



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:42 AM UTC

PDB ID : 4PS1 / pdb_00004ps1
Title : Caspase-8 specific unnatural amino acid peptides
Authors : Wolan, D.W.; Vickers, C.J.; Gonzalez-Paez, G.E.
Deposited on : 2014-03-06
Resolution : 1.73 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

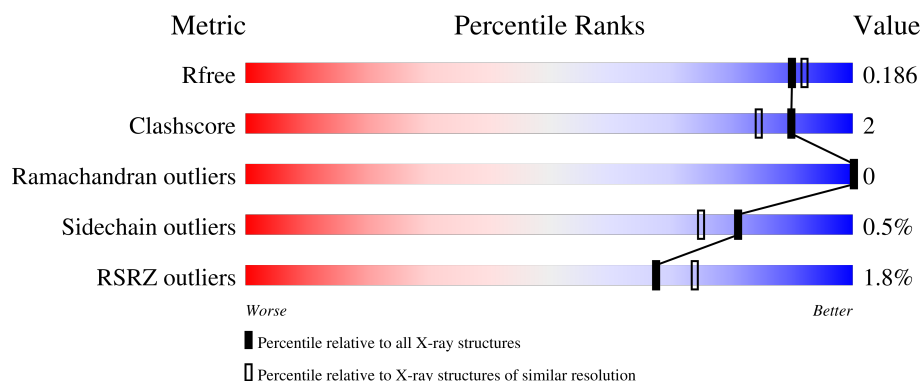
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.73 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	1187 (1.74-1.74)
Clashscore	190562	1207 (1.74-1.74)
Ramachandran outliers	187476	1200 (1.74-1.74)
Sidechain outliers	187428	1200 (1.74-1.74)
RSRZ outliers	180081	1188 (1.74-1.74)

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	275	0% 83% 13%
1	B	275	2% 81% 5% 13%
1	C	275	0% 80% 6% 14%
1	D	275	2% 83% 14%
2	E	5	60% 40%

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Mol	Chain	Length	Quality of chain
2	F	5	 40% 60%
2	G	5	 40% 60%
2	H	5	 80% 20%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8582 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 Caspase-8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	238	Total	C	N	O	S	0	4	0
			1885	1191	320	358	16			
1	B	238	Total	C	N	O	S	0	5	0
			1884	1190	318	360	16			
1	C	237	Total	C	N	O	S	0	4	0
			1883	1189	319	359	16			
1	D	236	Total	C	N	O	S	0	4	0
			1887	1194	321	356	16			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	216	MET	-	expression tag	UNP Q14790
A	480	ALA	-	expression tag	UNP Q14790
A	481	ALA	-	expression tag	UNP Q14790
A	482	ALA	-	expression tag	UNP Q14790
A	483	LEU	-	expression tag	UNP Q14790
A	484	GLU	-	expression tag	UNP Q14790
A	485	HIS	-	expression tag	UNP Q14790
A	486	HIS	-	expression tag	UNP Q14790
A	487	HIS	-	expression tag	UNP Q14790
A	488	HIS	-	expression tag	UNP Q14790
A	489	HIS	-	expression tag	UNP Q14790
A	490	HIS	-	expression tag	UNP Q14790
B	216	MET	-	expression tag	UNP Q14790
B	480	ALA	-	expression tag	UNP Q14790
B	481	ALA	-	expression tag	UNP Q14790
B	482	ALA	-	expression tag	UNP Q14790
B	483	LEU	-	expression tag	UNP Q14790
B	484	GLU	-	expression tag	UNP Q14790
B	485	HIS	-	expression tag	UNP Q14790
B	486	HIS	-	expression tag	UNP Q14790
B	487	HIS	-	expression tag	UNP Q14790

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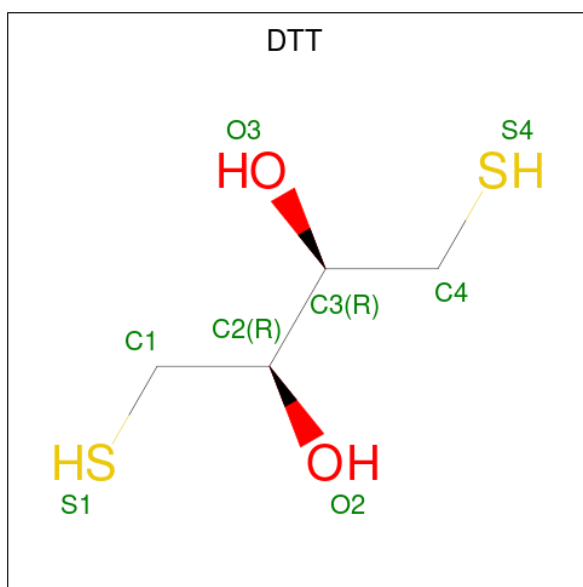
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Chain	Residue	Modelled	Actual	Comment	Reference
B	488	HIS	-	expression tag	UNP Q14790
B	489	HIS	-	expression tag	UNP Q14790
B	490	HIS	-	expression tag	UNP Q14790
C	216	MET	-	expression tag	UNP Q14790
C	480	ALA	-	expression tag	UNP Q14790
C	481	ALA	-	expression tag	UNP Q14790
C	482	ALA	-	expression tag	UNP Q14790
C	483	LEU	-	expression tag	UNP Q14790
C	484	GLU	-	expression tag	UNP Q14790
C	485	HIS	-	expression tag	UNP Q14790
C	486	HIS	-	expression tag	UNP Q14790
C	487	HIS	-	expression tag	UNP Q14790
C	488	HIS	-	expression tag	UNP Q14790
C	489	HIS	-	expression tag	UNP Q14790
C	490	HIS	-	expression tag	UNP Q14790
D	216	MET	-	expression tag	UNP Q14790
D	480	ALA	-	expression tag	UNP Q14790
D	481	ALA	-	expression tag	UNP Q14790
D	482	ALA	-	expression tag	UNP Q14790
D	483	LEU	-	expression tag	UNP Q14790
D	484	GLU	-	expression tag	UNP Q14790
D	485	HIS	-	expression tag	UNP Q14790
D	486	HIS	-	expression tag	UNP Q14790
D	487	HIS	-	expression tag	UNP Q14790
D	488	HIS	-	expression tag	UNP Q14790
D	489	HIS	-	expression tag	UNP Q14790
D	490	HIS	-	expression tag	UNP Q14790

- Molecule 2 is a protein called (BAL)LQ(HYP)(1U8) PEPTIDE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	5	Total	C	N	O	0	0	0
			39	24	6	9			
2	F	5	Total	C	N	O	0	0	0
			39	24	6	9			
2	G	5	Total	C	N	O	0	0	0
			39	24	6	9			
2	H	5	Total	C	N	O	0	0	0
			39	24	6	9			

- Molecule 3 is 2,3-DIHYDROXY-1,4-DITHIOBUTANE (CCD ID: DTT) (formula: C₄H₁₀O₂S₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	S	0	0
			8	4	2	2		
3	B	1	Total	C	O	S	0	0
			8	4	2	2		
3	C	1	Total	C	O	S	0	0
			8	4	2	2		
3	D	1	Total	C	O	S	0	0
			8	4	2	2		

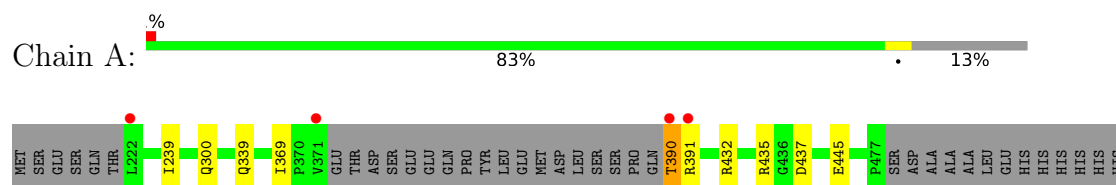
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	218	Total	O	0	0
			218	218		
4	B	221	Total	O	0	0
			221	221		
4	C	195	Total	O	0	0
			195	195		
4	D	209	Total	O	0	0
			209	209		
4	E	2	Total	O	0	0
			2	2		
4	F	6	Total	O	0	0
			6	6		
4	G	2	Total	O	0	0
			2	2		
4	H	2	Total	O	0	0
			2	2		

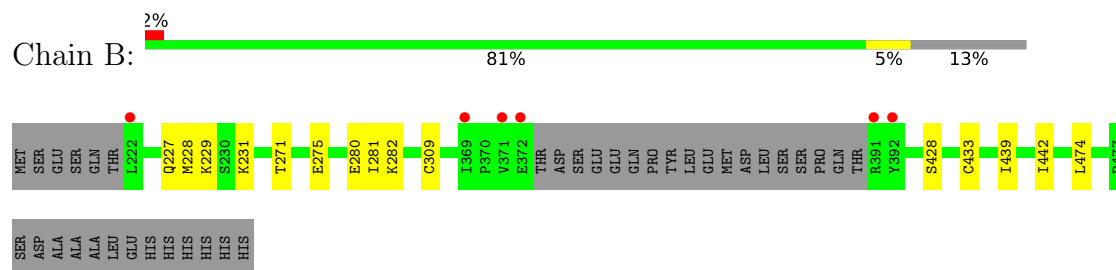
3 Residue-property plots [i](#)

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.

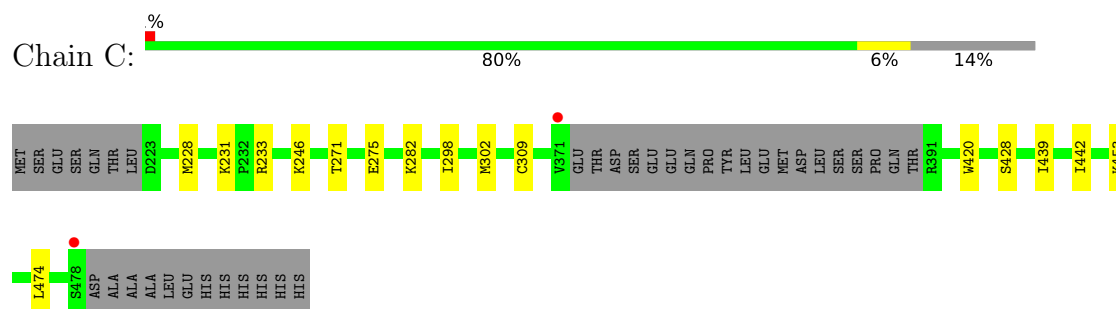
• Molecule 1: Caspase-8



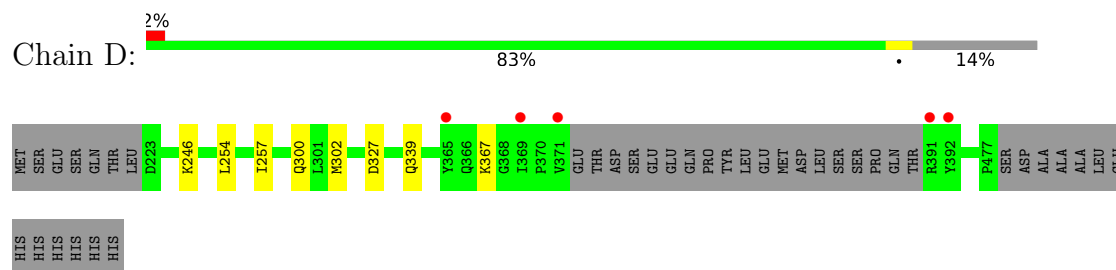
• Molecule 1: Caspase-8



• Molecule 1: Caspase-8



• Molecule 1: Caspase-8

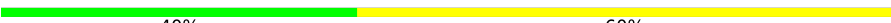


- Molecule 2: (BAL)LQ(HYP)(1U8) PEPTIDE

Chain E:  60% 40%



- Molecule 2: (BAL)LQ(HYP)(1U8) PEPTIDE

Chain F:  40% 60%



- Molecule 2: (BAL)LQ(HYP)(1U8) PEPTIDE

Chain G:  40% 60%



- Molecule 2: (BAL)LQ(HYP)(1U8) PEPTIDE

Chain H:  80% 20%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	115.87Å 144.60Å 86.19Å 90.00° 123.86° 90.00°	Depositor
Resolution (Å)	44.95 – 1.73 44.95 – 1.73	Depositor EDS
% Data completeness (in resolution range)	97.8 (44.95-1.73) 97.8 (44.95-1.73)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 1.73Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.152 , 0.185 0.155 , 0.186	Depositor DCC
R_{free} test set	5986 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	22.9	Xtriage
Anisotropy	0.117	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 40.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	8582	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.68% 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: HYP, 1U8, BAL, DTT

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	0.88	1/1942 (0.1%)	0.94	0/2627
1	B	0.82	0/1944	0.91	2/2632 (0.1%)
1	C	0.79	0/1940	0.87	0/2623
1	D	0.80	0/1943	0.89	0/2626
2	E	0.52	0/16	0.64	0/20
2	F	0.32	0/16	0.44	0/20
2	G	0.57	0/16	0.61	0/20
2	H	0.61	0/16	0.62	0/20
All	All	0.82	1/7833 (0.0%)	0.90	2/10588 (0.0%)

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
2	G	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	239	ILE	CA-CB	5.47	1.60	1.53

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	433	CYS	CA-C-N	-5.07	114.44	119.56
1	B	433	CYS	C-N-CA	-5.07	114.44	119.56

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	G	401	BAL	Mainchain

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	1885	0	1833	5	0
1	B	1884	0	1822	7	0
1	C	1883	0	1833	9	0
1	D	1887	0	1845	4	0
2	E	39	0	35	1	0
2	F	39	0	35	2	0
2	G	39	0	35	0	0
2	H	39	0	35	0	0
3	A	8	0	10	0	0
3	B	8	0	10	0	0
3	C	8	0	10	0	0
3	D	8	0	10	0	0
4	A	218	0	0	0	0
4	B	221	0	0	1	0
4	C	195	0	0	0	0
4	D	209	0	0	0	0
4	E	2	0	0	1	0
4	F	6	0	0	1	0
4	G	2	0	0	0	0
4	H	2	0	0	0	0
All	All	8582	0	7513	28	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 (28) 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:390:THR:HG22	1:A:391:ARG:H	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:401:BAL:N	4:E:502:HOH:O	2.29	0.60
1:B:227:GLN:HG3	1:B:229:LYS:HZ3	1.67	0.59
1:D:246:LYS:HB3	1:D:327:ASP:HA	1.86	0.57
1:C:271:THR:O	1:C:275:GLU:HB2	2.06	0.55
2:F:401:BAL:N	4:F:505:HOH:O	2.34	0.53
1:B:271:THR:O	1:B:275:GLU:HB2	2.12	0.49
1:B:280:GLU:HG2	1:B:282:LYS:HE2	1.95	0.49
1:B:275:GLU:HG3	1:B:281:ILE:HG12	1.97	0.47
1:C:428[A]:SER:OG	1:C:442:ILE:HG23	2.14	0.46
1:D:254:LEU:HD22	1:D:257:ILE:HD12	1.97	0.46
1:B:439:ILE:HG21	1:B:474:LEU:HD23	1.99	0.45
1:C:298:ILE:HG22	1:C:302:MET:HE3	1.99	0.45
1:C:228:MET:HE1	1:C:309:CYS:HB2	1.98	0.45
1:B:228:MET:HE1	1:B:309:CYS:HB2	1.99	0.45
1:C:439:ILE:HG22	1:C:474:LEU:HB3	1.99	0.45
1:A:300:GLN:HG3	1:A:339:GLN:O	2.18	0.43
1:C:231:LYS:HE3	1:C:233:ARG:HH12	1.84	0.42
1:C:231:LYS:CE	1:C:233:ARG:HH12	2.32	0.42
1:C:282:LYS:HA	1:C:282:LYS:HD2	1.83	0.42
1:A:432:ARG:HE	1:A:445:GLU:CD	2.28	0.42
1:C:420:TRP:CD1	1:C:453:LYS:HE2	2.55	0.41
1:B:428[A]:SER:OG	1:B:442:ILE:HG23	2.19	0.41
4:B:780:HOH:O	2:F:402:LEU:HD21	2.21	0.41
1:D:300:GLN:HG3	1:D:339:GLN:O	2.21	0.41
1:D:302:MET:HE3	1:D:302:MET:HB2	1.75	0.41
1:A:369:ILE:O	1:A:369:ILE:HG13	2.22	0.40
1:A:435:ARG:NH1	1:A:437:ASP:OD2	2.55	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	238/275 (86%)	232 (98%)	6 (2%)	0	100	100
1	B	239/275 (87%)	232 (97%)	7 (3%)	0	100	100
1	C	237/275 (86%)	229 (97%)	8 (3%)	0	100	100
1	D	236/275 (86%)	227 (96%)	9 (4%)	0	100	100
2	E	2/5 (40%)	2 (100%)	0	0	100	100
2	F	2/5 (40%)	2 (100%)	0	0	100	100
2	G	2/5 (40%)	2 (100%)	0	0	100	100
2	H	2/5 (40%)	2 (100%)	0	0	100	100
All	All	958/1120 (86%)	928 (97%)	30 (3%)	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	210/247 (85%)	209 (100%)	1 (0%)	81	75
1	B	210/247 (85%)	209 (100%)	1 (0%)	81	75
1	C	211/247 (85%)	210 (100%)	1 (0%)	81	75
1	D	211/247 (85%)	210 (100%)	1 (0%)	81	75
2	E	2/2 (100%)	2 (100%)	0	100	100
2	F	2/2 (100%)	2 (100%)	0	100	100
2	G	2/2 (100%)	2 (100%)	0	100	100
2	H	2/2 (100%)	2 (100%)	0	100	100
All	All	850/996 (85%)	846 (100%)	4 (0%)	81	75

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	390	THR
1	B	231	LYS

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Mol	Chain	Res	Type
1	C	246	LYS
1	D	367	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	358	GLN
1	B	278	HIS
1	B	407	ASN
1	B	465	GLN
1	C	407	ASN
1	C	427	GLN
1	C	465	GLN
1	D	227	GLN
1	D	407	ASN
1	D	465	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

12 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	$\# Z > 2$
2	HYP	E	404	2	7,8,9	5.69	6 (85%)	5,10,12	2.95	3 (60%)
2	HYP	H	404	2	7,8,9	5.63	6 (85%)	5,10,12	3.35	3 (60%)
2	BAL	E	401	2	3,4,5	0.81	0	3,3,5	0.82	0
2	HYP	F	404	2	7,8,9	5.37	5 (71%)	5,10,12	2.53	3 (60%)
2	1U8	G	405	2	7,8,20	0.87	0	7,10,27	1.39	2 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	BAL	G	401	2	3,4,5	0.75	0	3,3,5	0.86	0
2	1U8	H	405	2	7,8,20	0.77	0	7,10,27	1.02	0
2	1U8	E	405	2	7,8,20	0.61	0	7,10,27	1.15	0
2	BAL	F	401	2	3,4,5	0.73	0	3,3,5	0.63	0
2	HYP	G	404	2	7,8,9	5.60	4 (57%)	5,10,12	2.82	3 (60%)
2	1U8	F	405	2	7,8,20	0.80	0	7,10,27	0.84	0
2	BAL	H	401	2	3,4,5	0.74	0	3,3,5	1.06	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	HYP	E	404	2	-	0/0/11/13	0/1/1/1
2	HYP	H	404	2	-	0/0/11/13	0/1/1/1
2	BAL	E	401	2	-	0/1/2/3	-
2	HYP	F	404	2	-	0/0/11/13	0/1/1/1
2	1U8	G	405	2	-	1/7/8/17	-
2	BAL	G	401	2	-	1/1/2/3	-
2	1U8	H	405	2	-	2/7/8/17	-
2	1U8	E	405	2	-	2/7/8/17	-
2	BAL	F	401	2	-	0/1/2/3	-
2	HYP	G	404	2	-	0/0/11/13	0/1/1/1
2	1U8	F	405	2	-	2/7/8/17	-
2	BAL	H	401	2	-	0/1/2/3	-

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	404	HYP	CB-CG	-12.72	1.29	1.52
2	G	404	HYP	CB-CG	-12.55	1.30	1.52
2	H	404	HYP	CB-CG	-12.46	1.30	1.52
2	F	404	HYP	CB-CG	-11.72	1.31	1.52
2	F	404	HYP	CA-N	5.43	1.58	1.48
2	E	404	HYP	CD-N	-4.99	1.30	1.47
2	G	404	HYP	CD-N	-4.97	1.30	1.47
2	H	404	HYP	CD-N	-4.94	1.30	1.47
2	G	404	HYP	CA-N	4.82	1.57	1.48
2	H	404	HYP	CA-N	4.73	1.57	1.48
2	F	404	HYP	CD-N	-4.53	1.32	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	404	HYP	CA-N	4.49	1.56	1.48
2	H	404	HYP	OD1-CG	2.81	1.51	1.43
2	E	404	HYP	OD1-CG	2.57	1.50	1.43
2	G	404	HYP	OD1-CG	2.49	1.50	1.43
2	F	404	HYP	OD1-CG	2.46	1.50	1.43
2	E	404	HYP	CB-CA	2.28	1.59	1.54
2	H	404	HYP	O-C	2.26	1.28	1.20
2	F	404	HYP	CD-CG	2.19	1.58	1.53
2	E	404	HYP	CD-CG	2.15	1.58	1.53
2	H	404	HYP	CD-CG	2.12	1.58	1.53

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	404	HYP	CB-CG-CD	6.12	109.97	103.16
2	E	404	HYP	CB-CG-CD	5.29	109.05	103.16
2	G	404	HYP	CB-CG-CD	4.60	108.28	103.16
2	F	404	HYP	CB-CG-CD	3.53	107.08	103.16
2	F	404	HYP	CG-CB-CA	3.13	107.37	103.75
2	G	404	HYP	CG-CB-CA	3.04	107.26	103.75
2	H	404	HYP	CG-CB-CA	2.95	107.16	103.75
2	G	404	HYP	OD1-CG-CD	-2.70	104.79	110.30
2	E	404	HYP	CG-CB-CA	2.66	106.83	103.75
2	F	404	HYP	OD1-CG-CD	-2.58	105.02	110.30
2	H	404	HYP	OD1-CG-CD	-2.54	105.12	110.30
2	G	405	1U8	CB-CA-C	-2.35	107.89	110.72
2	E	404	HYP	OD1-CG-CD	-2.34	105.51	110.30
2	G	405	1U8	O-C-C9	-2.14	117.40	121.17

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	401	BAL	C-CA-CB-N
2	E	405	1U8	C-CA-CB-CG
2	F	405	1U8	C-CA-CB-CG
2	E	405	1U8	N-CA-CB-CG
2	F	405	1U8	N-CA-CB-CG
2	H	405	1U8	N-CA-CB-CG
2	G	405	1U8	N-CA-CB-CG
2	H	405	1U8	C-CA-CB-CG

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	401	BAL	1	0
2	F	401	BAL	1	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	$\# Z > 2$
3	DTT	A	501	-	7,7,7	0.96	1 (14%)	4,8,8	1.53	1 (25%)
3	DTT	D	501	-	7,7,7	1.04	1 (14%)	4,8,8	1.36	0
3	DTT	C	501	-	7,7,7	1.09	0	4,8,8	0.88	0
3	DTT	B	501	-	7,7,7	1.20	1 (14%)	4,8,8	0.98	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
3	DTT	A	501	-	-	0/8/8/8	-
3	DTT	D	501	-	-	0/8/8/8	-
3	DTT	C	501	-	-	0/8/8/8	-
3	DTT	B	501	-	-	0/8/8/8	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	501	DTT	O3-C3	-2.38	1.38	1.43
3	A	501	DTT	C4-S4	-2.22	1.76	1.81
3	B	501	DTT	C4-S4	-2.03	1.77	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	DTT	C3-C4-S4	-2.15	108.43	114.43

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 [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	238/275 (86%)	-0.30	4 (1%) 69 76	12, 23, 41, 78	4 (1%)
1	B	238/275 (86%)	-0.24	6 (2%) 58 66	14, 23, 42, 84	5 (2%)
1	C	237/275 (86%)	-0.18	2 (0%) 82 88	15, 26, 44, 59	4 (1%)
1	D	236/275 (85%)	-0.21	5 (2%) 63 70	13, 25, 42, 59	4 (1%)
2	E	2/5 (40%)	0.60	0 100 100	32, 32, 32, 35	0
2	F	2/5 (40%)	0.04	0 100 100	31, 31, 31, 32	0
2	G	2/5 (40%)	0.57	0 100 100	32, 32, 32, 35	0
2	H	2/5 (40%)	0.29	0 100 100	32, 32, 32, 36	0
All	All	957/1120 (85%)	-0.23	17 (1%) 67 74	12, 24, 42, 84	17 (1%)

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	222	LEU	6.1
1	A	222	LEU	4.8
1	A	390	THR	4.3
1	C	371	VAL	4.1
1	B	392	TYR	3.6
1	B	372	GLU	3.5
1	B	369	ILE	3.5
1	D	371	VAL	3.3
1	C	478	SER	3.2
1	A	371	VAL	2.9
1	B	391	ARG	2.9
1	D	392	TYR	2.7
1	A	391	ARG	2.5
1	D	391	ARG	2.4
1	D	369	ILE	2.4
1	D	365	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	371	VAL	2.1

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
2	BAL	G	401	5/6	0.82	0.17	37,41,50,52	0
2	BAL	F	401	5/6	0.85	0.16	36,43,51,53	0
2	BAL	H	401	5/6	0.87	0.14	38,45,49,51	0
2	BAL	E	401	5/6	0.88	0.14	38,41,50,51	0
2	HYP	E	404	8/9	0.90	0.11	22,24,38,38	0
2	HYP	F	404	8/9	0.92	0.09	19,23,30,32	0
2	HYP	H	404	8/9	0.93	0.09	20,24,33,35	0
2	HYP	G	404	8/9	0.95	0.07	21,25,32,34	0
2	1U8	E	405	9/20	0.95	0.06	19,19,21,28	0
2	1U8	G	405	9/20	0.96	0.06	19,21,24,28	0
2	1U8	F	405	9/20	0.97	0.06	18,19,22,31	0
2	1U8	H	405	9/20	0.97	0.05	20,21,24,29	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
3	DTT	A	501	8/8	0.97	0.07	20,31,32,34	0
3	DTT	B	501	8/8	0.97	0.07	22,29,30,31	0
3	DTT	C	501	8/8	0.97	0.07	23,32,34,36	0
3	DTT	D	501	8/8	0.97	0.07	24,30,32,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.