
1	B	408	ASN
1	B	462	ASN
1	C	47	HIS
1	C	162	ASN
1	C	285	GLN
1	C	302	GLN
1	C	362	ASN
1	C	372	GLN
1	C	462	ASN
1	C	621	GLN
1	D	372	GLN
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	2,1	11,13,14	2.92	4 (36%)	15,18,20	1.65	3 (20%)
1	MDO	A	175	2,1	11,13,14	2.94	4 (36%)	15,18,20	1.95	5 (33%)
1	MDO	C	175	2,1	11,13,14	2.89	5 (45%)	15,18,20	1.97	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MDO	B	175	2,1	11,13,14	2.82	4 (36%)	15,18,20	2.03	3 (20%)

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	2,1	-	2/4/23/24	0/1/1/1
1	MDO	A	175	2,1	-	3/4/23/24	0/1/1/1
1	MDO	C	175	2,1	-	2/4/23/24	0/1/1/1
1	MDO	B	175	2,1	-	2/4/23/24	0/1/1/1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	175	MDO	O2-C2	7.17	1.37	1.23
1	A	175	MDO	O2-C2	6.98	1.37	1.23
1	B	175	MDO	O2-C2	6.61	1.36	1.23
1	C	175	MDO	O2-C2	6.44	1.36	1.23
1	A	175	MDO	O3-C3	4.36	1.44	1.20
1	B	175	MDO	O3-C3	4.26	1.44	1.20
1	D	175	MDO	O3-C3	4.10	1.43	1.20
1	C	175	MDO	O3-C3	4.10	1.43	1.20
1	C	175	MDO	C2-N3	-3.19	1.32	1.40
1	C	175	MDO	CA2-N2	-3.18	1.33	1.39
1	A	175	MDO	C2-N3	-2.99	1.33	1.40
1	A	175	MDO	CA2-N2	-2.89	1.34	1.39
1	B	175	MDO	CA2-N2	-2.87	1.34	1.39
1	B	175	MDO	C2-N3	-2.84	1.33	1.40
1	D	175	MDO	CA2-N2	-2.77	1.34	1.39
1	D	175	MDO	C2-N3	-2.76	1.33	1.40
1	C	175	MDO	C1-N2	2.07	1.35	1.32

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	175	MDO	O2-C2-CA2	-5.80	127.32	131.02
1	C	175	MDO	O2-C2-CA2	-5.10	127.77	131.02
1	A	175	MDO	O2-C2-CA2	-4.31	128.27	131.02
1	D	175	MDO	O2-C2-CA2	-4.27	128.29	131.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	175	MDO	CA2-C2-N3	4.26	107.08	103.50
1	B	175	MDO	CA2-C2-N3	3.76	106.66	103.50
1	D	175	MDO	CA2-C2-N3	2.98	106.00	103.50
1	A	175	MDO	CB-CA1-C1	2.73	115.27	111.43
1	A	175	MDO	CA2-C2-N3	2.70	105.77	103.50
1	B	175	MDO	O3-C3-CA3	-2.55	113.99	125.47
1	C	175	MDO	O3-C3-CA3	-2.52	114.12	125.47
1	D	175	MDO	O3-C3-CA3	-2.36	114.84	125.47
1	A	175	MDO	CA1-C1-N2	2.14	126.71	124.04
1	A	175	MDO	CA1-C1-N3	-2.06	122.25	124.69

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	175	MDO	C3-CA3-N3-C2
1	A	175	MDO	N2-C1-CA1-CB
1	B	175	MDO	N2-C1-CA1-CB
1	C	175	MDO	N2-C1-CA1-CB
1	D	175	MDO	N2-C1-CA1-CB
1	A	175	MDO	N3-C1-CA1-CB
1	B	175	MDO	N3-C1-CA1-CB
1	C	175	MDO	N3-C1-CA1-CB
1	D	175	MDO	N3-C1-CA1-CB

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	175	MDO	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands 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
2	BQ7	B	1678	1	13,14,14	1.61	2 (15%)	17,20,20	1.51	3 (17%)
2	BQ7	C	1678	1	13,14,14	1.70	3 (23%)	17,20,20	1.71	4 (23%)
2	BQ7	D	1678	1	13,14,14	1.46	2 (15%)	17,20,20	1.75	3 (17%)
2	BQ7	A	1678	1	13,14,14	1.33	3 (23%)	17,20,20	1.85	3 (17%)

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
2	BQ7	B	1678	1	-	5/14/16/16	0/1/1/1
2	BQ7	C	1678	1	-	3/14/16/16	0/1/1/1
2	BQ7	D	1678	1	-	3/14/16/16	0/1/1/1
2	BQ7	A	1678	1	-	2/14/16/16	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1678	BQ7	CG-CB	3.99	1.57	1.52
2	C	1678	BQ7	CG-CB	3.79	1.56	1.52
2	D	1678	BQ7	CG-CB	3.05	1.56	1.52
2	B	1678	BQ7	FR-CA	-3.00	1.31	1.36
2	D	1678	BQ7	FR-CA	-2.88	1.31	1.36
2	C	1678	BQ7	FR-CA	-2.85	1.31	1.36
2	C	1678	BQ7	FS-CA	-2.77	1.31	1.36
2	A	1678	BQ7	FR-CA	-2.37	1.32	1.36
2	A	1678	BQ7	CG-CB	2.33	1.55	1.52
2	A	1678	BQ7	FS-CA	-2.08	1.33	1.36

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1678	BQ7	FR-CA-CB	-5.29	102.19	109.23
2	A	1678	BQ7	FR-CA-CB	-4.44	103.31	109.23
2	A	1678	BQ7	FS-CA-CB	4.30	114.95	109.23
2	C	1678	BQ7	FR-CA-CB	-4.15	103.70	109.23
2	B	1678	BQ7	FR-CA-CB	-4.08	103.81	109.23
2	C	1678	BQ7	FS-CA-CB	3.94	114.47	109.23
2	D	1678	BQ7	FS-CA-CB	2.73	112.86	109.23
2	B	1678	BQ7	FS-CA-CB	2.70	112.82	109.23
2	A	1678	BQ7	O-C-CA	2.23	117.82	112.54
2	D	1678	BQ7	O-C-CA	2.14	117.60	112.54
2	C	1678	BQ7	O-C-CA	2.10	117.52	112.54
2	B	1678	BQ7	O-C-CA	2.04	117.38	112.54
2	C	1678	BQ7	CD1-CG-CB	-2.03	117.12	120.82

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1678	BQ7	O-C-CA-FR
2	A	1678	BQ7	FS-CA-CB-N
2	B	1678	BQ7	O-C-CA-FR
2	B	1678	BQ7	FS-CA-CB-N
2	C	1678	BQ7	O-C-CA-FR
2	C	1678	BQ7	FS-CA-CB-N
2	D	1678	BQ7	O-C-CA-FR
2	D	1678	BQ7	FS-CA-CB-N
2	B	1678	BQ7	O-C-CA-FS
2	B	1678	BQ7	O1-C-CA-FR
2	D	1678	BQ7	O-C-CA-FS
2	B	1678	BQ7	FR-CA-CB-N
2	C	1678	BQ7	FR-CA-CB-N

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	174:SER	C	175:MDO	N1	1.79
1	A	175:MDO	C3	178:ASP	N	1.62

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	638/705 (90%)	-0.22	12 (1%) 66 70	9, 18, 35, 52	0
1	B	640/705 (90%)	-0.29	6 (0%) 81 84	9, 17, 32, 51	0
1	C	641/705 (90%)	-0.23	7 (1%) 78 81	8, 18, 34, 51	0
1	D	640/705 (90%)	-0.26	9 (1%) 73 77	8, 16, 37, 51	0
All	All	2559/2820 (90%)	-0.25	34 (1%) 75 79	8, 17, 35, 52	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	55	ALA	4.3
1	A	618	VAL	3.3
1	C	56	GLU	3.3
1	D	576	THR	3.1
1	C	576	THR	3.0
1	C	587	ARG	2.9
1	B	590	ASP	2.8
1	D	55	ALA	2.8
1	D	567	HIS	2.7
1	D	114	THR	2.6
1	A	567	HIS	2.5
1	A	202	ASP	2.5
1	B	605	LYS	2.5
1	A	574	THR	2.4
1	B	576	THR	2.4
1	D	574	THR	2.4
1	B	567	HIS	2.4
1	A	566	LEU	2.4
1	A	576	THR	2.4
1	D	524	THR	2.3
1	A	589	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	523	ASP	2.3
1	C	591	ARG	2.2
1	B	202	ASP	2.2
1	A	123	GLU	2.2
1	A	586	LYS	2.1
1	C	677	LEU	2.1
1	D	523	ASP	2.1
1	A	587	ARG	2.1
1	B	57	GLN	2.1
1	D	521	PRO	2.1
1	A	169	LEU	2.1
1	C	114	THR	2.0
1	D	566	LEU	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	MDO	A	175	13/14	0.84	0.16	19,23,25,25	0
1	MDO	B	175	13/14	0.85	0.14	18,22,23,23	0
1	MDO	D	175	13/14	0.86	0.14	19,22,23,23	0
1	MDO	C	175	13/14	0.91	0.10	19,21,22,23	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [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
2	BQ7	C	1678	14/14	0.94	0.07	18,21,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	BQ7	A	1678	14/14	0.95	0.07	19,20,24,24	0
2	BQ7	B	1678	14/14	0.96	0.06	19,20,22,23	0
2	BQ7	D	1678	14/14	0.96	0.06	17,18,21,22	0

6.5 Other polymers [i](#)

There are no such residues in this entry.