



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:09 PM UTC

PDB ID : 3CTM / pdb_00003ctm
Title : Crystal Structure of a Carbonyl Reductase from Candida Parapsilosis with anti-Prelog Stereo-specificity
Authors : Zhang, R.; Zhu, G.; Li, X.; Xu, Y.; Zhang, X.C.; Rao, Z.
Deposited on : 2008-04-14
Resolution : 2.69 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

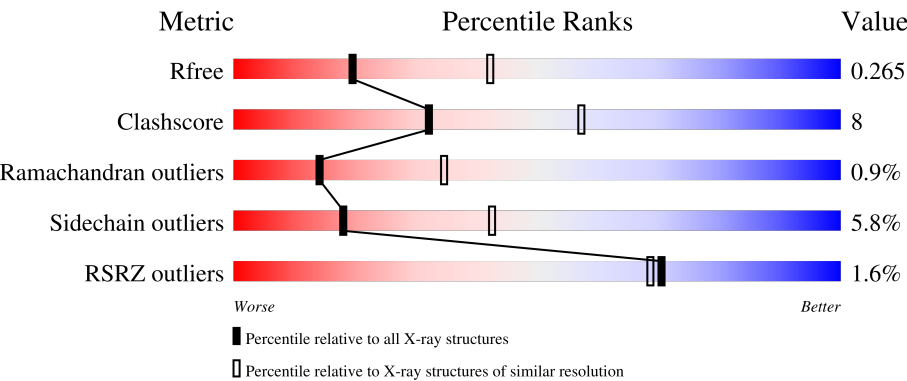
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.69 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	287	% 71%22%• 5%
1	B	287	% 76%17%• 6%
1	D	287	% 68%21%• 8%
1	E	287	% 75%17%• 8%
1	F	287	3% 72%20%• 6%

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Mol	Chain	Length	Quality of chain
1	G	287	
1	H	287	
2	C	287	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16741 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 Carbonyl Reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	272	Total	C	N	O	S	0	0	0
			2076	1320	339	410	7			
1	B	271	Total	C	N	O	S	0	0	0
			2054	1308	336	402	8			
1	D	265	Total	C	N	O	S	0	0	0
			2024	1289	331	397	7			
1	E	265	Total	C	N	O	S	0	0	0
			2024	1288	331	398	7			
1	F	269	Total	C	N	O	S	0	0	0
			2042	1301	335	399	7			
1	G	270	Total	C	N	O	S	0	0	0
			2065	1315	338	405	7			
1	H	270	Total	C	N	O	S	0	0	0
			2051	1308	335	401	7			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	280	LEU	-	expression tag	UNP B2KJ46
A	281	GLU	-	expression tag	UNP B2KJ46
A	282	HIS	-	expression tag	UNP B2KJ46
A	283	HIS	-	expression tag	UNP B2KJ46
A	284	HIS	-	expression tag	UNP B2KJ46
A	285	HIS	-	expression tag	UNP B2KJ46
A	286	HIS	-	expression tag	UNP B2KJ46
A	287	HIS	-	expression tag	UNP B2KJ46
B	280	LEU	-	expression tag	UNP B2KJ46
B	281	GLU	-	expression tag	UNP B2KJ46
B	282	HIS	-	expression tag	UNP B2KJ46
B	283	HIS	-	expression tag	UNP B2KJ46
B	284	HIS	-	expression tag	UNP B2KJ46
B	285	HIS	-	expression tag	UNP B2KJ46
B	286	HIS	-	expression tag	UNP B2KJ46

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Chain	Residue	Modelled	Actual	Comment	Reference
B	287	HIS	-	expression tag	UNP B2KJ46
D	280	LEU	-	expression tag	UNP B2KJ46
D	281	GLU	-	expression tag	UNP B2KJ46
D	282	HIS	-	expression tag	UNP B2KJ46
D	283	HIS	-	expression tag	UNP B2KJ46
D	284	HIS	-	expression tag	UNP B2KJ46
D	285	HIS	-	expression tag	UNP B2KJ46
D	286	HIS	-	expression tag	UNP B2KJ46
D	287	HIS	-	expression tag	UNP B2KJ46
E	280	LEU	-	expression tag	UNP B2KJ46
E	281	GLU	-	expression tag	UNP B2KJ46
E	282	HIS	-	expression tag	UNP B2KJ46
E	283	HIS	-	expression tag	UNP B2KJ46
E	284	HIS	-	expression tag	UNP B2KJ46
E	285	HIS	-	expression tag	UNP B2KJ46
E	286	HIS	-	expression tag	UNP B2KJ46
E	287	HIS	-	expression tag	UNP B2KJ46
F	280	LEU	-	expression tag	UNP B2KJ46
F	281	GLU	-	expression tag	UNP B2KJ46
F	282	HIS	-	expression tag	UNP B2KJ46
F	283	HIS	-	expression tag	UNP B2KJ46
F	284	HIS	-	expression tag	UNP B2KJ46
F	285	HIS	-	expression tag	UNP B2KJ46
F	286	HIS	-	expression tag	UNP B2KJ46
F	287	HIS	-	expression tag	UNP B2KJ46
G	280	LEU	-	expression tag	UNP B2KJ46
G	281	GLU	-	expression tag	UNP B2KJ46
G	282	HIS	-	expression tag	UNP B2KJ46
G	283	HIS	-	expression tag	UNP B2KJ46
G	284	HIS	-	expression tag	UNP B2KJ46
G	285	HIS	-	expression tag	UNP B2KJ46
G	286	HIS	-	expression tag	UNP B2KJ46
G	287	HIS	-	expression tag	UNP B2KJ46
H	280	LEU	-	expression tag	UNP B2KJ46
H	281	GLU	-	expression tag	UNP B2KJ46
H	282	HIS	-	expression tag	UNP B2KJ46
H	283	HIS	-	expression tag	UNP B2KJ46
H	284	HIS	-	expression tag	UNP B2KJ46
H	285	HIS	-	expression tag	UNP B2KJ46
H	286	HIS	-	expression tag	UNP B2KJ46
H	287	HIS	-	expression tag	UNP B2KJ46

- Molecule 2 is a protein called Carbonyl Reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	269	Total 2038	C 1299	N 334	O 399	S 6	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	280	LEU	-	expression tag	UNP B2KJ46
C	281	GLU	-	expression tag	UNP B2KJ46
C	282	HIS	-	expression tag	UNP B2KJ46
C	283	HIS	-	expression tag	UNP B2KJ46
C	284	HIS	-	expression tag	UNP B2KJ46
C	285	HIS	-	expression tag	UNP B2KJ46
C	286	HIS	-	expression tag	UNP B2KJ46
C	287	HIS	-	expression tag	UNP B2KJ46

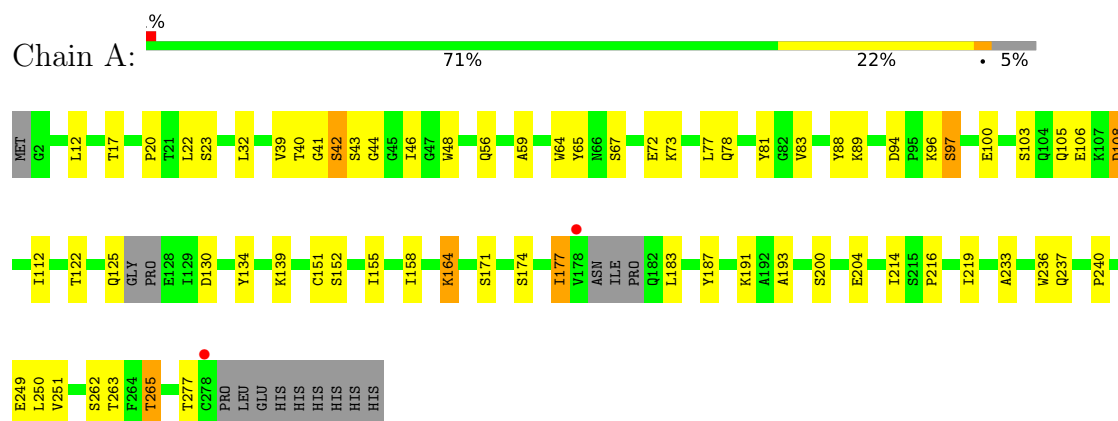
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	50	Total 50	O 50	0	0
3	B	58	Total 58	O 58	0	0
3	D	30	Total 30	O 30	0	0
3	C	43	Total 43	O 43	0	0
3	E	40	Total 40	O 40	0	0
3	F	55	Total 55	O 55	0	0
3	G	43	Total 43	O 43	0	0
3	H	48	Total 48	O 48	0	0

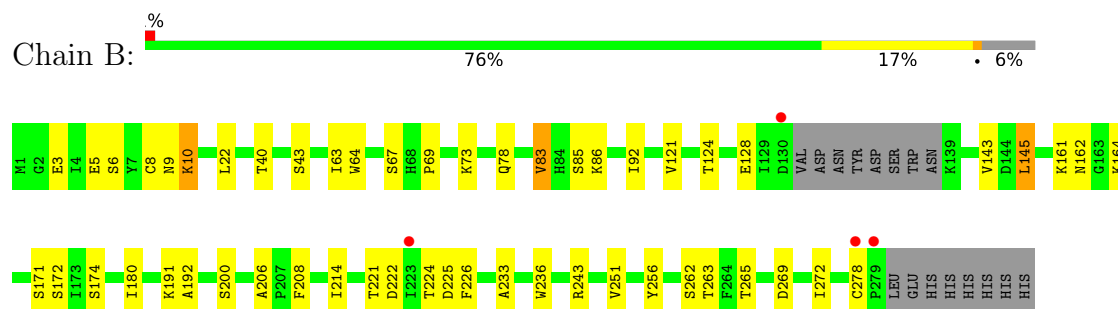
3 Residue-property plots [i](#)

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.

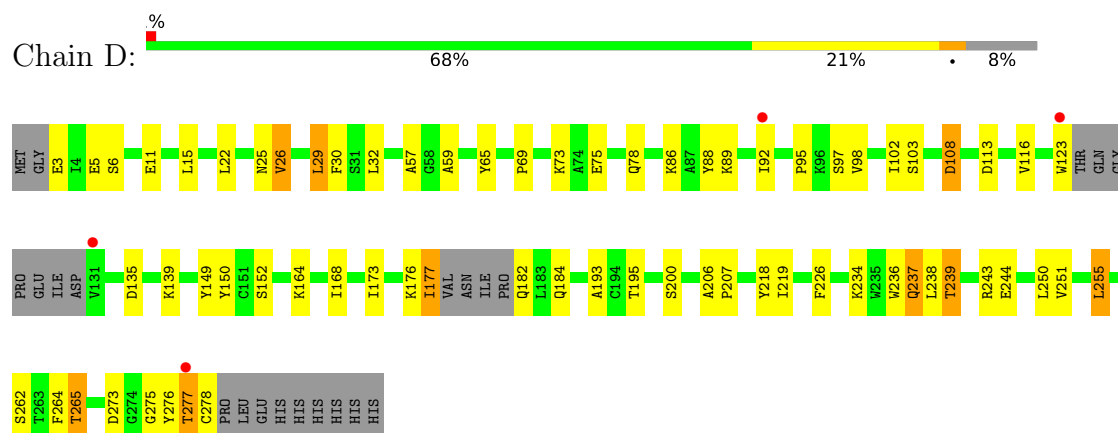
• Molecule 1: Carbonyl Reductase



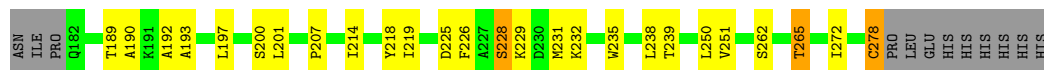
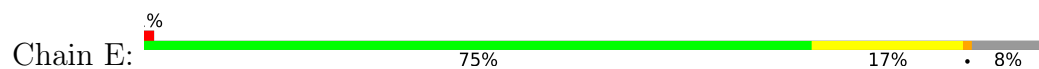
• Molecule 1: Carbonyl Reductase



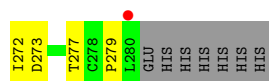
• Molecule 1: Carbonyl Reductase



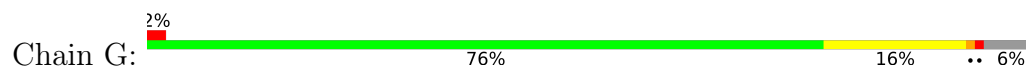
- Molecule 1: Carbonyl Reductase



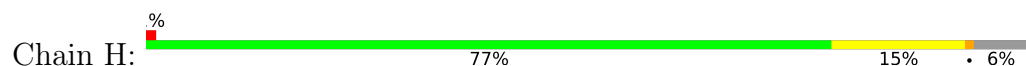
- Molecule 1: Carbonyl Reductase



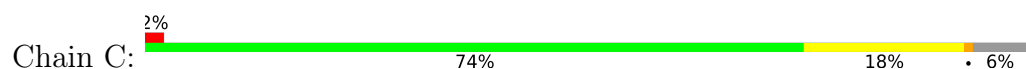
- Molecule 1: Carbonyl Reductase

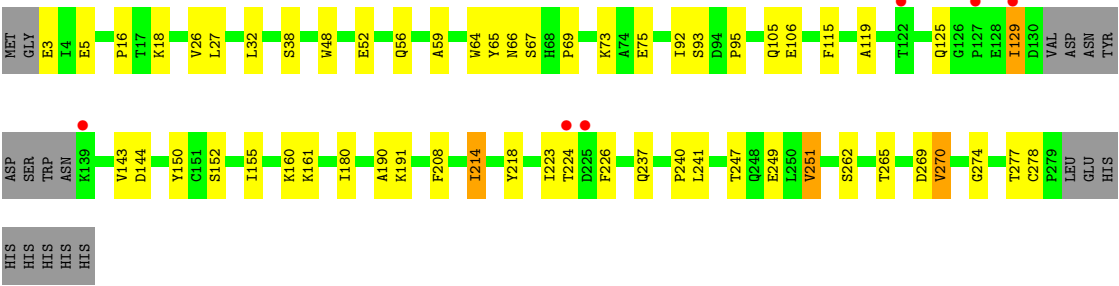


- Molecule 1: Carbonyl Reductase



- Molecule 2: Carbonyl Reductase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	104.73Å 142.76Å 151.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.66 – 2.69 41.66 – 2.69	Depositor EDS
% Data completeness (in resolution range)	99.4 (41.66-2.69) 99.4 (41.66-2.69)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.86 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158, PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.180 , 0.268 0.181 , 0.265	Depositor DCC
R_{free} test set	3215 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	43.6	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 44.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	16741	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.03% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.33	0/2110	0.52	0/2865
1	B	0.37	0/2089	0.54	0/2838
1	D	0.35	0/2058	0.56	0/2794
1	E	0.36	0/2058	0.54	0/2794
1	F	0.41	0/2077	0.60	0/2823
1	G	0.37	0/2101	0.58	0/2854
1	H	0.37	0/2086	0.56	0/2835
2	C	0.39	0/2084	0.60	0/2834
All	All	0.37	0/16663	0.56	0/22637

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	2076	0	2029	38	0
1	B	2054	0	2030	31	0
1	D	2024	0	1980	42	0
1	E	2024	0	1978	33	0
1	F	2042	0	2017	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	2065	0	2019	35	0
1	H	2051	0	2027	36	0
2	C	2038	0	2011	40	0
3	A	50	0	0	3	0
3	B	58	0	0	2	0
3	C	43	0	0	8	0
3	D	30	0	0	3	0
3	E	40	0	0	5	0
3	F	55	0	0	4	0
3	G	43	0	0	2	0
3	H	48	0	0	0	0
All	All	16741	0	16091	260	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 8.

All (260) 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:F:179:ASN:HA	1:F:189:THR:HG22	1.60	0.82
1:E:189:THR:O	3:E:301:HOH:O	1.96	0.81
1:A:106:GLU:HG3	1:A:158:ILE:HD12	1.63	0.81
1:E:228:SER:H	1:E:231:MET:HE3	1.47	0.80
1:G:265:THR:HG22	1:H:272:ILE:HG23	1.64	0.79
1:E:193:ALA:N	3:E:301:HOH:O	1.98	0.77
1:D:32:LEU:HB3	1:D:59:ALA:HB2	1.66	0.76
1:A:32:LEU:HB3	1:A:59:ALA:HB2	1.67	0.75
1:A:265:THR:HG22	1:B:272:ILE:HG23	1.71	0.73
1:B:6:SER:OG	1:B:8:CME:O	2.05	0.72
1:F:144:ASP:OD1	3:F:301:HOH:O	2.07	0.72
1:D:26:VAL:HG13	2:C:251:VAL:HG13	1.72	0.71
1:E:96:LYS:H	1:E:96:LYS:HD2	1.56	0.69
1:E:24:LYS:NZ	3:E:302:HOH:O	2.22	0.69
1:B:128:GLU:OE2	3:B:301:HOH:O	2.12	0.67
2:C:249:GLU:O	3:C:301:HOH:O	2.12	0.67
1:H:179:ASN:HA	1:H:189:THR:HG22	1.77	0.67
1:D:57:ALA:HA	2:C:27:LEU:HD21	1.77	0.66
1:E:192:ALA:N	3:E:301:HOH:O	2.28	0.66
1:G:73:LYS:NZ	3:G:302:HOH:O	2.27	0.66
2:C:119:ALA:HB3	2:C:143:VAL:HG23	1.77	0.66
1:D:92:ILE:HD12	1:D:92:ILE:H	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:269:ASP:OD2	3:C:303:HOH:O	2.15	0.65
1:H:235:TRP:O	1:H:239:THR:HG22	1.96	0.64
2:C:106:GLU:OE2	2:C:161:LYS:NZ	2.29	0.64
2:C:129:ILE:O	3:C:302:HOH:O	2.15	0.64
1:F:222:ASP:HA	1:F:225:ASP:HB3	1.79	0.64
1:G:22:LEU:HD21	1:G:263:THR:HG21	1.78	0.64
1:D:113:ASP:OD1	1:D:164:LYS:NZ	2.28	0.63
1:E:219:ILE:HG12	1:E:250:LEU:HD11	1.80	0.63
2:C:52:GLU:OE1	3:C:304:HOH:O	2.15	0.63
2:C:64:TRP:NE1	2:C:105:GLN:HE22	1.97	0.63
1:F:92:ILE:HG12	1:F:147:GLY:HA3	1.80	0.62
2:C:26:VAL:HG13	2:C:27:LEU:HD22	1.82	0.61
1:G:277:THR:C	1:G:279:PRO:HD2	2.25	0.61
1:B:161:LYS:HG2	1:B:162:ASN:ND2	2.14	0.61
1:F:262:SER:HB2	1:F:265:THR:HG23	1.82	0.61
1:D:219:ILE:HG13	1:D:250:LEU:HD11	1.80	0.61
2:C:152:SER:HA	2:C:155:ILE:HG22	1.82	0.61
1:E:235:TRP:O	1:E:239:THR:HG23	2.01	0.61
1:B:171:SER:OG	1:B:172:SER:N	2.27	0.60
1:B:262:SER:HB2	1:B:265:THR:HB	1.82	0.60
1:H:228:SER:H	1:H:231:MET:HE3	1.67	0.59
1:G:227:ALA:HB3	1:G:232:LYS:HE3	1.84	0.59
1:D:86:LYS:HD2	1:D:88:TYR:CZ	2.38	0.59
1:H:183:LEU:O	1:H:189:THR:HG21	2.02	0.59
1:G:279:PRO:HB3	1:H:8:CME:SD	2.43	0.59
1:D:78:GLN:NE2	3:D:304:HOH:O	2.36	0.58
1:D:239:THR:HG21	3:D:322:HOH:O	2.03	0.58
1:E:272:ILE:HG23	1:F:265:THR:HG22	1.84	0.58
1:G:32:LEU:HB3	1:G:59:ALA:HB2	1.84	0.58
1:A:78:GLN:NE2	3:A:305:HOH:O	2.37	0.57
1:A:171:SER:HB3	1:A:191:LYS:HD2	1.87	0.56
1:H:40:THR:O	1:H:118:ASN:ND2	2.34	0.56
1:H:75:GLU:HG3	1:H:79:LYS:HE3	1.87	0.56
1:H:233:ALA:O	1:H:237:GLN:HG3	2.05	0.56
1:A:112:ILE:H	1:A:158:ILE:HD11	1.70	0.56
1:F:64:TRP:NE1	1:F:105:GLN:HE22	2.03	0.55
2:C:95:PRO:HG3	2:C:150:TYR:CZ	2.42	0.55
1:E:228:SER:OG	1:E:229:LYS:N	2.39	0.55
1:G:235:TRP:O	1:G:239:THR:HG23	2.07	0.55
1:D:275:GLY:O	1:D:277:THR:N	2.39	0.54
1:G:277:THR:O	1:G:278:CYS:HB2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:32:LEU:HB3	1:F:59:ALA:HB2	1.90	0.54
1:A:56:GLN:HG2	1:A:81:TYR:CE1	2.43	0.54
2:C:3:GLU:OE1	3:C:305:HOH:O	2.18	0.54
1:F:65:TYR:CE1	1:F:69:PRO:HA	2.43	0.54
1:G:40:THR:HA	1:G:64:TRP:CG	2.42	0.53
1:A:216:PRO:HB2	1:A:219:ILE:HD13	1.89	0.53
1:G:239:THR:HG22	1:G:276:TYR:HD1	1.74	0.53
1:A:40:THR:HA	1:A:64:TRP:CG	2.43	0.53
1:E:265:THR:HG22	1:F:272:ILE:HG23	1.91	0.53
1:F:60:ASP:CG	1:F:84:HIS:HB2	2.33	0.53
1:G:26:VAL:HG13	1:H:251:VAL:CG1	2.38	0.53
1:A:78:GLN:HG3	1:A:83:VAL:O	2.09	0.53
1:F:5:GLU:OE1	1:F:10:LYS:NZ	2.38	0.53
1:B:43:SER:O	1:B:73:LYS:NZ	2.42	0.52
1:G:78:GLN:HG3	1:G:83:VAL:O	2.09	0.52
1:H:140:ILE:HG13	1:H:177:ILE:HG21	1.91	0.52
1:E:65:TYR:CE1	1:E:69:PRO:HA	2.45	0.52
1:B:222:ASP:HA	1:B:225:ASP:HB2	1.92	0.52
1:A:219:ILE:HG12	1:A:250:LEU:HD11	1.91	0.52
1:D:237:GLN:NE2	2:C:5:GLU:O	2.43	0.52
1:G:240:PRO:HD2	1:G:275:GLY:C	2.35	0.51
1:G:256:TYR:OH	1:G:265:THR:HG21	2.10	0.51
1:H:199:LYS:NZ	1:H:267:GLY:O	2.41	0.51
1:F:201:LEU:HD22	1:F:205:TRP:CE2	2.46	0.51
1:G:172:SER:O	1:G:191:LYS:NZ	2.39	0.51
1:H:99:GLU:HG3	1:H:154:ASN:HD21	1.74	0.51
2:C:32:LEU:HB3	2:C:59:ALA:HB2	1.91	0.51
1:H:48:TRP:CZ3	1:H:73:LYS:HB3	2.46	0.51
1:F:233:ALA:O	1:F:237:GLN:HG3	2.11	0.51
1:F:235:TRP:O	1:F:239:THR:HG22	2.11	0.51
1:F:273:ASP:OD2	1:F:277:THR:OG1	2.26	0.51
1:B:22:LEU:HD21	1:B:263:THR:HG21	1.92	0.51
1:B:78:GLN:HG2	1:B:83:VAL:O	2.10	0.51
1:G:6:SER:CB	1:G:15:LEU:HD11	2.41	0.51
1:A:94:ASP:HB3	1:A:97:SER:HB2	1.93	0.51
1:F:195:THR:O	1:F:199:LYS:HG2	2.10	0.51
1:G:26:VAL:HG13	1:H:251:VAL:HG13	1.93	0.50
1:H:38:SER:HB3	1:H:115:PHE:CD1	2.46	0.50
1:G:40:THR:HA	1:G:64:TRP:HB2	1.92	0.50
1:A:130:ASP:OD1	1:A:139:LYS:HE3	2.11	0.50
1:F:270:VAL:HG12	1:F:272:ILE:HD11	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:68:HIS:O	3:F:303:HOH:O	2.18	0.49
1:G:65:TYR:CZ	1:G:89:LYS:HB2	2.47	0.49
1:F:183:LEU:O	1:F:189:THR:HG21	2.12	0.49
1:A:249:GLU:OE2	1:B:263:THR:OG1	2.21	0.49
1:G:279:PRO:HB3	1:H:8:CME:HE3	1.95	0.49
1:D:264:PHE:HB2	2:C:249:GLU:CD	2.38	0.49
1:F:161:LYS:NZ	3:F:304:HOH:O	2.29	0.49
1:E:96:LYS:H	1:E:96:LYS:CD	2.24	0.49
1:E:197:LEU:O	1:E:201:LEU:HG	2.12	0.48
1:E:262:SER:HB2	1:E:265:THR:HG23	1.95	0.48
1:A:193:ALA:HB2	1:D:193:ALA:HB2	1.94	0.48
1:F:46:ILE:HD12	1:F:250:LEU:CD1	2.43	0.48
1:B:224:THR:HG22	1:B:224:THR:O	2.13	0.48
2:C:214:ILE:HD13	2:C:270:VAL:CG2	2.43	0.48
1:A:164:LYS:HD2	1:A:164:LYS:HA	1.67	0.48
1:A:22:LEU:HD21	1:A:263:THR:HG21	1.95	0.48
1:A:233:ALA:HA	1:A:236:TRP:CE3	2.48	0.48
1:D:65:TYR:CZ	1:D:89:LYS:HB2	2.49	0.48
2:C:262:SER:HB2	2:C:265:THR:HB	1.96	0.48
2:C:143:VAL:HG11	2:C:190:ALA:HB1	1.95	0.48
1:E:278:CYS:HB3	1:F:199:LYS:NZ	2.28	0.48
1:G:6:SER:HB3	1:G:15:LEU:HD11	1.96	0.48
1:E:71:ASP:O	1:E:75:GLU:HG3	2.13	0.48
1:E:7:TYR:CD2	1:F:237:GLN:HB3	2.48	0.48
1:F:222:ASP:HA	1:F:225:ASP:CB	2.43	0.48
1:D:30:PHE:HB3	1:D:255:LEU:HD13	1.96	0.48
1:A:240:PRO:O	1:B:206:ALA:HB1	2.14	0.47
1:B:5:GLU:HB3	1:B:10:LYS:HD3	1.95	0.47
1:D:95:PRO:HG3	1:D:150:TYR:CZ	2.50	0.47
1:G:183:LEU:O	1:G:186:PRO:HD2	2.15	0.47
1:G:281:GLU:H	1:G:281:GLU:HG3	1.47	0.47
2:C:125:GLN:O	2:C:125:GLN:NE2	2.48	0.47
1:E:26:VAL:HG21	1:F:53:ALA:HB1	1.97	0.47
1:H:121:VAL:HG22	1:H:143:VAL:HG12	1.97	0.47
1:B:121:VAL:HG22	1:B:143:VAL:HG12	1.96	0.47
1:D:177:ILE:HG13	1:D:226:PHE:HZ	1.80	0.47
2:C:241:LEU:HD12	2:C:274:GLY:HA2	1.97	0.47
1:E:190:ALA:C	3:E:301:HOH:O	2.58	0.46
1:H:75:GLU:HG3	1:H:79:LYS:CE	2.45	0.46
1:D:75:GLU:OE1	3:D:301:HOH:O	2.20	0.46
1:B:161:LYS:HG2	1:B:162:ASN:HD22	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:6:SER:HB2	1:D:15:LEU:HD11	1.97	0.46
1:G:278:CYS:N	1:G:279:PRO:HD2	2.31	0.46
1:A:262:SER:HB2	1:A:265:THR:HG23	1.96	0.46
1:G:139:LYS:HE2	1:G:139:LYS:HB3	1.73	0.46
1:D:236:TRP:CZ3	2:C:16:PRO:HD3	2.51	0.46
2:C:129:ILE:HB	3:C:329:HOH:O	2.16	0.46
1:E:32:LEU:HB3	1:E:59:ALA:HB2	1.96	0.46
1:E:176:LYS:HB3	1:E:218:TYR:OH	2.16	0.46
1:G:278:CYS:HB3	1:G:282:HIS:NE2	2.31	0.46
1:D:11:GLU:HB2	1:D:207:PRO:HG2	1.98	0.46
1:E:118:ASN:ND2	1:E:170:THR:OG1	2.49	0.45
1:D:206:ALA:HB1	2:C:240:PRO:O	2.16	0.45
1:B:40:THR:HG22	1:B:64:TRP:CD2	2.52	0.45
1:F:123:TRP:HB2	1:F:140:ILE:O	2.16	0.45
1:H:145:LEU:HD23	1:H:145:LEU:HA	1.70	0.45
1:H:239:THR:HB	1:H:276:TYR:HD1	1.81	0.45
1:A:39:VAL:O	1:A:42:SER:OG	2.31	0.45
1:D:108:ASP:N	1:D:108:ASP:OD1	2.49	0.45
1:D:176:LYS:HB3	1:D:218:TYR:CE1	2.51	0.45
1:E:174:SER:HA	1:E:177:ILE:HG12	1.99	0.45
1:E:238:LEU:HD22	1:F:7:TYR:HD2	1.82	0.45
1:F:90:CYS:HB2	1:F:101:THR:OG1	2.17	0.45
1:A:152:SER:HA	1:A:155:ILE:HG22	1.99	0.45
1:B:164:LYS:HA	1:B:208:PHE:O	2.17	0.45
2:C:214:ILE:HD13	2:C:270:VAL:HG22	1.98	0.45
1:H:115:PHE:CE2	1:H:151:CYS:HB3	2.52	0.45
2:C:48:TRP:CZ3	2:C:73:LYS:HB3	2.52	0.44
1:D:182:GLN:N	1:D:184:GLN:HE21	2.15	0.44
1:G:264:PHE:HB2	1:H:249:GLU:CD	2.42	0.44
1:G:185:ALA:HB3	1:G:186:PRO:HD3	2.00	0.44
1:A:20:PRO:HD3	1:B:243:ARG:CZ	2.48	0.44
1:D:26:VAL:O	1:D:29:LEU:HB2	2.18	0.44
1:E:90:CYS:HB2	1:E:101:THR:OG1	2.17	0.44
1:A:73:LYS:NZ	3:A:311:HOH:O	2.50	0.44
1:A:96:LYS:O	1:A:100:GLU:HG3	2.18	0.44
1:D:238:LEU:HD23	1:D:238:LEU:HA	1.78	0.44
1:F:106:GLU:CD	1:F:158:ILE:HD12	2.43	0.44
1:F:119:ALA:HB2	1:F:148:VAL:CG2	2.47	0.44
1:A:237:GLN:HG2	1:B:5:GLU:O	2.18	0.43
1:B:221:THR:HB	1:B:222:ASP:H	1.49	0.43
1:D:25:ASN:HA	2:C:56:GLN:OE1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:52:GLU:O	1:E:56:GLN:HG3	2.17	0.43
1:H:48:TRP:CE3	1:H:73:LYS:HD3	2.53	0.43
1:D:5:GLU:O	2:C:237:GLN:HG2	2.18	0.43
1:D:237:GLN:HE21	1:D:237:GLN:HB3	1.70	0.43
1:B:256:TYR:CZ	1:B:262:SER:HB3	2.53	0.43
2:C:38:SER:HB3	2:C:115:PHE:CD2	2.53	0.43
1:F:107:LYS:NZ	3:F:312:HOH:O	2.50	0.43
1:F:201:LEU:HD22	1:F:205:TRP:CZ2	2.53	0.43
1:B:191:LYS:NZ	1:B:269:ASP:OD2	2.49	0.43
1:D:243:ARG:HG3	1:D:244:GLU:O	2.18	0.43
1:E:278:CYS:HB3	1:F:199:LYS:HZ3	1.83	0.43
1:A:88:TYR:CZ	1:A:105:GLN:HG2	2.53	0.43
1:D:98:VAL:O	1:D:102:ILE:HG13	2.19	0.43
2:C:224:THR:C	2:C:226:PHE:H	2.26	0.43
1:G:71:ASP:N	3:G:313:HOH:O	2.51	0.43
1:H:78:GLN:HG2	1:H:83:VAL:O	2.18	0.43
1:G:272:ILE:HG23	1:H:265:THR:HG22	2.01	0.43
1:B:67:SER:O	1:B:69:PRO:HD3	2.19	0.43
2:C:95:PRO:HG3	2:C:150:TYR:CE1	2.53	0.43
1:E:118:ASN:HD22	1:E:118:ASN:HA	1.68	0.42
3:A:339:HOH:O	1:B:265:THR:HA	2.19	0.42
2:C:93:SER:OG	2:C:144:ASP:OD2	2.35	0.42
1:H:117:ALA:HB1	1:H:148:VAL:HG22	2.01	0.42
1:A:183:LEU:HD23	1:A:183:LEU:HA	1.85	0.42
1:D:116:VAL:HG13	1:D:168:ILE:HB	2.01	0.42
2:C:65:TYR:CD2	2:C:69:PRO:HA	2.54	0.42
1:E:177:ILE:HD12	1:E:226:PHE:CZ	2.55	0.42
1:G:278:CYS:HB2	1:H:199:LYS:HE3	2.01	0.42
1:A:151:CYS:O	1:A:155:ILE:HG22	2.19	0.42
1:E:232:LYS:HG2	1:E:235:TRP:CZ3	2.55	0.42
1:G:137:TRP:HE3	1:G:186:PRO:HG3	1.84	0.42
1:G:142:SER:HA	1:G:146:ASN:HB2	2.01	0.42
1:A:174:SER:HA	1:A:177:ILE:HG13	2.02	0.42
1:B:224:THR:O	1:B:224:THR:CG2	2.67	0.42
1:A:12:LEU:HD22	1:A:17:THR:HG21	2.00	0.42
1:E:12:LEU:HG	1:E:207:PRO:HG3	2.01	0.42
1:H:75:GLU:HG3	1:H:79:LYS:NZ	2.35	0.42
2:C:18:LYS:HD2	2:C:18:LYS:C	2.45	0.42
1:H:221:THR:HG23	1:H:223:ILE:HG12	2.01	0.42
2:C:52:GLU:O	2:C:56:GLN:HG3	2.19	0.42
1:D:262:SER:HB2	1:D:265:THR:HG23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:273:ASP:OD2	1:D:278:CYS:HA	2.19	0.42
2:C:218:TYR:HB2	3:C:321:HOH:O	2.20	0.41
2:C:223:ILE:HD13	2:C:223:ILE:HA	1.73	0.41
1:H:8:CME:HE2	1:H:8:CME:HA	2.02	0.41
1:G:237:GLN:HE21	1:H:4:ILE:HG23	1.85	0.41
1:F:65:TYR:CZ	1:F:69:PRO:HA	2.55	0.41
1:H:99:GLU:HG3	1:H:154:ASN:ND2	2.35	0.41
1:A:125:GLN:HE21	1:A:187:TYR:HE1	1.68	0.41
1:A:44:GLY:HA2	1:A:48:TRP:HB2	2.01	0.41
1:A:134:TYR:CD2	1:D:95:PRO:HB2	2.55	0.41
1:D:22:LEU:HD23	1:D:22:LEU:HA	1.90	0.41
1:B:233:ALA:HA	1:B:236:TRP:CE3	2.56	0.41
1:D:65:TYR:CE1	1:D:69:PRO:HA	2.55	0.41
1:D:149:TYR:O	1:D:152:SER:HB3	2.20	0.41
1:F:160:LYS:HG3	1:F:208:PHE:CE2	2.56	0.41
1:H:176:LYS:HE3	1:H:176:LYS:HB2	1.59	0.41
1:A:108:ASP:OD1	1:A:108:ASP:N	2.50	0.41
2:C:160:LYS:HG3	2:C:208:PHE:CE2	2.56	0.41
1:B:145:LEU:HG	1:B:180:ILE:HG21	2.03	0.41
1:D:234:LYS:HE2	1:D:237:GLN:OE1	2.21	0.41
2:C:92:ILE:H	2:C:92:ILE:HG22	1.63	0.41
1:E:238:LEU:HD22	1:F:7:TYR:CD2	2.56	0.41
1:A:46:ILE:HG12	1:A:250:LEU:HD12	2.01	0.41
1:A:65:TYR:CE1	1:A:89:LYS:HG3	2.56	0.41
1:H:231:MET:HG3	1:H:234:LYS:NZ	2.36	0.41
1:A:41:GLY:HA3	1:A:122:THR:OG1	2.20	0.40
1:B:3:GLU:HA	3:B:307:HOH:O	2.20	0.40
1:B:192:ALA:HB3	3:C:309:HOH:O	2.20	0.40
2:C:155:ILE:HD12	2:C:155:ILE:HA	1.88	0.40
1:H:183:LEU:HB2	1:H:189:THR:HG21	2.04	0.40
1:B:143:VAL:O	1:B:180:ILE:HG22	2.21	0.40
1:D:123:TRP:HH2	1:D:139:LYS:HZ1	1.67	0.40
1:D:264:PHE:O	1:D:264:PHE:CG	2.74	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	265/287 (92%)	256 (97%)	7 (3%)	2 (1%)	16	37
1	B	266/287 (93%)	252 (95%)	12 (4%)	2 (1%)	16	37
1	D	258/287 (90%)	248 (96%)	8 (3%)	2 (1%)	16	37
1	E	258/287 (90%)	246 (95%)	11 (4%)	1 (0%)	30	54
1	F	264/287 (92%)	242 (92%)	19 (7%)	3 (1%)	11	29
1	G	263/287 (92%)	246 (94%)	12 (5%)	5 (2%)	6	17
1	H	265/287 (92%)	253 (96%)	12 (4%)	0	100	100
2	C	265/287 (92%)	247 (93%)	14 (5%)	4 (2%)	8	22
All	All	2104/2296 (92%)	1990 (95%)	95 (4%)	19 (1%)	14	35

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	9	ASN
1	D	276	TYR
1	D	277	THR
1	G	123	TRP
1	G	278	CYS
1	G	279	PRO
1	G	281	GLU
2	C	67	SER
2	C	277	THR
1	E	228	SER
1	A	67	SER
1	B	226	PHE
1	F	226	PHE
2	C	66	ASN
2	C	278	CYS
1	F	221	THR
1	F	279	PRO

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Mol	Chain	Res	Type
1	G	174	SER
1	A	177	ILE

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	221/235 (94%)	206 (93%)	15 (7%)	14	35
1	B	219/235 (93%)	206 (94%)	13 (6%)	18	42
1	D	215/235 (92%)	198 (92%)	17 (8%)	11	28
1	E	215/235 (92%)	205 (95%)	10 (5%)	23	51
1	F	218/235 (93%)	203 (93%)	15 (7%)	14	34
1	G	220/235 (94%)	207 (94%)	13 (6%)	18	42
1	H	219/235 (93%)	209 (95%)	10 (5%)	24	51
2	C	219/236 (93%)	211 (96%)	8 (4%)	30	59
All	All	1746/1881 (93%)	1645 (94%)	101 (6%)	18	42

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	SER
1	A	42	SER
1	A	43	SER
1	A	72	GLU
1	A	77	LEU
1	A	97	SER
1	A	103	SER
1	A	108	ASP
1	A	164	LYS
1	A	200	SER
1	A	204	GLU
1	A	214	ILE
1	A	251	VAL

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Mol	Chain	Res	Type
1	A	265	THR
1	A	277	THR
1	B	10	LYS
1	B	63	ILE
1	B	83	VAL
1	B	85	SER
1	B	86	LYS
1	B	92	ILE
1	B	124	THR
1	B	145	LEU
1	B	174	SER
1	B	200	SER
1	B	214	ILE
1	B	251	VAL
1	B	278	CYS
1	D	3	GLU
1	D	26	VAL
1	D	29	LEU
1	D	73	LYS
1	D	97	SER
1	D	103	SER
1	D	108	ASP
1	D	135	ASP
1	D	173	ILE
1	D	177	ILE
1	D	195	THR
1	D	200	SER
1	D	237	GLN
1	D	239	THR
1	D	251	VAL
1	D	255	LEU
1	D	265	THR
2	C	75	GLU
2	C	129	ILE
2	C	180	ILE
2	C	191	LYS
2	C	214	ILE
2	C	247	THR
2	C	251	VAL
2	C	270	VAL
1	E	27	LEU
1	E	43	SER

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Mol	Chain	Res	Type
1	E	124	THR
1	E	155	ILE
1	E	200	SER
1	E	214	ILE
1	E	225	ASP
1	E	251	VAL
1	E	265	THR
1	E	278	CYS
1	F	21	THR
1	F	71	ASP
1	F	84	HIS
1	F	124	THR
1	F	142	SER
1	F	143	VAL
1	F	174	SER
1	F	189	THR
1	F	221	THR
1	F	223	ILE
1	F	239	THR
1	F	241	LEU
1	F	247	THR
1	F	251	VAL
1	F	265	THR
1	G	26	VAL
1	G	67	SER
1	G	131	VAL
1	G	132	ASP
1	G	174	SER
1	G	200	SER
1	G	214	ILE
1	G	247	THR
1	G	251	VAL
1	G	265	THR
1	G	270	VAL
1	G	278	CYS
1	G	281	GLU
1	H	67	SER
1	H	92	ILE
1	H	124	THR
1	H	129	ILE
1	H	189	THR
1	H	214	ILE

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Mol	Chain	Res	Type
1	H	239	THR
1	H	247	THR
1	H	251	VAL
1	H	265	THR

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	91	ASN
1	A	125	GLN
1	A	133	ASN
1	A	138	ASN
1	B	25	ASN
1	B	91	ASN
1	B	153	HIS
1	B	196	HIS
2	C	25	ASN
2	C	237	GLN
1	E	104	GLN
1	E	118	ASN
1	E	153	HIS
1	F	68	HIS
1	G	138	ASN
1	G	237	GLN
1	H	76	HIS
1	H	78	GLN
1	H	162	ASN
1	H	179	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

7 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	CME	G	8	1	8,9,10	1.04	0	6,9,11	0.84	0
1	CME	F	8	1	8,9,10	0.95	0	6,9,11	0.92	0
1	CME	B	8	1	8,9,10	0.92	0	6,9,11	0.88	0
1	CME	A	8	1	8,9,10	0.90	0	6,9,11	0.94	0
1	CME	H	8	1	8,9,10	0.97	0	6,9,11	0.86	0
1	CME	E	8	1	8,9,10	1.01	0	6,9,11	1.56	1 (16%)
1	CME	D	8	1	8,9,10	1.02	0	6,9,11	1.08	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
1	CME	G	8	1	-	1/5/8/10	-
1	CME	F	8	1	-	2/5/8/10	-
1	CME	B	8	1	-	3/5/8/10	-
1	CME	A	8	1	-	1/5/8/10	-
1	CME	H	8	1	-	4/5/8/10	-
1	CME	E	8	1	-	2/5/8/10	-
1	CME	D	8	1	-	3/5/8/10	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	8	CME	CB-SG-SD	3.14	111.98	103.86

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	8	CME	N-CA-CB-SG
1	D	8	CME	SD-CE-CZ-OH
1	E	8	CME	N-CA-CB-SG
1	D	8	CME	CE-SD-SG-CB

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Mol	Chain	Res	Type	Atoms
1	F	8	CME	CE-SD-SG-CB
1	A	8	CME	SD-CE-CZ-OH
1	B	8	CME	SD-CE-CZ-OH
1	E	8	CME	CA-CB-SG-SD
1	H	8	CME	CA-CB-SG-SD
1	B	8	CME	CE-SD-SG-CB
1	H	8	CME	CE-SD-SG-CB
1	G	8	CME	SD-CE-CZ-OH
1	H	8	CME	SD-CE-CZ-OH
1	D	8	CME	CZ-CE-SD-SG
1	F	8	CME	CZ-CE-SD-SG
1	H	8	CME	CZ-CE-SD-SG

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	8	CME	1	0
1	H	8	CME	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	271/287 (94%)	-0.20	2 (0%) 84 83	26, 44, 73, 87	1 (0%)
1	B	270/287 (94%)	-0.50	4 (1%) 72 70	20, 33, 68, 92	0
1	D	264/287 (91%)	-0.18	4 (1%) 72 70	26, 44, 71, 94	0
1	E	264/287 (91%)	-0.31	3 (1%) 78 76	22, 38, 70, 96	0
1	F	268/287 (93%)	-0.46	8 (2%) 52 49	19, 32, 69, 87	0
1	G	269/287 (93%)	-0.23	6 (2%) 62 59	25, 41, 80, 94	0
1	H	269/287 (93%)	-0.47	2 (0%) 84 83	22, 35, 68, 90	0
2	C	269/287 (93%)	-0.29	6 (2%) 62 59	23, 38, 64, 100	0
All	All	2144/2296 (93%)	-0.33	35 (1%) 70 68	19, 38, 71, 100	1 (0%)

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	131	VAL	4.4
1	F	120	GLY	3.8
1	E	123	TRP	3.5
1	G	131	VAL	3.5
1	A	178	VAL	3.5
1	G	280	LEU	3.3
1	B	223	ILE	3.1
2	C	129	ILE	3.0
1	H	129	ILE	2.9
1	E	124	THR	2.9
1	F	280	LEU	2.9
1	G	282	HIS	2.6
2	C	225	ASP	2.6
1	G	68	HIS	2.5
2	C	224	THR	2.4
2	C	139	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
2	C	127	PRO	2.3
1	G	175	GLY	2.3
2	C	122	THR	2.3
1	F	222	ASP	2.3
1	G	279	PRO	2.3
1	F	139	LYS	2.2
1	A	278	CYS	2.2
1	D	123	TRP	2.2
1	D	92	ILE	2.2
1	F	140	ILE	2.2
1	F	221	THR	2.2
1	B	130	ASP	2.2
1	H	281	GLU	2.1
1	E	177	ILE	2.1
1	D	277	THR	2.1
1	F	122	THR	2.1
1	B	279	PRO	2.1
1	B	278	CYS	2.1
1	F	123	TRP	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	CME	E	8	10/11	0.87	0.13	49,57,65,65	1
1	CME	F	8	10/11	0.87	0.12	36,49,65,74	0
1	CME	H	8	10/11	0.90	0.11	45,53,74,82	4
1	CME	B	8	10/11	0.91	0.10	36,47,61,68	1
1	CME	A	8	10/11	0.91	0.10	43,54,58,61	2
1	CME	D	8	10/11	0.92	0.10	45,51,58,63	1
1	CME	G	8	10/11	0.93	0.11	38,48,77,79	1

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.