



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:16 AM UTC

PDB ID : 4CQ5 / pdb_00004cq5
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 : 2014-02-11
Resolution : 1.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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

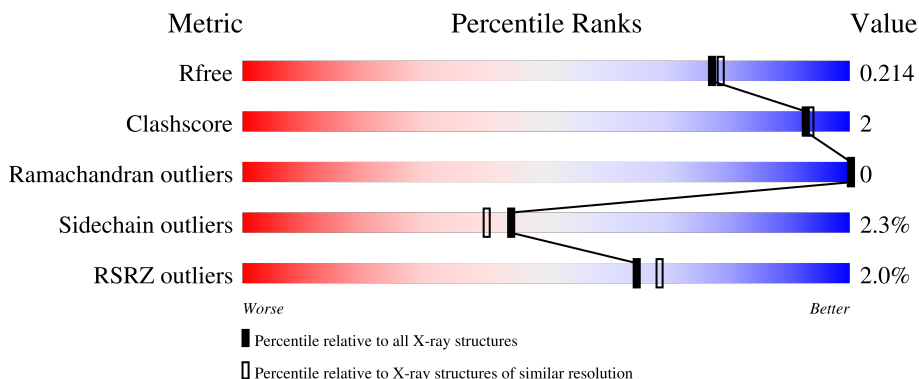
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	2% 85% 5% 9%
1	B	705	2% 85% 5% 10%
1	C	705	% 85% 5% 9%
1	D	705	2% 86% 5% 9%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 20824 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	639	Total	C	N	O	S	0	0	0
			4955	3144	855	933	23			
1	B	638	Total	C	N	O	S	0	0	0
			4946	3138	855	930	23			
1	C	641	Total	C	N	O	S	0	0	0
			4965	3149	856	937	23			
1	D	642	Total	C	N	O	S	0	0	0
			4980	3159	859	939	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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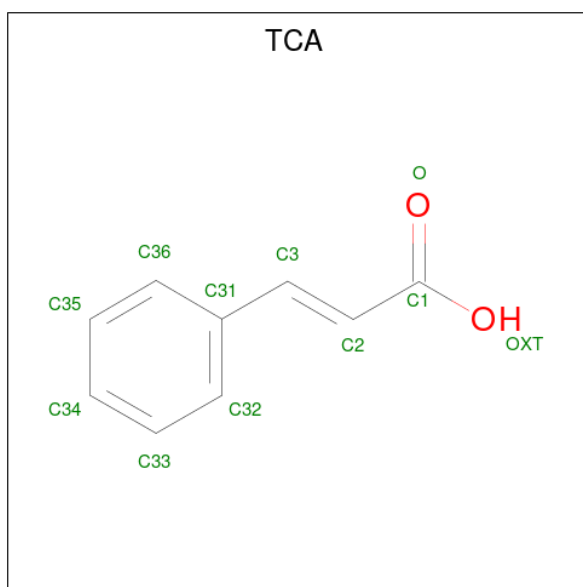
Chain	Residue	Modelled	Actual	Comment	Reference
A	175	MDO	SER	chromophore	UNP Q68G84
A	175	MDO	GLY	chromophore	UNP Q68G84
B	-19	MET	-	expression tag	UNP Q68G84
B	-18	GLY	-	expression tag	UNP Q68G84
B	-17	SER	-	expression tag	UNP Q68G84
B	-16	SER	-	expression tag	UNP Q68G84
B	-15	HIS	-	expression tag	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
A	80	ALA	TYR	engineered mutation	UNP Q68G84
B	80	ALA	TYR	engineered mutation	UNP Q68G84
C	80	ALA	TYR	engineered mutation	UNP Q68G84
D	80	ALA	TYR	engineered mutation	UNP Q68G84

- Molecule 2 is PHENYLETHYLENECARBOXYLIC ACID (CCD ID: TCA) (formula: C₉H₈O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			11	9	2		
2	A	1	Total	C	O	0	0
			11	9	2		
2	B	1	Total	C	O	0	0
			11	9	2		
2	B	1	Total	C	O	0	0
			11	9	2		
2	C	1	Total	C	O	0	0
			11	9	2		
2	C	1	Total	C	O	0	0
			11	9	2		
2	D	1	Total	C	O	0	0
			11	9	2		
2	D	1	Total	C	O	0	0
			11	9	2		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	C	O	0	0
			4	2	2		

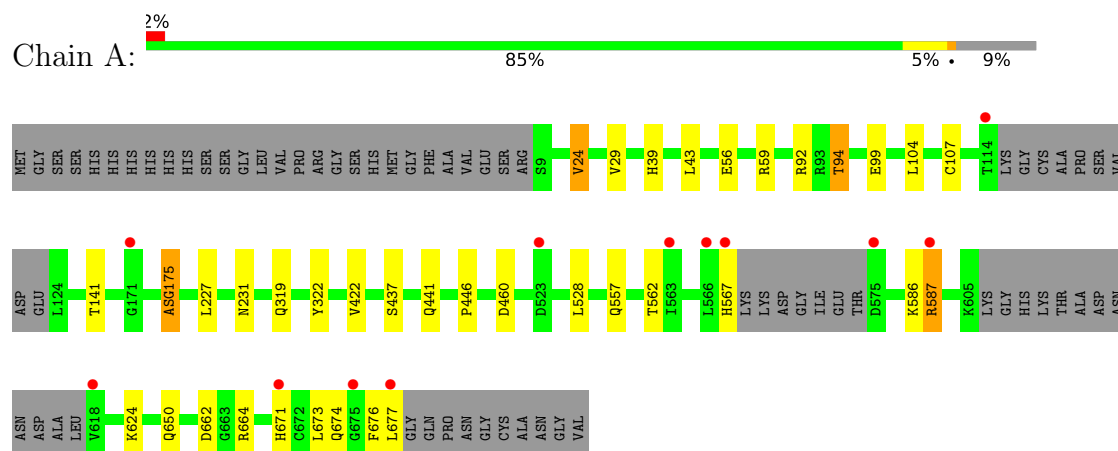
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	245	Total 245	O 245	0	0
5	B	220	Total 220	O 220	0	0
5	C	212	Total 212	O 212	0	0
5	D	203	Total 203	O 203	0	0

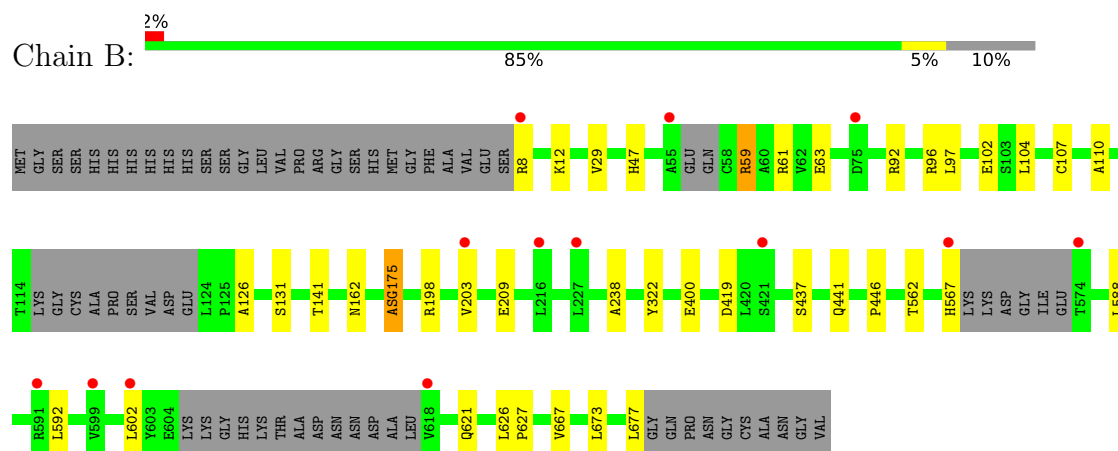
3 Residue-property plots [i](#)

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.

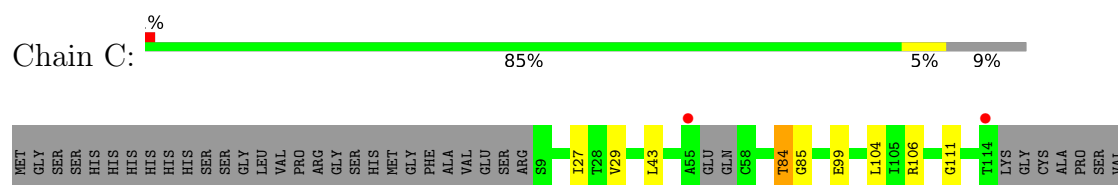
• Molecule 1: PHENYLALANINE AMINOMUTASE

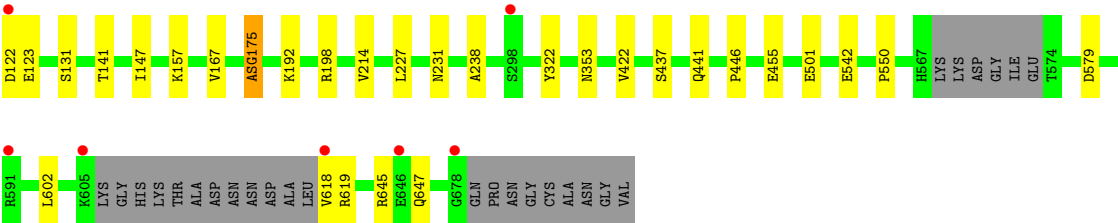


• Molecule 1: PHENYLALANINE AMINOMUTASE

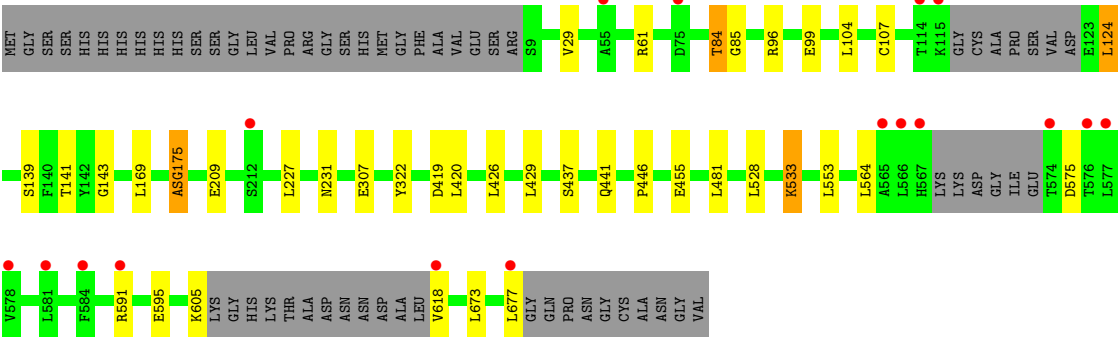
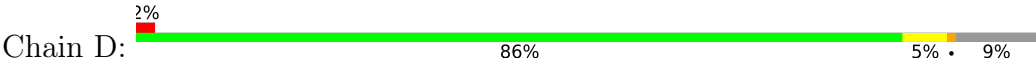


• Molecule 1: PHENYLALANINE AMINOMUTASE





● Molecule 1: PHENYLALANINE AMINOMUTASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	99.88Å 146.42Å 100.48Å 90.00° 99.59° 90.00°	Depositor
Resolution (Å)	33.91 – 1.90 33.91 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.5 (33.91-1.90) 99.5 (33.91-1.90)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.178 , 0.207 0.186 , 0.214	Depositor DCC
R_{free} test set	11126 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	22.3	Xtriage
Anisotropy	0.146	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 29.4	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	20824	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.43% 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: GOL, MDO, EDO, TCA

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	0/5026	0.78	1/6819 (0.0%)
1	B	0.60	0/5016	0.77	2/6805 (0.0%)
1	C	0.60	0/5035	0.76	1/6830 (0.0%)
1	D	0.59	0/5051	0.77	0/6852
All	All	0.59	0/20128	0.77	4/27306 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	94	THR	CB-CA-C	-5.95	97.66	110.45
1	B	667	VAL	CA-C-N	-5.31	113.44	119.28
1	B	667	VAL	C-N-CA	-5.31	113.44	119.28
1	C	550	PRO	N-CA-C	5.02	120.43	113.65

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	5019	19	0
1	B	4946	0	5011	19	0
1	C	4965	0	5024	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	4980	0	5045	19	0
2	A	22	0	9	1	0
2	B	22	0	7	1	0
2	C	22	0	6	1	0
2	D	22	0	7	1	0
3	B	6	0	8	0	0
4	D	4	0	6	0	0
5	A	245	0	0	0	0
5	B	220	0	0	1	0
5	C	212	0	0	0	0
5	D	203	0	0	0	0
All	All	20824	0	20142	60	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 (60) 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:96:ARG:NH1	1:D:419:ASP:OD2	2.18	0.76
1:A:104:LEU:HD11	2:A:1680:TCA:H35	1.81	0.62
1:B:567:HIS:NE2	1:C:579:ASP:OD1	2.26	0.61
1:C:123:GLU:OE2	1:C:198:ARG:NH2	2.33	0.61
1:D:104:LEU:HD11	2:D:1680:TCA:H35	1.83	0.60
1:C:99:GLU:OE2	1:C:106:ARG:NH2	2.36	0.59
1:C:446:PRO:HD3	1:D:446:PRO:HD3	1.88	0.56
1:C:175:MDO:HB21	1:D:322:TYR:OH	2.05	0.56
1:C:322:TYR:OH	1:D:175:MDO:HB21	2.09	0.53
1:C:104:LEU:HD11	2:C:1681:TCA:H33	1.91	0.52
1:A:446:PRO:HD3	1:B:446:PRO:HD3	1.90	0.52
1:D:307:GLU:OE2	1:D:533:LYS:NZ	2.37	0.51
1:A:175:MDO:HB21	1:B:322:TYR:OH	2.11	0.50
1:A:92:ARG:HH22	1:C:542:GLU:CD	2.19	0.50
1:A:671:HIS:O	1:A:674:GLN:HG2	2.12	0.50
1:A:322:TYR:OH	1:B:175:MDO:HB21	2.11	0.50
1:A:24:VAL:HG11	1:A:39:HIS:CD2	2.48	0.48
1:B:92:ARG:NH2	1:D:420:LEU:HD12	2.29	0.48
1:C:131:SER:HB2	1:C:238:ALA:HB1	1.94	0.47
1:A:227:LEU:O	1:A:231:ASN:HB2	2.15	0.47
1:B:47:HIS:CE1	1:B:162:ASN:OD1	2.68	0.47
1:D:29:VAL:HG12	1:D:141:THR:HG21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:437:SER:O	1:D:441:GLN:HG2	2.15	0.47
1:A:567:HIS:NE2	1:D:575:ASP:OD1	2.48	0.46
1:B:59:ARG:HD2	1:B:63:GLU:CD	2.41	0.45
1:C:84:THR:HG22	1:C:85:GLY:O	2.16	0.45
1:C:645:ARG:CZ	1:C:647:GLN:HG3	2.47	0.45
1:D:124:LEU:HD13	1:D:169:LEU:HD12	1.98	0.45
1:D:426:LEU:HD12	1:D:426:LEU:N	2.32	0.45
1:A:676:PHE:O	1:A:677:LEU:HD23	2.17	0.45
1:B:29:VAL:HG12	1:B:141:THR:HG21	1.99	0.45
1:B:419:ASP:OD2	1:D:96:ARG:NH1	2.44	0.44
1:D:84:THR:HG22	1:D:85:GLY:O	2.16	0.44
1:C:29:VAL:HG12	1:C:141:THR:HG21	1.98	0.44
1:B:8:ARG:HD2	1:B:12:LYS:HE3	2.00	0.44
1:A:29:VAL:HG12	1:A:141:THR:HG21	2.00	0.44
1:B:126:ALA:HB2	1:B:198:ARG:HD2	2.00	0.44
1:A:662:ASP:OD1	1:A:664:ARG:HD3	2.18	0.44
1:A:650:GLN:HG3	1:C:111:GLY:O	2.19	0.43
1:A:437:SER:O	1:A:441:GLN:HG2	2.18	0.43
1:D:591:ARG:NH1	1:D:595:GLU:OE2	2.52	0.43
1:A:587:ARG:HH11	1:A:587:ARG:HG2	1.84	0.42
1:A:422:VAL:HG11	1:C:99:GLU:HG3	2.02	0.42
1:A:460:ASP:OD2	1:B:400:GLU:OE2	2.38	0.42
1:B:131:SER:HB2	1:B:238:ALA:HB1	2.01	0.42
1:C:437:SER:O	1:C:441:GLN:HG2	2.20	0.42
1:B:626:LEU:HB3	1:B:627:PRO:HD3	2.01	0.41
1:C:501:GLU:OE1	1:C:619:ARG:HD3	2.20	0.41
1:C:123:GLU:HB2	1:C:167:VAL:O	2.20	0.41
1:C:157:LYS:HE2	1:C:214:VAL:O	2.21	0.41
1:A:99:GLU:HG3	1:C:422:VAL:HG11	2.02	0.41
1:B:104:LEU:HD11	2:B:1679:TCA:H35	2.03	0.41
1:B:198:ARG:NH1	5:B:2063:HOH:O	2.50	0.41
1:B:437:SER:O	1:B:441:GLN:HG2	2.21	0.41
1:B:110:ALA:HB1	1:D:429:LEU:HD23	2.03	0.41
1:C:27:ILE:CD1	1:C:43:LEU:HB2	2.51	0.41
1:D:61:ARG:HG2	1:D:143:GLY:HA3	2.03	0.40
1:D:227:LEU:O	1:D:231:ASN:HB2	2.22	0.40
1:A:557:GLN:OE1	1:D:553:LEU:HD22	2.22	0.40
1:C:227:LEU:O	1:C:231:ASN:HB2	2.21	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	625/705 (89%)	612 (98%)	13 (2%)	0	100	100
1	C	628/705 (89%)	618 (98%)	10 (2%)	0	100	100
1	D	631/705 (90%)	617 (98%)	14 (2%)	0	100	100
All	All	2512/2820 (89%)	2463 (98%)	49 (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%)	527 (98%)	13 (2%)	43	38
1	B	539/591 (91%)	525 (97%)	14 (3%)	40	35
1	C	541/591 (92%)	533 (98%)	8 (2%)	57	56
1	D	543/591 (92%)	528 (97%)	15 (3%)	38	32
All	All	2163/2364 (92%)	2113 (98%)	50 (2%)	44	40

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	VAL
1	A	43	LEU

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Mol	Chain	Res	Type
1	A	56	GLU
1	A	59	ARG
1	A	94	THR
1	A	107	CYS
1	A	319	GLN
1	A	528	LEU
1	A	562	THR
1	A	586	LYS
1	A	587	ARG
1	A	624	LYS
1	A	673	LEU
1	B	59	ARG
1	B	61	ARG
1	B	97	LEU
1	B	102	GLU
1	B	107	CYS
1	B	203	VAL
1	B	209	GLU
1	B	562	THR
1	B	588	LEU
1	B	592	LEU
1	B	602	LEU
1	B	621	GLN
1	B	673	LEU
1	B	677	LEU
1	C	84	THR
1	C	122	ASP
1	C	147	ILE
1	C	192	LYS
1	C	353	ASN
1	C	455	GLU
1	C	602	LEU
1	C	618	VAL
1	D	84	THR
1	D	99	GLU
1	D	107	CYS
1	D	124	LEU
1	D	139	SER
1	D	209	GLU
1	D	455	GLU
1	D	481	LEU
1	D	528	LEU

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Mol	Chain	Res	Type
1	D	533	LYS
1	D	564	LEU
1	D	605	LYS
1	D	618	VAL
1	D	673	LEU
1	D	677	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	285	GLN
1	A	362	ASN
1	A	372	GLN
1	B	302	GLN
1	B	372	GLN
1	C	162	ASN
1	C	285	GLN
1	C	360	HIS
1	C	362	ASN
1	C	372	GLN
1	C	462	ASN
1	C	621	GLN
1	D	277	HIS
1	D	285	GLN
1	D	302	GLN
1	D	360	HIS
1	D	372	GLN
1	D	522	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	4.15	4 (36%)	15,18,20	4.70	5 (33%)
1	MDO	C	175	1	11,13,14	4.08	5 (45%)	15,18,20	4.53	5 (33%)
1	MDO	B	175	1	11,13,14	4.07	5 (45%)	15,18,20	5.16	5 (33%)
1	MDO	A	175	1	11,13,14	4.25	5 (45%)	15,18,20	5.21	5 (33%)

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

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	175	MDO	O2-C2	12.59	1.48	1.23
1	D	175	MDO	O2-C2	12.32	1.48	1.23
1	B	175	MDO	O2-C2	12.07	1.47	1.23
1	C	175	MDO	O2-C2	11.94	1.47	1.23
1	A	175	MDO	C1-N2	4.14	1.38	1.32
1	C	175	MDO	C1-N2	3.84	1.37	1.32
1	D	175	MDO	C1-N2	3.56	1.37	1.32
1	C	175	MDO	C2-N3	-3.51	1.31	1.40
1	B	175	MDO	C1-N2	3.41	1.37	1.32
1	D	175	MDO	C2-N3	-3.36	1.32	1.40
1	B	175	MDO	C2-N3	-3.16	1.32	1.40
1	A	175	MDO	C2-N3	-3.04	1.33	1.40
1	B	175	MDO	CA2-N2	-2.43	1.35	1.39
1	A	175	MDO	CA2-N2	-2.23	1.35	1.39
1	B	175	MDO	CA2-C2	2.22	1.47	1.43
1	C	175	MDO	CA2-C2	2.13	1.47	1.43
1	D	175	MDO	CA2-C2	2.11	1.47	1.43
1	C	175	MDO	CA2-N2	-2.11	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	175	MDO	CA2-C2	2.10	1.47	1.43

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	175	MDO	O2-C2-CA2	-12.33	123.15	131.02
1	B	175	MDO	CA2-C2-N3	10.48	112.30	103.50
1	C	175	MDO	CA2-C2-N3	10.34	112.18	103.50
1	B	175	MDO	O2-C2-CA2	-10.33	124.43	131.02
1	A	175	MDO	CA2-C2-N3	10.15	112.02	103.50
1	D	175	MDO	CA2-C2-N3	9.91	111.82	103.50
1	D	175	MDO	O2-C2-CA2	-9.71	124.83	131.02
1	C	175	MDO	C2-CA2-N2	-9.33	102.27	108.95
1	B	175	MDO	C2-CA2-N2	-9.22	102.35	108.95
1	D	175	MDO	C2-CA2-N2	-8.71	102.71	108.95
1	A	175	MDO	C2-CA2-N2	-8.56	102.82	108.95
1	B	175	MDO	C2-N3-C1	-8.25	104.25	108.07
1	A	175	MDO	C2-N3-C1	-7.06	104.80	108.07
1	C	175	MDO	O2-C2-CA2	-6.67	126.76	131.02
1	D	175	MDO	C2-N3-C1	-6.49	105.06	108.07
1	C	175	MDO	C2-N3-C1	-6.15	105.22	108.07
1	C	175	MDO	CA2-N2-C1	4.84	109.73	105.39
1	B	175	MDO	CA2-N2-C1	4.76	109.66	105.39
1	A	175	MDO	CA2-N2-C1	4.50	109.42	105.39
1	D	175	MDO	CA2-N2-C1	4.20	109.16	105.39

There are no chirality outliers.

All (6) torsion outliers are listed below:

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

There are no ring outliers.

4 monomers are involved in 4 short contacts:

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

10 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	TCA	C	1679	-	11,11,11	2.73	3 (27%)	13,13,13	1.16	1 (7%)
2	TCA	A	1680	-	11,11,11	2.54	3 (27%)	13,13,13	1.63	2 (15%)
2	TCA	B	1679	-	11,11,11	2.56	2 (18%)	13,13,13	1.61	1 (7%)
2	TCA	B	1680	-	11,11,11	2.65	3 (27%)	13,13,13	1.15	1 (7%)
2	TCA	A	1679	-	11,11,11	2.75	3 (27%)	13,13,13	1.22	1 (7%)
2	TCA	D	1680	-	11,11,11	2.50	3 (27%)	13,13,13	1.51	1 (7%)
3	GOL	B	1681	-	5,5,5	0.26	0	5,5,5	0.19	0
2	TCA	C	1681	-	11,11,11	2.53	3 (27%)	13,13,13	1.53	1 (7%)
2	TCA	D	1679	-	11,11,11	2.72	2 (18%)	13,13,13	1.28	1 (7%)
4	EDO	D	1681	-	3,3,3	0.49	0	2,2,2	0.31	0

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	TCA	C	1679	-	-	0/5/5/5	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TCA	A	1680	-	-	0/5/5/5	0/1/1/1
2	TCA	B	1679	-	-	0/5/5/5	0/1/1/1
2	TCA	B	1680	-	-	0/5/5/5	0/1/1/1
2	TCA	A	1679	-	-	0/5/5/5	0/1/1/1
2	TCA	D	1680	-	-	0/5/5/5	0/1/1/1
3	GOL	B	1681	-	-	2/4/4/4	-
2	TCA	C	1681	-	-	0/5/5/5	0/1/1/1
2	TCA	D	1679	-	-	0/5/5/5	0/1/1/1
4	EDO	D	1681	-	-	0/1/1/1	-

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1679	TCA	C2-C3	8.10	1.53	1.33
2	C	1679	TCA	C2-C3	8.02	1.53	1.33
2	D	1679	TCA	C2-C3	8.02	1.53	1.33
2	B	1680	TCA	C2-C3	7.71	1.52	1.33
2	B	1679	TCA	C2-C3	7.56	1.52	1.33
2	A	1680	TCA	C2-C3	7.30	1.51	1.33
2	C	1681	TCA	C2-C3	7.30	1.51	1.33
2	D	1680	TCA	C2-C3	7.17	1.51	1.33
2	D	1680	TCA	C31-C3	-3.01	1.39	1.47
2	A	1680	TCA	C31-C3	-3.01	1.39	1.47
2	C	1681	TCA	C31-C3	-2.87	1.39	1.47
2	D	1679	TCA	C31-C3	-2.76	1.39	1.47
2	A	1679	TCA	C31-C3	-2.74	1.39	1.47
2	B	1679	TCA	C31-C3	-2.73	1.39	1.47
2	B	1680	TCA	C31-C3	-2.62	1.40	1.47
2	C	1679	TCA	C31-C3	-2.55	1.40	1.47
2	A	1680	TCA	OXT-C1	-2.34	1.24	1.30
2	C	1679	TCA	C2-C1	2.32	1.54	1.48
2	C	1681	TCA	OXT-C1	-2.18	1.24	1.30
2	D	1680	TCA	OXT-C1	-2.18	1.24	1.30
2	A	1679	TCA	C2-C1	2.04	1.53	1.48
2	B	1680	TCA	C2-C1	2.03	1.53	1.48

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1680	TCA	C31-C3-C2	-5.11	115.75	126.92
2	B	1679	TCA	C31-C3-C2	-5.09	115.80	126.92
2	C	1681	TCA	C31-C3-C2	-4.78	116.47	126.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1680	TCA	C31-C3-C2	-4.75	116.53	126.92
2	D	1679	TCA	C31-C3-C2	-3.88	118.45	126.92
2	A	1679	TCA	C31-C3-C2	-3.50	119.27	126.92
2	B	1680	TCA	C31-C3-C2	-3.46	119.36	126.92
2	C	1679	TCA	C31-C3-C2	-3.34	119.62	126.92
2	A	1680	TCA	C36-C31-C32	2.05	120.70	117.65

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1681	GOL	O1-C1-C2-C3
3	B	1681	GOL	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1680	TCA	1	0
2	B	1679	TCA	1	0
2	D	1680	TCA	1	0
2	C	1681	TCA	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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%)	0.06	12 (1%) 66 70	12, 23, 43, 67	0
1	B	637/705 (90%)	0.03	13 (2%) 65 69	12, 23, 38, 56	0
1	C	640/705 (90%)	0.03	9 (1%) 73 76	12, 23, 41, 55	0
1	D	641/705 (90%)	0.09	17 (2%) 56 60	12, 23, 46, 61	0
All	All	2556/2820 (90%)	0.05	51 (1%) 65 69	12, 23, 42, 67	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	55	ALA	5.1
1	D	55	ALA	3.9
1	B	55	ALA	3.8
1	B	618	VAL	3.4
1	A	618	VAL	3.4
1	D	576	THR	3.3
1	B	591	ARG	3.2
1	A	677	LEU	3.0
1	D	75	ASP	3.0
1	D	567	HIS	2.9
1	A	171	GLY	2.9
1	A	575	ASP	2.8
1	B	567	HIS	2.7
1	D	677	LEU	2.6
1	C	618	VAL	2.6
1	D	566	LEU	2.6
1	C	122	ASP	2.6
1	D	114	THR	2.6
1	A	587	ARG	2.5
1	D	574	THR	2.5
1	C	605	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	591	ARG	2.4
1	D	577	LEU	2.4
1	A	114	THR	2.4
1	C	591	ARG	2.4
1	A	567	HIS	2.4
1	A	675	GLY	2.4
1	D	212	SER	2.3
1	D	618	VAL	2.3
1	D	581	LEU	2.3
1	D	565	ALA	2.3
1	B	75	ASP	2.2
1	A	671	HIS	2.2
1	C	114	THR	2.2
1	A	523	ASP	2.2
1	B	574	THR	2.2
1	C	298	SER	2.2
1	C	646	GLU	2.1
1	B	599	VAL	2.1
1	B	8	ARG	2.1
1	D	584	PHE	2.1
1	D	115	LYS	2.1
1	A	566	LEU	2.1
1	C	678	GLY	2.1
1	B	227	LEU	2.1
1	B	203	VAL	2.0
1	D	578	VAL	2.0
1	B	216	LEU	2.0
1	B	602	LEU	2.0
1	B	421	SER	2.0
1	A	563	ILE	2.0

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

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	0.85	0.14	24,28,31,32	0
1	MDO	B	175	13/14	0.86	0.12	22,25,26,29	0
1	MDO	D	175	13/14	0.88	0.11	21,25,27,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	MDO	C	175	13/14	0.91	0.09	18,21,23,24	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($\text{\AA}^2$)	Q<0.9
2	TCA	C	1679	11/11	0.86	0.15	33,34,35,35	11
2	TCA	A	1679	11/11	0.87	0.12	31,31,32,32	11
2	TCA	B	1680	11/11	0.88	0.10	23,24,24,24	11
2	TCA	D	1680	11/11	0.88	0.11	26,28,28,29	11
2	TCA	C	1681	11/11	0.89	0.10	24,25,26,26	11
2	TCA	B	1679	11/11	0.90	0.11	28,29,29,29	11
3	GOL	B	1681	6/6	0.91	0.10	36,41,42,43	0
2	TCA	A	1680	11/11	0.92	0.10	25,26,27,27	11
4	EDO	D	1681	4/4	0.92	0.09	29,31,31,34	0
2	TCA	D	1679	11/11	0.93	0.09	24,26,27,27	11

6.5 Other polymers [i](#)

There are no such residues in this entry.