



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 03:34 AM EDT

PDB ID : 1XV8 / pdb_00001xv8
Title : Crystal Structure of Human Salivary Alpha-Amylase Dimer
Authors : Fisher, S.Z.; Govindasamy, L.; Tu, C.K.; Silverman, D.N.; Rajaniemi, H.; McKenna, R.
Deposited on : 2004-10-27
Resolution : 3.00 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

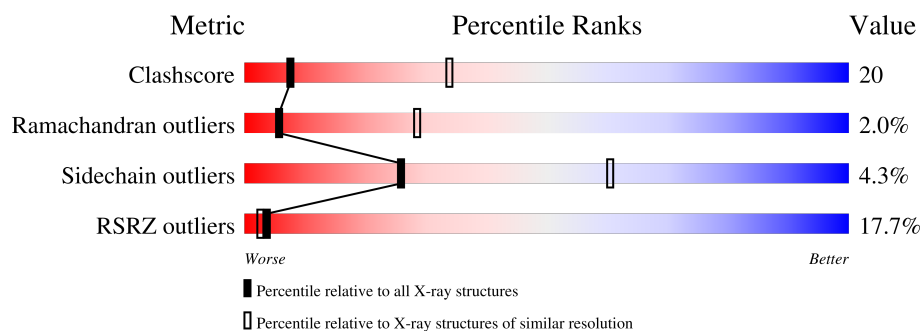
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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))
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	8% 60% 35% 5%
1	B	496	27% 61% 34% 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8024 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 Alpha-amylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	496	Total	C	N	O	S	0	0	0
			3945	2493	696	735	21			
1	B	496	Total	C	N	O	S	0	0	0
			3945	2493	696	735	21			

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		
2	B	1	Total	Ca	0	0
			1	1		

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		
3	B	1	Total	Cl	0	0
			1	1		

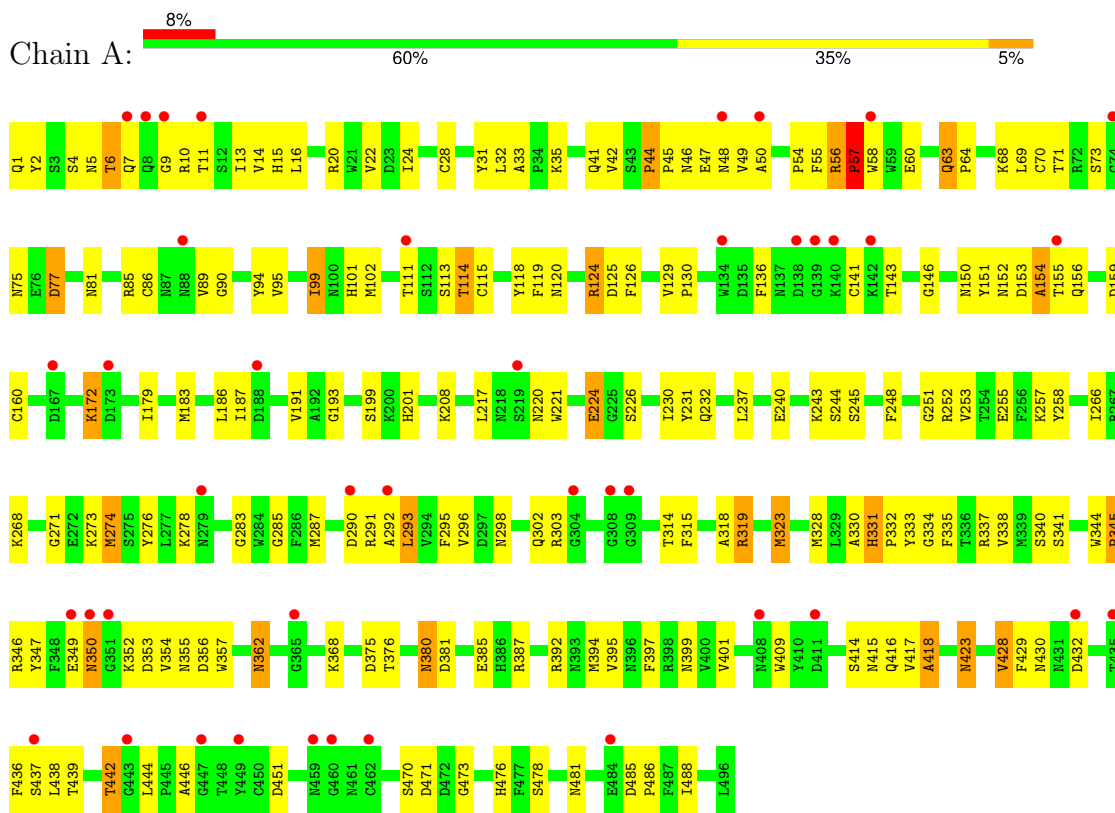
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	69	Total	O	0	0
			69	69		
4	B	61	Total	O	0	0
			61	61		

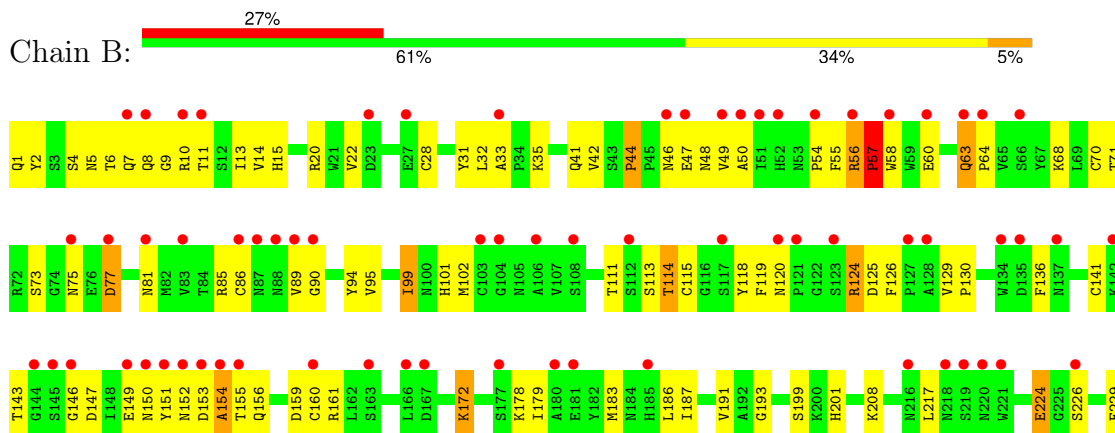
3 Residue-property plots [i](#)

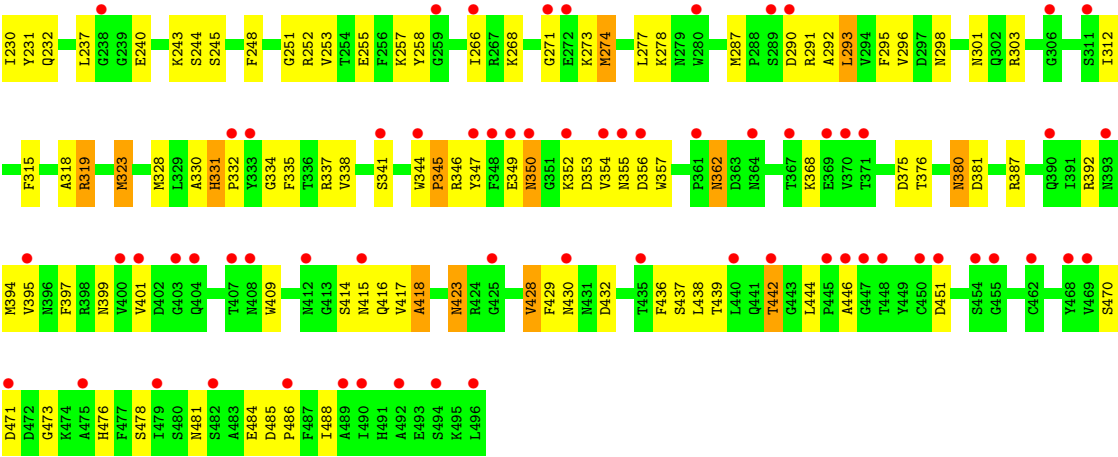
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Alpha-amylase



• Molecule 1: Alpha-amylase





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	150.81Å 72.27Å 91.11Å 90.00° 102.80° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00 20.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-3.00) 95.9 (20.00-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 2.98Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.228 , 0.271 0.279 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	19.3	Xtriage
Anisotropy	0.173	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 23.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.77	EDS
Total number of atoms	8024	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 4.86% 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, CA, PCA

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	0.50	0/4052	1.03	19/5502 (0.3%)
1	B	0.50	0/4052	1.03	19/5502 (0.3%)
All	All	0.50	0/8104	1.03	38/11004 (0.3%)

There are no bond length outliers.

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	331	HIS	CA-C-N	8.63	128.77	119.28
1	A	331	HIS	C-N-CA	8.63	128.77	119.28
1	B	331	HIS	CA-C-N	8.61	128.75	119.28
1	B	331	HIS	C-N-CA	8.61	128.75	119.28
1	B	63	GLN	O-C-N	6.91	127.04	121.17
1	A	63	GLN	O-C-N	6.90	127.04	121.17
1	A	362	ASN	N-CA-C	6.13	116.65	108.38
1	B	362	ASN	N-CA-C	6.09	116.60	108.38
1	A	291	ARG	N-CA-C	-6.01	105.67	114.39
1	B	291	ARG	N-CA-C	-6.01	105.68	114.39
1	A	146	GLY	N-CA-C	-5.91	107.17	115.32
1	B	146	GLY	N-CA-C	-5.88	107.20	115.32
1	B	485	ASP	CA-C-N	5.83	127.12	119.84
1	B	485	ASP	C-N-CA	5.83	127.12	119.84
1	A	99	ILE	N-CA-C	5.81	119.34	113.47
1	A	485	ASP	CA-C-N	5.81	127.10	119.84
1	A	485	ASP	C-N-CA	5.81	127.10	119.84
1	B	99	ILE	N-CA-C	5.81	119.33	113.47
1	B	126	PHE	CA-C-N	5.55	126.78	119.84
1	B	126	PHE	C-N-CA	5.55	126.78	119.84
1	A	126	PHE	CA-C-N	5.54	126.77	119.84
1	A	126	PHE	C-N-CA	5.54	126.77	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	318	ALA	N-CA-C	5.46	117.66	111.11
1	A	318	ALA	N-CA-C	5.44	117.64	111.11
1	A	57	PRO	CA-N-CD	-5.44	104.39	112.00
1	A	230	ILE	N-CA-C	5.42	116.35	107.24
1	B	230	ILE	N-CA-C	5.41	116.33	107.24
1	B	57	PRO	CA-N-CD	-5.39	104.45	112.00
1	B	240	GLU	CA-C-N	5.31	124.82	119.19
1	B	240	GLU	C-N-CA	5.31	124.82	119.19
1	A	240	GLU	CA-C-N	5.28	124.78	119.19
1	A	240	GLU	C-N-CA	5.28	124.78	119.19
1	A	274	MET	N-CA-C	5.16	117.81	111.82
1	B	274	MET	N-CA-C	5.14	117.78	111.82
1	A	296	VAL	N-CA-C	-5.08	106.12	110.74
1	B	296	VAL	N-CA-C	-5.08	106.12	110.74
1	B	57	PRO	N-CA-C	5.06	119.18	111.34
1	A	57	PRO	N-CA-C	5.04	119.14	111.34

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	3945	0	3707	159	4
1	B	3945	0	3707	158	4
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	69	0	0	6	1
4	B	61	0	0	6	1
All	All	8024	0	7414	309	5

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 20.

All (309) 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:56:ARG:HG3	1:A:56:ARG:HH11	1.16	1.09
1:B:56:ARG:HH11	1:B:56:ARG:HG3	1.16	1.06
1:B:56:ARG:HH11	1:B:56:ARG:CG	1.76	0.97
1:A:56:ARG:HH11	1:A:56:ARG:CG	1.76	0.96
1:B:56:ARG:HG3	1:B:56:ARG:NH1	1.76	0.92
1:A:319:ARG:HG2	1:A:319:ARG:HH11	1.37	0.90
1:B:7:GLN:OE1	1:B:90:GLY:HA2	1.73	0.89
1:B:319:ARG:HG2	1:B:319:ARG:HH11	1.37	0.89
1:B:7:GLN:O	1:B:10:ARG:HG3	1.74	0.88
1:A:7:GLN:OE1	1:A:90:GLY:HA2	1.73	0.87
1:A:7:GLN:O	1:A:10:ARG:HG3	1.74	0.87
1:A:285:GLY:HA3	1:B:152:ASN:ND2	1.90	0.87
1:A:56:ARG:HG3	1:A:56:ARG:NH1	1.76	0.86
1:A:276:TYR:CD1	1:B:149:GLU:HG2	2.13	0.84
1:A:349:GLU:C	1:A:350:ASN:HD22	1.91	0.77
1:B:349:GLU:O	1:B:350:ASN:ND2	2.17	0.77
1:A:217:LEU:HD12	1:A:226:SER:HB3	1.67	0.77
1:B:217:LEU:HD12	1:B:226:SER:HB3	1.67	0.77
1:B:349:GLU:C	1:B:350:ASN:HD22	1.91	0.76
1:A:285:GLY:CA	1:B:152:ASN:ND2	2.50	0.74
1:A:35:LYS:HD2	1:A:392:ARG:HD3	1.70	0.74
1:B:28:CYS:HA	1:B:32:LEU:HB2	1.69	0.74
1:B:397:PHE:O	1:B:401:VAL:HG22	1.88	0.74
1:A:349:GLU:O	1:A:350:ASN:ND2	2.17	0.74
1:A:397:PHE:O	1:A:401:VAL:HG22	1.88	0.73
1:A:418:ALA:HB2	1:A:428:VAL:HG13	1.71	0.73
1:B:35:LYS:HD2	1:B:392:ARG:HD3	1.70	0.72
1:A:28:CYS:HA	1:A:32:LEU:HB2	1.69	0.72
1:B:418:ALA:HB2	1:B:428:VAL:HG13	1.71	0.71
1:A:99:ILE:HB	1:A:179:ILE:HD13	1.73	0.70
1:B:99:ILE:HB	1:B:179:ILE:HD13	1.73	0.70
1:B:319:ARG:HG2	1:B:319:ARG:NH1	2.06	0.69
1:A:4:SER:O	1:A:5:ASN:HB2	1.94	0.66
1:B:4:SER:O	1:B:5:ASN:HB2	1.94	0.66
1:A:319:ARG:HG2	1:A:319:ARG:NH1	2.06	0.66
1:B:380:ASN:O	1:B:381:ASP:HB2	1.96	0.65
1:A:380:ASN:O	1:A:381:ASP:HB2	1.96	0.65
1:A:56:ARG:HD2	1:A:60:GLU:OE1	1.98	0.63
1:B:237:LEU:HD22	1:B:257:LYS:HG2	1.80	0.63
1:B:56:ARG:HD2	1:B:60:GLU:OE1	1.98	0.63
1:B:172:LYS:NZ	1:B:172:LYS:HB3	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:349:GLU:C	1:A:350:ASN:ND2	2.57	0.62
1:A:237:LEU:HD22	1:A:257:LYS:HG2	1.80	0.62
1:B:258:TYR:CE1	1:B:328:MET:HG3	2.35	0.62
1:A:258:TYR:CE1	1:A:328:MET:HG3	2.35	0.61
1:B:11:THR:H	1:B:399:ASN:HD21	1.49	0.61
1:A:172:LYS:NZ	1:A:172:LYS:HB3	2.14	0.61
1:A:293:LEU:HD23	1:A:335:PHE:O	2.01	0.61
1:B:349:GLU:C	1:B:350:ASN:ND2	2.57	0.61
1:A:153:ASP:HB3	1:A:156:GLN:HG2	1.83	0.60
1:B:293:LEU:HD23	1:B:335:PHE:O	2.01	0.60
1:B:153:ASP:HB3	1:B:156:GLN:HG2	1.83	0.60
1:B:199:SER:OG	1:B:232:GLN:HB3	2.01	0.60
1:A:224:GLU:HA	1:A:224:GLU:OE1	2.02	0.60
1:A:186:LEU:HB3	1:A:191:VAL:HG21	1.83	0.60
1:A:331:HIS:CG	1:A:332:PRO:HD2	2.37	0.59
1:B:186:LEU:HB3	1:B:191:VAL:HG21	1.83	0.59
1:A:199:SER:OG	1:A:232:GLN:HB3	2.01	0.59
1:A:11:THR:H	1:A:399:ASN:HD21	1.49	0.59
1:A:11:THR:H	1:A:399:ASN:ND2	2.01	0.59
1:A:268:LYS:HD3	1:A:415:ASN:ND2	2.18	0.59
1:B:268:LYS:HD3	1:B:415:ASN:ND2	2.18	0.59
1:B:201:HIS:HB3	4:B:513:HOH:O	2.03	0.59
1:B:15:HIS:HD2	1:B:41:GLN:O	1.85	0.59
1:B:224:GLU:OE1	1:B:224:GLU:HA	2.02	0.59
1:B:331:HIS:CG	1:B:332:PRO:HD2	2.37	0.58
1:A:15:HIS:HD2	1:A:41:GLN:O	1.85	0.58
1:A:201:HIS:HB3	4:A:510:HOH:O	2.03	0.58
1:B:11:THR:H	1:B:399:ASN:ND2	2.01	0.58
1:B:75:ASN:OD1	1:B:77:ASP:HB2	2.05	0.57
1:A:101:HIS:HD2	1:A:102:MET:O	1.88	0.57
1:B:141:CYS:HB2	1:B:159:ASP:O	2.05	0.57
1:A:75:ASN:OD1	1:A:77:ASP:HB2	2.05	0.57
1:A:141:CYS:HB2	1:A:159:ASP:O	2.05	0.57
1:B:101:HIS:HD2	1:B:102:MET:O	1.88	0.57
1:B:31:TYR:OH	1:B:387:ARG:HA	2.06	0.56
1:B:303:ARG:HG3	1:B:303:ARG:HH11	1.71	0.56
1:A:303:ARG:HG3	1:A:303:ARG:HH11	1.71	0.56
1:B:417:VAL:HG22	1:B:429:PHE:HB2	1.88	0.56
1:B:58:TRP:NE1	1:B:356:ASP:O	2.39	0.56
1:A:46:ASN:O	1:A:71:THR:HG22	2.06	0.56
1:B:46:ASN:O	1:B:71:THR:HG22	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:TRP:NE1	1:A:356:ASP:O	2.39	0.55
1:A:231:TYR:CD2	1:A:293:LEU:HD12	2.41	0.55
1:B:231:TYR:CD2	1:B:293:LEU:HD12	2.41	0.55
1:A:31:TYR:OH	1:A:387:ARG:HA	2.06	0.55
1:A:54:PRO:HG2	1:A:57:PRO:HG3	1.89	0.55
1:A:417:VAL:HG22	1:A:429:PHE:HB2	1.88	0.55
1:B:423:ASN:C	1:B:423:ASN:HD22	2.14	0.55
1:B:54:PRO:HG2	1:B:57:PRO:HG3	1.89	0.54
1:A:423:ASN:C	1:A:423:ASN:HD22	2.14	0.53
1:A:217:LEU:HB2	1:A:226:SER:HB2	1.91	0.53
1:A:293:LEU:C	1:A:293:LEU:HD22	2.33	0.53
1:B:217:LEU:HB2	1:B:226:SER:HB2	1.91	0.53
1:B:111:THR:O	1:B:113:SER:N	2.42	0.52
1:A:330:ALA:HB2	1:A:394:MET:HE1	1.91	0.52
1:A:56:ARG:NH2	4:A:535:HOH:O	2.25	0.52
1:A:111:THR:O	1:A:113:SER:N	2.42	0.52
1:B:293:LEU:C	1:B:293:LEU:HD22	2.34	0.52
1:A:330:ALA:HB2	1:A:394:MET:CE	2.41	0.51
1:A:470:SER:O	1:A:473:GLY:N	2.35	0.51
1:B:330:ALA:HB2	1:B:394:MET:CE	2.41	0.51
1:B:330:ALA:HB2	1:B:394:MET:HE1	1.91	0.51
1:A:129:VAL:H	1:A:130:PRO:HA	1.75	0.51
1:A:278:LYS:HE2	1:B:149:GLU:OE1	2.11	0.51
1:B:2:TYR:CE1	1:B:251:GLY:HA2	2.46	0.51
1:A:150:ASN:C	1:A:152:ASN:H	2.19	0.51
1:B:470:SER:O	1:B:473:GLY:N	2.36	0.51
1:A:2:TYR:CE1	1:A:251:GLY:HA2	2.46	0.51
1:A:153:ASP:OD1	1:A:155:THR:HG22	2.11	0.51
1:B:54:PRO:HB2	1:B:357:TRP:CZ3	2.46	0.51
1:B:129:VAL:H	1:B:130:PRO:HA	1.76	0.51
1:B:153:ASP:OD1	1:B:155:THR:HG22	2.11	0.51
1:A:258:TYR:CZ	1:A:328:MET:HG3	2.46	0.51
1:A:54:PRO:HB2	1:A:357:TRP:CZ3	2.46	0.51
1:A:81:ASN:OD1	1:A:85:ARG:HD3	2.11	0.51
1:A:95:VAL:HG11	1:A:186:LEU:HD13	1.92	0.50
1:B:81:ASN:OD1	1:B:85:ARG:HD3	2.11	0.50
1:B:150:ASN:C	1:B:152:ASN:H	2.19	0.50
1:B:191:VAL:HG12	1:B:193:GLY:H	1.77	0.50
1:A:362:ASN:HA	1:A:368:LYS:HG3	1.94	0.49
1:B:258:TYR:CZ	1:B:328:MET:HG3	2.46	0.49
1:B:353:ASP:HB3	1:B:356:ASP:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:362:ASN:HA	1:B:368:LYS:HG3	1.94	0.49
1:A:353:ASP:HB3	1:A:356:ASP:HB3	1.94	0.49
1:B:95:VAL:HG11	1:B:186:LEU:HD13	1.92	0.49
1:A:191:VAL:HG12	1:A:193:GLY:H	1.77	0.49
1:B:172:LYS:HB3	1:B:172:LYS:HZ2	1.77	0.49
1:B:63:GLN:N	1:B:64:PRO:CD	2.75	0.49
1:A:63:GLN:N	1:A:64:PRO:CD	2.75	0.49
1:A:439:THR:HA	1:A:476:HIS:HA	1.95	0.49
1:B:20:ARG:HD2	4:B:504:HOH:O	2.12	0.49
1:B:56:ARG:CG	1:B:56:ARG:NH1	2.45	0.49
1:B:208:LYS:HG3	4:B:546:HOH:O	2.13	0.49
1:B:28:CYS:HA	1:B:32:LEU:HD12	1.95	0.49
1:B:129:VAL:HB	1:B:130:PRO:HA	1.94	0.49
1:A:208:LYS:HG3	4:A:545:HOH:O	2.13	0.48
1:A:436:PHE:O	1:A:478:SER:HA	2.13	0.48
1:A:437:SER:O	1:A:438:LEU:HB2	2.13	0.48
1:A:49:VAL:HG12	1:A:50:ALA:N	2.27	0.48
1:B:49:VAL:HG12	1:B:50:ALA:N	2.27	0.48
1:B:437:SER:O	1:B:438:LEU:HB2	2.13	0.48
1:A:323:MET:HE2	1:A:486:PRO:CG	2.44	0.48
1:A:28:CYS:HA	1:A:32:LEU:HD12	1.95	0.48
1:B:153:ASP:O	1:B:154:ALA:C	2.57	0.48
1:B:439:THR:HA	1:B:476:HIS:HA	1.95	0.48
1:A:129:VAL:HB	1:A:130:PRO:HA	1.94	0.48
1:A:153:ASP:O	1:A:154:ALA:C	2.57	0.48
1:B:63:GLN:N	1:B:64:PRO:HD3	2.29	0.48
1:B:323:MET:HE2	1:B:486:PRO:CG	2.44	0.48
1:B:436:PHE:O	1:B:478:SER:HA	2.13	0.48
1:B:31:TYR:CE1	1:B:35:LYS:HG3	2.49	0.48
1:A:20:ARG:HD2	4:A:501:HOH:O	2.12	0.47
1:A:346:ARG:HG3	1:A:353:ASP:OD2	2.14	0.47
1:A:423:ASN:C	1:A:423:ASN:ND2	2.72	0.47
1:B:124:ARG:HG2	1:B:136:PHE:CD1	2.50	0.47
1:B:346:ARG:HG3	1:B:353:ASP:OD2	2.14	0.47
1:A:319:ARG:NH1	1:A:319:ARG:CG	2.76	0.47
1:A:63:GLN:N	1:A:64:PRO:HD3	2.29	0.47
1:A:31:TYR:CE1	1:A:35:LYS:HG3	2.49	0.47
1:A:124:ARG:HG2	1:A:136:PHE:CD1	2.50	0.47
1:B:423:ASN:C	1:B:423:ASN:ND2	2.72	0.47
1:A:285:GLY:CA	1:B:152:ASN:HD21	2.27	0.46
1:B:56:ARG:NH2	4:B:537:HOH:O	2.26	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:352:LYS:HG2	1:B:353:ASP:N	2.30	0.46
1:A:352:LYS:HG2	1:A:353:ASP:N	2.30	0.46
1:A:266:ILE:HD11	1:A:274:MET:HE3	1.97	0.46
1:A:442:THR:OG1	1:A:444:LEU:HB2	2.15	0.46
1:A:143:THR:HG23	1:A:160:CYS:SG	2.55	0.46
1:A:355:ASN:C	1:A:357:TRP:H	2.24	0.46
1:B:143:THR:HG23	1:B:160:CYS:SG	2.55	0.46
1:B:266:ILE:HD11	1:B:274:MET:HE3	1.97	0.46
1:A:328:MET:HE1	4:A:550:HOH:O	2.16	0.46
1:A:56:ARG:HD2	1:A:56:ARG:HA	1.59	0.46
1:A:129:VAL:HB	1:A:130:PRO:CA	2.45	0.46
1:B:183:MET:O	1:B:187:ILE:HG13	2.16	0.46
1:A:183:MET:O	1:A:187:ILE:HG13	2.16	0.46
1:A:295:PHE:CE2	1:A:298:ASN:HB3	2.51	0.46
1:B:129:VAL:HB	1:B:130:PRO:CA	2.45	0.46
1:A:42:VAL:HG22	1:A:94:TYR:O	2.16	0.45
1:B:442:THR:OG1	1:B:444:LEU:HB2	2.15	0.45
1:B:42:VAL:HG22	1:B:94:TYR:O	2.16	0.45
1:B:295:PHE:CE2	1:B:298:ASN:HB3	2.51	0.45
1:A:153:ASP:O	1:A:155:THR:N	2.50	0.45
1:B:33:ALA:CB	1:B:89:VAL:HB	2.47	0.45
1:A:56:ARG:CG	1:A:56:ARG:NH1	2.45	0.45
1:B:7:GLN:OE1	1:B:90:GLY:CA	2.56	0.45
1:B:153:ASP:O	1:B:155:THR:N	2.50	0.45
1:A:20:ARG:HG2	1:A:73:SER:HA	1.98	0.45
1:A:33:ALA:CB	1:A:89:VAL:HB	2.47	0.45
1:A:255:GLU:OE1	1:A:257:LYS:HG3	2.17	0.45
1:A:344:TRP:O	1:A:346:ARG:N	2.50	0.45
1:B:355:ASN:C	1:B:357:TRP:H	2.24	0.45
1:A:44:PRO:O	1:A:71:THR:HG21	2.17	0.45
1:A:276:TYR:CE1	1:B:149:GLU:HG2	2.51	0.45
1:B:56:ARG:HD2	1:B:56:ARG:HA	1.59	0.45
1:B:328:MET:HE1	4:B:551:HOH:O	2.16	0.45
1:A:338:VAL:HG13	4:A:537:HOH:O	2.17	0.45
1:B:20:ARG:HG2	1:B:73:SER:HA	1.98	0.45
1:B:338:VAL:HG13	4:B:539:HOH:O	2.17	0.44
1:B:344:TRP:O	1:B:346:ARG:N	2.50	0.44
1:B:44:PRO:O	1:B:71:THR:HG21	2.17	0.44
1:A:42:VAL:CG2	1:A:95:VAL:HA	2.47	0.44
1:A:268:LYS:CD	1:A:415:ASN:ND2	2.80	0.44
1:A:287:MET:O	1:A:333:TYR:OH	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:VAL:HG23	1:B:63:GLN:O	2.18	0.44
1:A:49:VAL:HG23	1:A:63:GLN:O	2.18	0.44
1:B:287:MET:HG3	1:B:292:ALA:HB2	1.99	0.44
1:B:417:VAL:O	1:B:418:ALA:HB2	2.17	0.44
1:A:287:MET:HG3	1:A:292:ALA:HB2	1.99	0.44
1:A:417:VAL:O	1:A:418:ALA:HB2	2.17	0.44
1:B:42:VAL:CG2	1:B:95:VAL:HA	2.48	0.43
1:B:258:TYR:OH	1:B:328:MET:HG3	2.18	0.43
1:A:47:GLU:OE2	1:A:115:CYS:HB3	2.18	0.43
1:B:95:VAL:HG11	1:B:186:LEU:CD1	2.48	0.43
1:A:4:SER:O	1:A:5:ASN:CB	2.62	0.43
1:B:255:GLU:OE1	1:B:257:LYS:HG3	2.17	0.43
1:A:258:TYR:OH	1:A:328:MET:HG3	2.18	0.43
1:B:252:ARG:NH1	1:B:292:ALA:O	2.50	0.43
1:A:276:TYR:OH	1:B:147:ASP:HB3	2.18	0.43
1:A:283:GLY:O	1:B:150:ASN:ND2	2.48	0.43
1:A:11:THR:OG1	1:A:399:ASN:ND2	2.52	0.43
1:A:252:ARG:NH1	1:A:292:ALA:O	2.50	0.43
1:A:344:TRP:HB2	1:A:345:PRO:HD2	2.00	0.43
1:B:11:THR:OG1	1:B:399:ASN:ND2	2.52	0.43
1:B:55:PHE:C	1:B:57:PRO:HD3	2.44	0.43
1:B:430:ASN:HD21	1:B:481:ASN:HA	1.84	0.43
1:A:451:ASP:CG	1:A:488:ILE:HG23	2.44	0.43
1:B:13:ILE:O	1:B:337:ARG:HA	2.19	0.43
1:B:451:ASP:CG	1:B:488:ILE:HG23	2.44	0.43
1:A:95:VAL:HG11	1:A:186:LEU:CD1	2.48	0.43
1:B:312:ILE:HD13	1:B:312:ILE:HA	1.82	0.43
1:B:120:ASN:OD1	1:B:120:ASN:C	2.62	0.43
1:A:48:ASN:OD1	1:A:114:THR:HG21	2.19	0.42
1:A:64:PRO:HB2	1:A:102:MET:HA	2.01	0.42
1:B:268:LYS:CD	1:B:415:ASN:ND2	2.80	0.42
1:B:178:LYS:HD3	1:B:178:LYS:HA	1.84	0.42
1:B:414:SER:HB3	1:B:432:ASP:OD2	2.19	0.42
1:A:237:LEU:CD2	1:A:257:LYS:HG2	2.47	0.42
1:B:47:GLU:OE2	1:B:115:CYS:HB3	2.18	0.42
1:A:245:SER:HA	1:A:248:PHE:CE2	2.54	0.42
1:A:414:SER:HB3	1:A:432:ASP:OD2	2.19	0.42
1:B:245:SER:HA	1:B:248:PHE:CE2	2.54	0.42
1:A:13:ILE:O	1:A:337:ARG:HA	2.19	0.42
1:A:55:PHE:C	1:A:57:PRO:HD3	2.44	0.42
1:A:315:PHE:CD1	1:A:315:PHE:C	2.97	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:GLY:O	1:A:11:THR:HG23	2.19	0.42
1:A:118:TYR:CG	1:A:119:PHE:N	2.88	0.42
1:A:349:GLU:O	1:A:350:ASN:C	2.62	0.42
1:A:446:ALA:HB2	1:A:471:ASP:N	2.35	0.42
1:B:344:TRP:HB2	1:B:345:PRO:HD2	2.00	0.42
1:A:253:VAL:CG1	1:A:287:MET:HE1	2.50	0.42
1:B:315:PHE:CD1	1:B:315:PHE:C	2.97	0.42
1:B:375:ASP:C	1:B:376:THR:HG23	2.45	0.42
1:A:375:ASP:C	1:A:376:THR:HG23	2.45	0.42
1:A:409:TRP:CD1	1:A:409:TRP:C	2.98	0.42
1:B:86:CYS:O	1:B:89:VAL:HG23	2.20	0.42
1:B:409:TRP:CD1	1:B:409:TRP:C	2.98	0.42
1:B:9:GLY:O	1:B:11:THR:HG23	2.19	0.42
1:A:86:CYS:O	1:A:89:VAL:HG23	2.20	0.41
1:B:64:PRO:HB2	1:B:102:MET:HA	2.01	0.41
1:A:120:ASN:OD1	1:A:120:ASN:C	2.62	0.41
1:B:48:ASN:OD1	1:B:114:THR:HG21	2.19	0.41
1:B:253:VAL:CG1	1:B:287:MET:HE1	2.50	0.41
1:B:301:ASN:C	1:B:303:ARG:N	2.78	0.41
1:A:430:ASN:HD21	1:A:481:ASN:HA	1.84	0.41
1:A:5:ASN:C	1:A:6:THR:O	2.62	0.41
1:B:4:SER:O	1:B:5:ASN:CB	2.62	0.41
1:B:33:ALA:HB2	1:B:89:VAL:HB	2.02	0.41
1:B:243:LYS:O	1:B:244:SER:C	2.64	0.41
1:B:237:LEU:CD2	1:B:257:LYS:HG2	2.47	0.41
1:B:273:LYS:HB2	1:B:415:ASN:OD1	2.21	0.41
1:A:416:GLN:HG3	1:A:432:ASP:OD2	2.21	0.41
1:B:68:LYS:O	1:B:70:CYS:N	2.54	0.41
1:B:349:GLU:O	1:B:350:ASN:C	2.62	0.41
1:A:14:VAL:HG22	1:A:15:HIS:N	2.36	0.41
1:A:13:ILE:HG23	1:A:335:PHE:CE1	2.56	0.41
1:A:68:LYS:O	1:A:70:CYS:N	2.54	0.41
1:A:347:TYR:O	1:A:354:VAL:HG22	2.20	0.41
1:B:13:ILE:HG23	1:B:335:PHE:CE1	2.56	0.41
1:B:161:ARG:HE	1:B:161:ARG:HB2	1.68	0.41
1:B:446:ALA:HB2	1:B:471:ASP:N	2.35	0.41
1:A:44:PRO:HA	1:A:45:PRO:HD2	2.00	0.41
1:A:45:PRO:O	1:A:69:LEU:HA	2.21	0.41
1:B:118:TYR:CG	1:B:119:PHE:N	2.88	0.41
1:B:150:ASN:ND2	1:B:152:ASN:HB3	2.36	0.41
1:A:243:LYS:O	1:A:244:SER:C	2.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:ASN:C	1:A:357:TRP:N	2.78	0.40
1:B:319:ARG:NH1	1:B:319:ARG:CG	2.76	0.40
1:A:172:LYS:HB3	1:A:172:LYS:HZ2	1.85	0.40
1:B:347:TYR:O	1:B:354:VAL:HG22	2.20	0.40
1:A:58:TRP:HD1	1:A:357:TRP:O	2.04	0.40
1:A:340:SER:HA	1:A:385:GLU:OE1	2.22	0.40
1:B:277:LEU:O	1:B:278:LYS:C	2.65	0.40
1:B:323:MET:HE2	1:B:486:PRO:HG2	2.04	0.40
1:A:4:SER:OG	1:A:6:THR:HG23	2.22	0.40
1:A:451:ASP:OD1	1:A:488:ILE:HG23	2.21	0.40
1:B:229:PHE:CE1	1:B:252:ARG:HD2	2.57	0.40
1:B:416:GLN:HG3	1:B:432:ASP:OD2	2.21	0.40
1:A:7:GLN:OE1	1:A:90:GLY:CA	2.56	0.40
1:A:16:LEU:HD12	1:A:24:ILE:HG23	2.04	0.40
1:A:33:ALA:HB2	1:A:89:VAL:HB	2.02	0.40
1:A:129:VAL:N	1:A:130:PRO:HA	2.34	0.40
1:A:273:LYS:HB2	1:A:415:ASN:OD1	2.21	0.40
1:A:302:GLN:HB2	1:A:314:THR:CG2	2.52	0.40
1:B:8:GLN:OE1	1:B:8:GLN:HA	2.22	0.40
1:B:14:VAL:HG22	1:B:15:HIS:N	2.36	0.40
1:B:323:MET:HE2	1:B:486:PRO:HG3	2.02	0.40
1:B:430:ASN:ND2	1:B:481:ASN:HA	2.37	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:ASN:O	1:B:8:GLN:OE1[3_445]	1.35	0.85
4:A:499:HOH:O	4:B:547:HOH:O[3_445]	1.62	0.58
1:A:111:THR:OG1	1:B:484:GLU:OE2[2_655]	2.04	0.16
1:A:220:ASN:O	1:B:8:GLN:CD[3_445]	2.13	0.07
1:A:221:TRP:CA	1:B:8:GLN:NE2[3_445]	2.16	0.04

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	494/496 (100%)	427 (86%)	57 (12%)	10 (2%)	6	28
1	B	494/496 (100%)	428 (87%)	56 (11%)	10 (2%)	6	28
All	All	988/992 (100%)	855 (86%)	113 (11%)	20 (2%)	6	28

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	154	ALA
1	A	380	ASN
1	B	154	ALA
1	B	380	ASN
1	A	6	THR
1	A	114	THR
1	B	6	THR
1	B	114	THR
1	A	418	ALA
1	B	418	ALA
1	A	44	PRO
1	A	334	GLY
1	B	44	PRO
1	B	334	GLY
1	A	151	TYR
1	A	345	PRO
1	B	151	TYR
1	B	345	PRO
1	A	271	GLY
1	B	271	GLY

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	418/418 (100%)	400 (96%)	18 (4%)	26	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	418/418 (100%)	400 (96%)	18 (4%)	26	60
All	All	836/836 (100%)	800 (96%)	36 (4%)	26	60

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	VAL
1	A	56	ARG
1	A	57	PRO
1	A	77	ASP
1	A	124	ARG
1	A	125	ASP
1	A	172	LYS
1	A	224	GLU
1	A	290	ASP
1	A	293	LEU
1	A	319	ARG
1	A	323	MET
1	A	341	SER
1	A	350	ASN
1	A	395	VAL
1	A	423	ASN
1	A	428	VAL
1	A	442	THR
1	B	22	VAL
1	B	56	ARG
1	B	57	PRO
1	B	77	ASP
1	B	124	ARG
1	B	125	ASP
1	B	172	LYS
1	B	224	GLU
1	B	290	ASP
1	B	293	LEU
1	B	319	ARG
1	B	323	MET
1	B	341	SER
1	B	350	ASN
1	B	395	VAL
1	B	423	ASN
1	B	428	VAL
1	B	442	THR

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	15	HIS
1	A	88	ASN
1	A	201	HIS
1	A	216	ASN
1	A	270	ASN
1	A	350	ASN
1	A	399	ASN
1	A	408	ASN
1	A	423	ASN
1	A	476	HIS
1	B	15	HIS
1	B	152	ASN
1	B	185	HIS
1	B	201	HIS
1	B	216	ASN
1	B	270	ASN
1	B	350	ASN
1	B	399	ASN
1	B	408	ASN
1	B	423	ASN
1	B	476	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 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	PCA	B	1	1	7,8,9	2.39	2 (28%)	9,10,12	2.35	4 (44%)

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	2.39	2 (28%)	9,10,12	2.36	4 (44%)

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1	PCA	CD-N	4.79	1.46	1.34
1	A	1	PCA	CD-N	4.78	1.46	1.34
1	A	1	PCA	CA-N	3.95	1.51	1.46
1	B	1	PCA	CA-N	3.92	1.51	1.46

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1	PCA	CB-CA-C	-4.29	106.77	112.66
1	B	1	PCA	CB-CA-C	-4.28	106.78	112.66
1	A	1	PCA	OE-CD-CG	-3.16	121.08	126.72
1	B	1	PCA	OE-CD-CG	-3.15	121.10	126.72
1	B	1	PCA	CA-N-CD	-2.99	103.34	113.58
1	A	1	PCA	CA-N-CD	-2.98	103.37	113.58
1	A	1	PCA	CG-CD-N	2.18	113.72	108.39
1	B	1	PCA	CG-CD-N	2.17	113.70	108.39

There are no chirality outliers.

There are no torsion outliers.

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

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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

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%)	0.99	42 (8%) 16 8	7, 19, 33, 50	0
1	B	495/496 (99%)	1.54	133 (26%) 1 1	7, 19, 33, 50	0
All	All	990/992 (99%)	1.27	175 (17%) 4 2	7, 19, 33, 50	0

All (175) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	8	GLN	6.1
1	B	88	ASN	4.7
1	A	58	TRP	4.4
1	A	7	GLN	4.3
1	B	81	ASN	4.2
1	A	88	ASN	4.1
1	B	23	ASP	4.1
1	B	7	GLN	4.0
1	B	87	ASN	4.0
1	B	496	LEU	4.0
1	A	134	TRP	3.9
1	A	349	GLU	3.8
1	B	63	GLN	3.7
1	A	408	ASN	3.7
1	B	51	ILE	3.6
1	B	489	ALA	3.6
1	B	482	SER	3.5
1	B	435	THR	3.5
1	B	90	GLY	3.5
1	B	425	GLY	3.5
1	B	364	ASN	3.4
1	B	446	ALA	3.4
1	A	9	GLY	3.3
1	A	350	ASN	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	77	ASP	3.3
1	A	8	GLN	3.3
1	B	163	SER	3.2
1	B	150	ASN	3.2
1	B	469	VAL	3.2
1	B	58	TRP	3.2
1	A	484	GLU	3.2
1	B	347	TYR	3.1
1	A	459	ASN	3.1
1	B	462	CYS	3.1
1	A	279	ASN	3.1
1	B	134	TRP	3.1
1	B	142	LYS	3.0
1	B	154	ALA	3.0
1	B	400	VAL	3.0
1	B	401	VAL	2.9
1	B	117	SER	2.9
1	B	348	PHE	2.9
1	B	104	GLY	2.9
1	B	494	SER	2.9
1	B	50	ALA	2.8
1	B	218	ASN	2.8
1	B	221	TRP	2.8
1	B	306	GLY	2.8
1	B	219	SER	2.8
1	B	146	GLY	2.7
1	B	128	ALA	2.7
1	B	83	VAL	2.7
1	B	350	ASN	2.7
1	B	11	THR	2.7
1	B	108	SER	2.7
1	A	462	CYS	2.7
1	A	447	GLY	2.7
1	B	33	ALA	2.7
1	A	290	ASP	2.7
1	A	435	THR	2.6
1	B	442	THR	2.6
1	B	112	SER	2.6
1	B	412	ASN	2.6
1	A	139	GLY	2.6
1	B	344	TRP	2.6
1	B	354	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	454	SER	2.6
1	B	167	ASP	2.6
1	A	11	THR	2.6
1	B	475	ALA	2.6
1	B	290	ASP	2.6
1	B	370	VAL	2.6
1	B	492	ALA	2.6
1	B	369	GLU	2.5
1	B	486	PRO	2.5
1	A	304	GLY	2.5
1	B	66	SER	2.5
1	B	455	GLY	2.5
1	B	266	ILE	2.5
1	B	144	GLY	2.5
1	B	447	GLY	2.5
1	B	259	GLY	2.5
1	B	103	CYS	2.4
1	B	64	PRO	2.4
1	B	49	VAL	2.4
1	B	89	VAL	2.4
1	B	271	GLY	2.4
1	A	437	SER	2.4
1	B	404	GLN	2.4
1	B	52	HIS	2.4
1	B	468	TYR	2.4
1	B	180	ALA	2.4
1	B	27	GLU	2.4
1	A	138	ASP	2.4
1	A	432	ASP	2.4
1	B	10	ARG	2.4
1	B	341	SER	2.4
1	A	167	ASP	2.3
1	B	149	GLU	2.3
1	A	351	GLY	2.3
1	B	407	THR	2.3
1	A	188	ASP	2.3
1	B	127	PRO	2.3
1	A	74	GLY	2.3
1	B	75	ASN	2.3
1	B	415	ASN	2.3
1	B	349	GLU	2.3
1	B	56	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	54	PRO	2.3
1	B	121	PRO	2.3
1	A	292	ALA	2.3
1	A	155	THR	2.3
1	B	137	ASN	2.3
1	B	135	ASP	2.3
1	A	443	GLY	2.3
1	B	151	TYR	2.3
1	B	220	ASN	2.3
1	A	173	ASP	2.3
1	B	451	ASP	2.3
1	B	280	TRP	2.2
1	B	311	SER	2.2
1	B	216	ASN	2.2
1	B	471	ASP	2.2
1	A	309	GLY	2.2
1	A	365	GLY	2.2
1	B	238	GLY	2.2
1	B	46	ASN	2.2
1	B	408	ASN	2.2
1	B	60	GLU	2.2
1	B	479	ILE	2.2
1	B	47	GLU	2.2
1	B	152	ASN	2.2
1	B	430	ASN	2.2
1	B	160	CYS	2.2
1	B	356	ASP	2.2
1	B	155	THR	2.2
1	B	440	LEU	2.2
1	A	48	ASN	2.2
1	B	355	ASN	2.2
1	A	460	GLY	2.2
1	B	106	ALA	2.1
1	B	185	HIS	2.1
1	B	395	VAL	2.1
1	B	333	TYR	2.1
1	A	219	SER	2.1
1	B	445	PRO	2.1
1	A	140	LYS	2.1
1	B	166	LEU	2.1
1	B	371	THR	2.1
1	B	361	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	177	SER	2.1
1	B	120	ASN	2.1
1	B	393	ASN	2.1
1	B	86	CYS	2.1
1	B	450	CYS	2.1
1	A	111	THR	2.1
1	B	367	THR	2.1
1	B	123	SER	2.1
1	B	145	SER	2.1
1	B	226	SER	2.1
1	A	142	LYS	2.1
1	A	411	ASP	2.1
1	B	181	GLU	2.1
1	B	332	PRO	2.1
1	B	289	SER	2.0
1	A	50	ALA	2.0
1	A	449	TYR	2.0
1	B	448	THR	2.0
1	B	272	GLU	2.0
1	B	352	LYS	2.0
1	B	153	ASP	2.0
1	A	308	GLY	2.0
1	B	403	GLY	2.0
1	B	390	GLN	2.0
1	B	490	ILE	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	B	1	8/9	0.83	0.16	23,29,30,32	0
1	PCA	A	1	8/9	0.85	0.16	23,29,30,32	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	CA	B	497	1/1	0.48	0.23	12,12,12,12	0
2	CA	A	497	1/1	0.78	0.10	12,12,12,12	0
3	CL	B	498	1/1	0.85	0.08	16,16,16,16	0
3	CL	A	498	1/1	0.91	0.09	16,16,16,16	0

6.5 Other polymers [i](#)

There are no such residues in this entry.