



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 07:52 PM UTC

PDB ID : 4GQQ / pdb_00004gqq
Title : Human pancreatic alpha-amylase with bound ethyl caffeate
Authors : Williams, L.K.; Brayer, G.D.
Deposited on : 2012-08-23
Resolution : 1.35 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

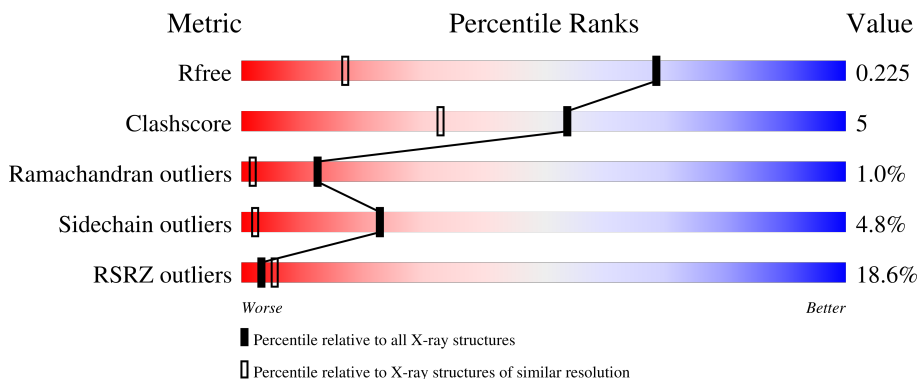
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.35 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	1216 (1.36-1.36)
Clashscore	190562	1232 (1.36-1.36)
Ramachandran outliers	187476	1220 (1.36-1.36)
Sidechain outliers	187428	1220 (1.36-1.36)
RSRZ outliers	180081	1214 (1.36-1.36)

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	496	19% 81% 16% ..

2 Entry composition [i](#)

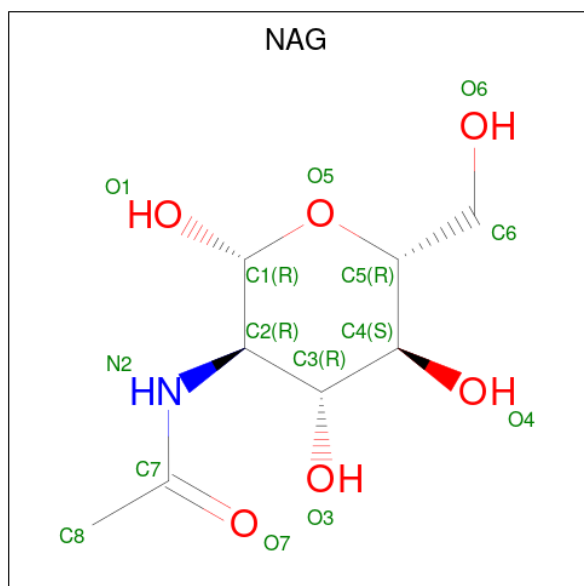
There are 6 unique types of molecules in this entry. The entry contains 4247 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Pancreatic alpha-amylase.

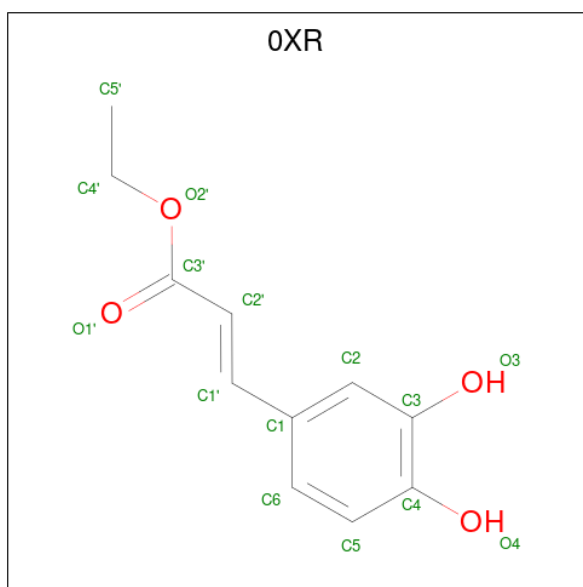
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	496	Total	C	N	O	S	0	0	0
			3946	2497	696	733	20			

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is ethyl (2E)-3-(3,4-dihydroxyphenyl)prop-2-enoate (CCD ID: 0XR) (formula: $C_{11}H_{12}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			15	11	4		
3	A	1	Total	C	O	0	0
			15	11	4		
3	A	1	Total	C	O	0	0
			15	11	4		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Ca	0	0
			1	1		

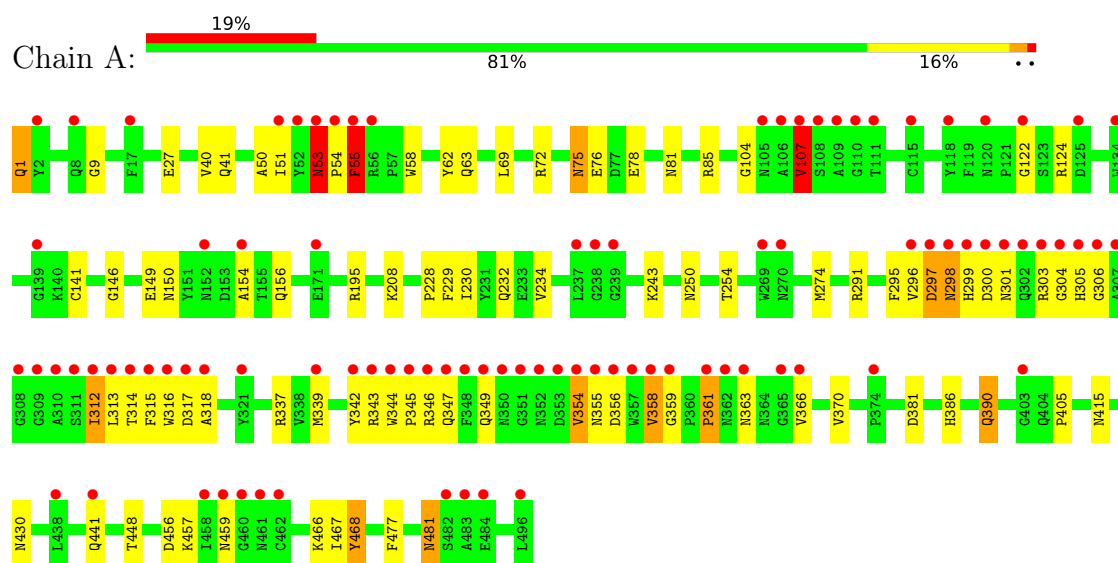
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	240	Total	O	0	0
			240	240		

3 Residue-property plots

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: Pancreatic alpha-amylase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	52.06Å 68.12Å 125.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	52.06 – 1.35 52.06 – 1.35	Depositor EDS
% Data completeness (in resolution range)	99.4 (52.06-1.35) 99.3 (52.06-1.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.37 (at 1.35Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.197 , 0.227 0.196 , 0.225	Depositor DCC
R_{free} test set	4938 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	11.7	Xtriage
Anisotropy	0.210	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 74.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4247	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.71% 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: CL, OXR, PCA, NAG, CA

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	0.91	2/4053 (0.0%)	1.71	72/5506 (1.3%)

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	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	313	LEU	CA-C	6.30	1.60	1.52
1	A	53	ASN	CA-C	5.45	1.59	1.52

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	361	PRO	CA-C-N	-7.43	111.02	122.62
1	A	361	PRO	C-N-CA	-7.43	111.02	122.62
1	A	354	VAL	CA-C-N	-6.70	112.00	121.99
1	A	354	VAL	C-N-CA	-6.70	112.00	121.99
1	A	313	LEU	N-CA-C	6.44	120.00	109.24
1	A	456	ASP	CA-C-N	-6.43	113.91	122.85
1	A	456	ASP	C-N-CA	-6.43	113.91	122.85
1	A	295	PHE	CA-C-N	-6.35	114.15	122.16
1	A	295	PHE	C-N-CA	-6.35	114.15	122.16
1	A	457	LYS	CA-C-N	-6.34	114.67	123.10
1	A	457	LYS	C-N-CA	-6.34	114.67	123.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	154	ALA	N-CA-C	6.24	118.08	111.28
1	A	124	ARG	CA-C-N	-6.18	114.40	123.05
1	A	124	ARG	C-N-CA	-6.18	114.40	123.05
1	A	254	THR	CA-C-N	-6.03	114.47	122.85
1	A	254	THR	C-N-CA	-6.03	114.47	122.85
1	A	467	ILE	CA-C-N	-5.96	114.70	123.05
1	A	467	ILE	C-N-CA	-5.96	114.70	123.05
1	A	55	PHE	CA-C-N	-5.89	107.42	121.80
1	A	55	PHE	C-N-CA	-5.89	107.42	121.80
1	A	316	TRP	N-CA-C	-5.81	105.29	112.38
1	A	53	ASN	N-CA-C	5.78	122.57	109.81
1	A	346	ARG	CA-C-N	-5.76	111.96	121.92
1	A	346	ARG	C-N-CA	-5.76	111.96	121.92
1	A	304	GLY	CA-C-N	-5.72	113.18	122.34
1	A	304	GLY	C-N-CA	-5.72	113.18	122.34
1	A	229	PHE	CA-C-N	-5.72	115.65	123.14
1	A	229	PHE	C-N-CA	-5.72	115.65	123.14
1	A	234	VAL	CA-C-N	-5.70	115.25	122.43
1	A	234	VAL	C-N-CA	-5.70	115.25	122.43
1	A	405	PRO	N-CA-C	5.69	120.43	111.38
1	A	359	GLY	CA-C-N	5.63	126.17	120.38
1	A	359	GLY	C-N-CA	5.63	126.17	120.38
1	A	477	PHE	CA-C-N	-5.62	115.07	123.00
1	A	477	PHE	C-N-CA	-5.62	115.07	123.00
1	A	53	ASN	CA-C-N	5.62	140.48	127.00
1	A	53	ASN	C-N-CA	5.62	140.48	127.00
1	A	299	HIS	CA-C-N	-5.62	112.06	121.39
1	A	299	HIS	C-N-CA	-5.62	112.06	121.39
1	A	122	GLY	CA-C-N	-5.50	113.85	122.65
1	A	122	GLY	C-N-CA	-5.50	113.85	122.65
1	A	291	ARG	CA-C-N	-5.47	114.99	122.93
1	A	291	ARG	C-N-CA	-5.47	114.99	122.93
1	A	468	TYR	CA-C-N	-5.45	116.07	122.93
1	A	468	TYR	C-N-CA	-5.45	116.07	122.93
1	A	230	ILE	CA-C-N	-5.44	115.09	122.77
1	A	230	ILE	C-N-CA	-5.44	115.09	122.77
1	A	306	GLY	CA-C-N	-5.43	114.87	123.12
1	A	306	GLY	C-N-CA	-5.43	114.87	123.12
1	A	141	CYS	CA-C-N	-5.39	114.11	122.67
1	A	141	CYS	C-N-CA	-5.39	114.11	122.67
1	A	50	ALA	CA-C-N	-5.33	112.97	120.75
1	A	50	ALA	C-N-CA	-5.33	112.97	120.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	296	VAL	CA-C-N	-5.31	114.12	122.08
1	A	296	VAL	C-N-CA	-5.31	114.12	122.08
1	A	448	THR	CA-C-N	-5.30	114.36	122.62
1	A	448	THR	C-N-CA	-5.30	114.36	122.62
1	A	9	GLY	CA-C-N	-5.27	115.76	122.77
1	A	9	GLY	C-N-CA	-5.27	115.76	122.77
1	A	107	VAL	CA-C-N	-5.26	113.52	122.56
1	A	107	VAL	C-N-CA	-5.26	113.52	122.56
1	A	312	ILE	CA-C-N	-5.26	114.21	122.73
1	A	312	ILE	C-N-CA	-5.26	114.21	122.73
1	A	40	VAL	CA-C-N	-5.18	115.31	122.30
1	A	40	VAL	C-N-CA	-5.18	115.31	122.30
1	A	370	VAL	CA-C-N	-5.04	114.76	122.87
1	A	370	VAL	C-N-CA	-5.04	114.76	122.87
1	A	146	GLY	N-CA-C	-5.03	108.67	115.21
1	A	430	ASN	CA-C-N	-5.01	114.70	122.67
1	A	430	ASN	C-N-CA	-5.01	114.70	122.67
1	A	195	ARG	CA-C-N	-5.00	115.06	122.41
1	A	195	ARG	C-N-CA	-5.00	115.06	122.41

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	107	VAL	Mainchain
1	A	468	TYR	Sidechain
1	A	55	PHE	Sidechain
1	A	62	TYR	Sidechain

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	3946	0	3717	37	0
2	A	14	0	13	0	0
3	A	45	0	30	1	0
4	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	1	0	0	0	0
6	A	240	0	0	2	0
All	All	4247	0	3760	38	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 5.

All (38) 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:53:ASN:HB3	1:A:55:PHE:HB2	1.58	0.86
1:A:314:THR:H	1:A:317:ASP:HB2	1.46	0.79
1:A:481:ASN:H	1:A:481:ASN:HD22	1.30	0.78
1:A:314:THR:N	1:A:317:ASP:HB2	2.00	0.77
1:A:81:ASN:HD21	1:A:85:ARG:HH11	1.34	0.76
1:A:390:GLN:NE2	1:A:390:GLN:H	1.92	0.67
1:A:390:GLN:H	1:A:390:GLN:HE21	1.41	0.67
1:A:208:LYS:HD3	1:A:250:ASN:HD22	1.62	0.65
1:A:150:ASN:H	1:A:156:GLN:NE2	1.97	0.60
1:A:300:ASP:HA	1:A:312:ILE:HD11	1.83	0.60
1:A:314:THR:O	1:A:318:ALA:HB2	2.01	0.60
1:A:149:GLU:H	1:A:156:GLN:NE2	2.00	0.60
1:A:274:MET:H	1:A:415:ASN:ND2	2.01	0.59
1:A:58:TRP:HE1	1:A:303:ARG:HG3	1.67	0.59
1:A:274:MET:H	1:A:415:ASN:HD22	1.51	0.59
1:A:481:ASN:H	1:A:481:ASN:ND2	1.99	0.58
1:A:27:GLU:OE2	1:A:386:HIS:HE1	1.85	0.58
1:A:63:GLN:NE2	1:A:104:GLY:H	2.02	0.57
1:A:69:LEU:HD12	1:A:76:GLU:HG3	1.88	0.56
1:A:75:ASN:ND2	1:A:78:GLU:H	2.05	0.55
1:A:342:TYR:OH	1:A:358:VAL:HG23	2.11	0.51
1:A:208:LYS:HD3	1:A:250:ASN:ND2	2.26	0.50
1:A:315:PHE:C	1:A:317:ASP:N	2.66	0.49
1:A:41:GLN:HE22	1:A:337:ARG:HH11	1.60	0.48
1:A:51:ILE:HD11	1:A:55:PHE:CD1	2.49	0.48
1:A:343:ARG:NH1	1:A:381:ASP:OD2	2.47	0.47
1:A:27:GLU:OE2	1:A:386:HIS:CE1	2.68	0.45
1:A:75:ASN:HD22	1:A:78:GLU:H	1.65	0.45
1:A:75:ASN:HD22	1:A:75:ASN:C	2.26	0.44
1:A:363:ASN:N	1:A:366:VAL:O	2.42	0.44
1:A:297:ASP:OD2	1:A:339:MET:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:ASN:ND2	1:A:85:ARG:HH11	2.10	0.43
1:A:301:ASN:C	1:A:303:ARG:HE	2.27	0.42
1:A:1:PCA:HA	1:A:228:PRO:O	2.19	0.42
1:A:72:ARG:HG2	6:A:625:HOH:O	2.19	0.42
1:A:361:PRO:HG2	6:A:793:HOH:O	2.19	0.41
3:A:502:OXR:H10	3:A:502:OXR:H6	1.84	0.41
1:A:208:LYS:HB2	1:A:250:ASN:HD21	1.86	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	494/496 (100%)	460 (93%)	29 (6%)	5 (1%)	12 2

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	54	PRO
1	A	107	VAL
1	A	298	ASN
1	A	53	ASN
1	A	55	PHE

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	418/418 (100%)	398 (95%)	20 (5%)	23 2

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	75	ASN
1	A	107	VAL
1	A	232	GLN
1	A	243	LYS
1	A	297	ASP
1	A	298	ASN
1	A	305	HIS
1	A	344	TRP
1	A	345	PRO
1	A	347	GLN
1	A	349	GLN
1	A	354	VAL
1	A	355	ASN
1	A	356	ASP
1	A	358	VAL
1	A	390	GLN
1	A	441	GLN
1	A	459	ASN
1	A	466	LYS
1	A	481	ASN

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	7	GLN
1	A	8	GLN
1	A	41	GLN
1	A	63	GLN
1	A	75	ASN
1	A	81	ASN
1	A	105	ASN
1	A	156	GLN
1	A	216	ASN
1	A	250	ASN
1	A	302	GLN
1	A	347	GLN
1	A	349	GLN

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Mol	Chain	Res	Type
1	A	355	ASN
1	A	386	HIS
1	A	390	GLN
1	A	404	GLN
1	A	415	ASN
1	A	416	GLN
1	A	481	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	PCA	A	1	1	7,8,9	1.18	1 (14%)	9,10,12	1.64	2 (22%)

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	PCA	A	1	1	-	0/0/11/13	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1	PCA	CB-CG	-2.43	1.47	1.53

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1	PCA	CB-CA-C	-3.07	108.44	112.66
1	A	1	PCA	OE-CD-CG	-2.43	122.37	126.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1	PCA	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

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
3	0XR	A	503	-	15,15,15	2.24	3 (20%)	19,19,19	2.02	4 (21%)
2	NAG	A	501	1	14,14,15	2.05	3 (21%)	17,19,21	1.25	3 (17%)
3	0XR	A	502	-	15,15,15	2.26	2 (13%)	19,19,19	2.11	4 (21%)
3	0XR	A	504	-	15,15,15	2.33	3 (20%)	19,19,19	2.09	4 (21%)

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
3	0XR	A	503	-	-	0/8/8/8	0/1/1/1
2	NAG	A	501	1	-	0/6/23/26	0/1/1/1
3	0XR	A	502	-	-	0/8/8/8	0/1/1/1
3	0XR	A	504	-	-	2/8/8/8	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	504	0XR	C2'-C1'	8.11	1.53	1.33
3	A	502	0XR	C2'-C1'	7.95	1.53	1.33
3	A	503	0XR	C2'-C1'	7.78	1.52	1.33
2	A	501	NAG	C1-C2	4.89	1.59	1.52
2	A	501	NAG	C2-N2	3.65	1.52	1.46
2	A	501	NAG	O5-C5	3.21	1.49	1.43
3	A	504	0XR	C2'-C3'	2.56	1.53	1.48
3	A	503	0XR	C2'-C3'	2.45	1.53	1.48
3	A	502	0XR	C2'-C3'	2.36	1.53	1.48
3	A	503	0XR	C1-C1'	2.06	1.53	1.47
3	A	504	0XR	C1-C1'	2.06	1.53	1.47

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	0XR	C1-C1'-C2'	-6.87	111.92	126.92
3	A	503	0XR	C1-C1'-C2'	-6.54	112.62	126.92
3	A	504	0XR	C1-C1'-C2'	-5.98	113.85	126.92
3	A	504	0XR	C1'-C2'-C3'	-4.29	110.01	122.28
3	A	502	0XR	C1'-C2'-C3'	-4.10	110.55	122.28
2	A	501	NAG	C1-O5-C5	3.58	116.98	112.19
3	A	503	0XR	C1'-C2'-C3'	-3.57	112.06	122.28
3	A	504	0XR	O2'-C3'-C2'	3.23	119.51	111.55
3	A	503	0XR	O2'-C3'-C2'	3.07	119.12	111.55
3	A	504	0XR	C4'-O2'-C3'	-2.95	110.54	116.38
3	A	502	0XR	O2'-C3'-C2'	2.75	118.34	111.55
3	A	503	0XR	C4'-O2'-C3'	-2.66	111.11	116.38
3	A	502	0XR	C4'-O2'-C3'	-2.48	111.47	116.38
2	A	501	NAG	C8-C7-N2	-2.08	112.67	116.12
2	A	501	NAG	O7-C7-N2	2.04	125.58	121.98

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	504	0XR	C1'-C2'-C3'-O2'
3	A	504	0XR	C1'-C2'-C3'-O1'

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	0XR	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	495/496 (99%)	1.11	92 (18%) 3 5	7, 13, 73, 100	0

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	315	PHE	13.7
1	A	344	TRP	12.3
1	A	314	THR	11.0
1	A	312	ILE	10.3
1	A	358	VAL	9.7
1	A	354	VAL	9.5
1	A	55	PHE	9.2
1	A	345	PRO	9.2
1	A	313	LEU	9.1
1	A	54	PRO	8.6
1	A	348	PHE	8.3
1	A	357	TRP	8.2
1	A	298	ASN	7.0
1	A	307	ALA	6.7
1	A	300	ASP	6.3
1	A	301	ASN	5.9
1	A	107	VAL	5.9
1	A	304	GLY	5.8
1	A	459	ASN	5.8
1	A	310	ALA	5.7
1	A	306	GLY	5.7
1	A	108	SER	5.6
1	A	109	ALA	5.5
1	A	311	SER	5.5
1	A	308	GLY	5.5
1	A	355	ASN	5.5
1	A	53	ASN	5.4

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Mol	Chain	Res	Type	RSRZ
1	A	106	ALA	5.4
1	A	356	ASP	5.3
1	A	309	GLY	5.3
1	A	305	HIS	5.2
1	A	350	ASN	5.2
1	A	52	TYR	5.0
1	A	299	HIS	4.9
1	A	316	TRP	4.8
1	A	349	GLN	4.7
1	A	303	ARG	4.7
1	A	353	ASP	4.7
1	A	363	ASN	4.6
1	A	51	ILE	4.4
1	A	110	GLY	4.3
1	A	461	ASN	4.3
1	A	352	ASN	4.3
1	A	346	ARG	4.0
1	A	297	ASP	3.9
1	A	458	ILE	3.9
1	A	302	GLN	3.8
1	A	359	GLY	3.7
1	A	343	ARG	3.5
1	A	365	GLY	3.5
1	A	460	GLY	3.5
1	A	351	GLY	3.4
1	A	482	SER	3.4
1	A	317	ASP	3.3
1	A	238	GLY	3.3
1	A	2	TYR	3.3
1	A	374	PRO	3.3
1	A	56	ARG	3.2
1	A	483	ALA	3.2
1	A	366	VAL	3.2
1	A	484	GLU	3.1
1	A	134	TRP	3.1
1	A	296	VAL	3.1
1	A	237	LEU	3.0
1	A	239	GLY	2.9
1	A	115	CYS	2.9
1	A	496	LEU	2.9
1	A	270	ASN	2.9
1	A	152	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	362	ASN	2.7
1	A	125	ASP	2.7
1	A	347	GLN	2.7
1	A	111	THR	2.6
1	A	403	GLY	2.6
1	A	342	TYR	2.5
1	A	154	ALA	2.5
1	A	139	GLY	2.4
1	A	171	GLU	2.4
1	A	17	PHE	2.4
1	A	339	MET	2.3
1	A	122	GLY	2.3
1	A	118	TYR	2.3
1	A	321	TYR	2.2
1	A	462	CYS	2.2
1	A	361	PRO	2.2
1	A	441	GLN	2.1
1	A	8	GLN	2.1
1	A	318	ALA	2.1
1	A	438	LEU	2.1
1	A	120	ASN	2.0
1	A	105	ASN	2.0
1	A	269	TRP	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	PCA	A	1	8/9	0.90	0.12	12,15,18,22	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	NAG	A	501	14/15	0.49	0.22	55,58,60,60	0
4	CL	A	505	1/1	0.82	0.14	24,24,24,24	1
3	0XR	A	504	15/15	0.88	0.11	17,19,21,24	0
3	0XR	A	502	15/15	0.93	0.09	11,13,18,21	0
3	0XR	A	503	15/15	0.94	0.09	11,12,21,22	0
5	CA	A	506	1/1	1.00	0.01	8,8,8,8	0

6.5 Other polymers [i](#)

There are no such residues in this entry.