



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:16 PM UTC

PDB ID : 1G5C / pdb_00001g5c
Title : CRYSTAL STRUCTURE OF THE 'CAB' TYPE BETA CLASS CARBONIC ANHYDRASE FROM METHANOBACTERIUM THERMOAUTOTROPHICUM
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Deposited on : 2000-10-31
Resolution : 2.10 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

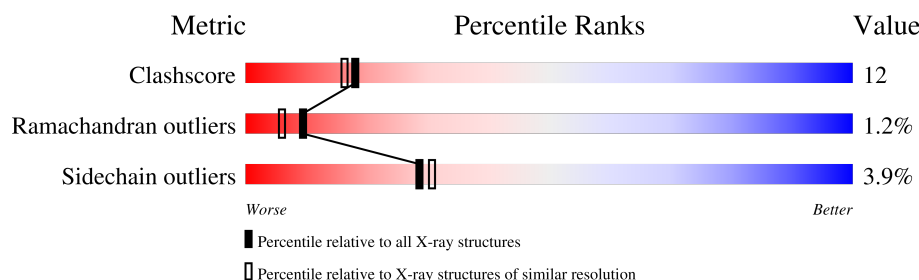
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	170	74% 23% ...
1	B	170	69% 22% 7%
1	C	170	74% 21% 5%
1	D	170	69% 23% 7%
1	E	170	74% 20% 5%
1	F	170	64% 24% 9%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8010 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 BETA-CARBONIC ANHYDRASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	169	Total	C	N	O	S	61	0	0
			1311	820	228	257	6			
1	B	158	Total	C	N	O	S	31	0	0
			1210	755	208	241	6			
1	C	169	Total	C	N	O	S	78	0	0
			1311	820	228	257	6			
1	D	158	Total	C	N	O	S	59	0	0
			1210	755	208	241	6			
1	E	169	Total	C	N	O	S	151	0	0
			1311	820	228	257	6			
1	F	155	Total	C	N	O	S	42	0	0
			1187	743	204	234	6			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	79	ASP	VAL	conflict	UNP Q50565
B	79	ASP	VAL	conflict	UNP Q50565
C	79	ASP	VAL	conflict	UNP Q50565
D	79	ASP	VAL	conflict	UNP Q50565
E	79	ASP	VAL	conflict	UNP Q50565
F	79	ASP	VAL	conflict	UNP Q50565

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

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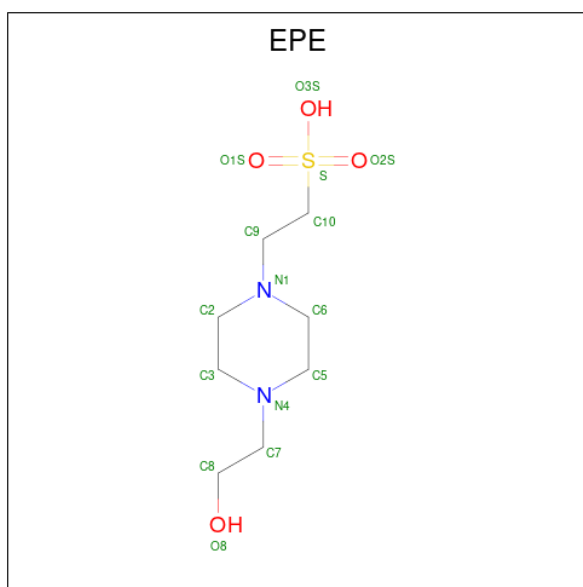
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total	Zn	0	0
			1	1		
2	E	1	Total	Zn	0	0
			1	1		
2	F	1	Total	Zn	0	0
			1	1		

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Ca	0	0
			2	2		
3	B	1	Total	Ca	0	0
			1	1		
3	C	1	Total	Ca	0	0
			1	1		
3	E	1	Total	Ca	0	0
			1	1		
3	F	1	Total	Ca	0	0
			1	1		

- Molecule 4 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: C₈H₁₈N₂O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	C	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
4	E	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	83	Total	O	0	0
			83	83		
5	B	73	Total	O	0	0
			73	73		
5	C	58	Total	O	0	0
			58	58		
5	D	49	Total	O	0	0
			49	49		
5	E	84	Total	O	0	0
			84	84		
5	F	66	Total	O	0	0
			66	66		

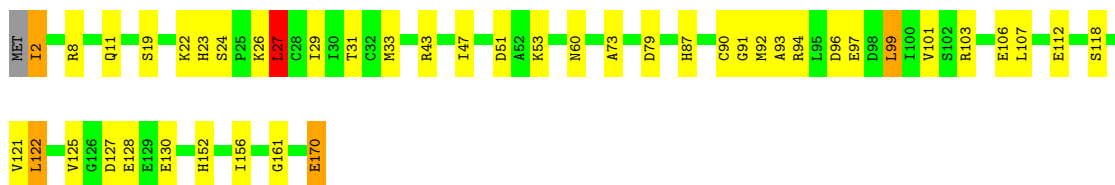
3 Residue-property plots

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

Note EDS was not executed.

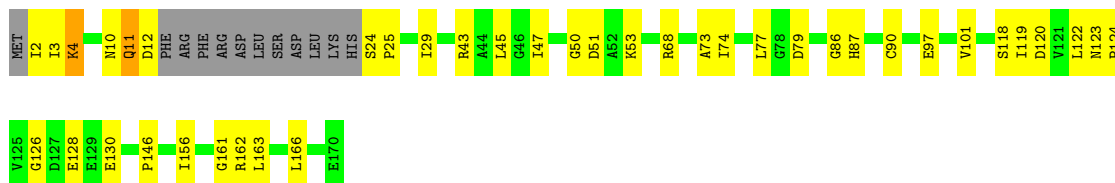
• Molecule 1: BETA-CARBONIC ANHYDRASE

Chain A: 



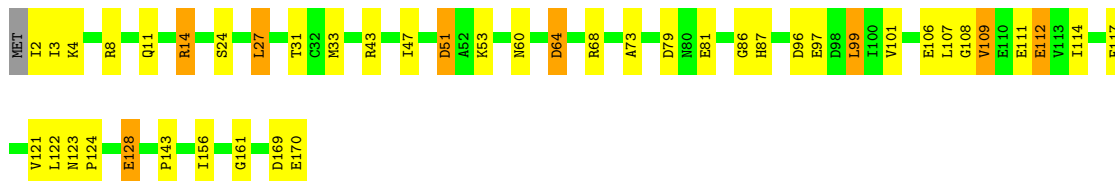
• Molecule 1: BETA-CARBONIC ANHYDRASE

Chain B: 



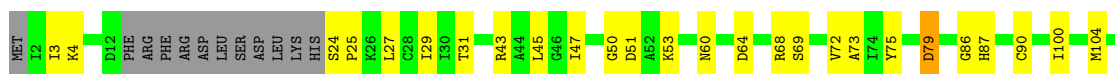
• Molecule 1: BETA-CARBONIC ANHYDRASE

Chain C: 



• Molecule 1: BETA-CARBONIC ANHYDRASE

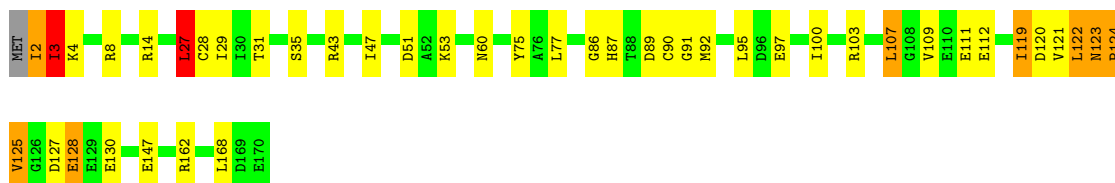
Chain D: 





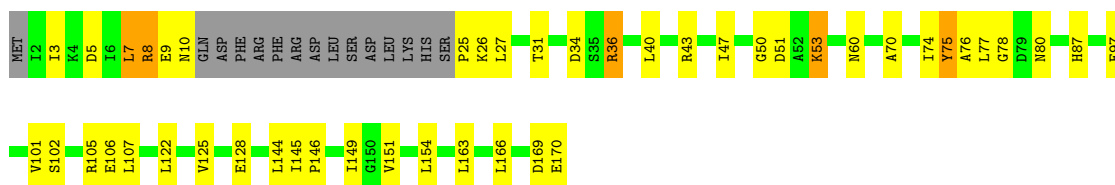
• Molecule 1: BETA-CARBONIC ANHYDRASE

Chain E: 74% 20% 5% ..



• Molecule 1: BETA-CARBONIC ANHYDRASE

Chain F: 64% 24% 9%



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	54.67Å 113.21Å 156.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	18.00 – 2.10	Depositor
% Data completeness (in resolution range)	98.8 (18.00-2.10)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.211 , 0.248	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8010	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

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: EPE, CA, ZN

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	3.24	1/1323 (0.1%)	0.97	4/1783 (0.2%)
1	B	0.53	0/1218	0.94	3/1642 (0.2%)
1	C	0.48	0/1323	0.95	6/1783 (0.3%)
1	D	0.46	0/1218	0.93	2/1642 (0.1%)
1	E	0.61	0/1323	1.09	13/1783 (0.7%)
1	F	0.48	0/1195	1.03	7/1610 (0.4%)
All	All	1.43	1/7600 (0.0%)	0.99	35/10243 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	170	GLU	C-OXT	116.03	3.55	1.23

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	92	MET	N-CA-C	-8.72	102.40	112.87
1	F	75	TYR	N-CA-C	8.39	120.51	111.36
1	B	11	GLN	N-CA-C	-8.02	103.64	113.19
1	F	145	ILE	CA-C-N	8.01	128.06	119.89
1	F	145	ILE	C-N-CA	8.01	128.06	119.89
1	E	125	VAL	N-CA-C	8.01	118.58	110.82
1	E	111	GLU	N-CA-C	7.43	122.63	112.90
1	F	8	ARG	N-CA-C	6.58	118.14	110.97
1	E	97	GLU	N-CA-C	-6.42	105.33	113.43
1	C	86	GLY	N-CA-C	-6.13	103.21	112.60
1	C	27	LEU	N-CA-C	6.12	119.45	109.59
1	C	51	ASP	N-CA-C	6.08	120.43	112.89
1	A	27	LEU	N-CA-C	6.08	119.73	109.76
1	F	166	LEU	N-CA-C	-6.04	106.55	114.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	112	GLU	N-CA-C	-5.96	106.65	112.97
1	E	122	LEU	N-CA-C	5.87	120.49	112.68
1	D	86	GLY	N-CA-C	-5.85	103.65	112.60
1	C	128	GLU	N-CA-C	5.80	118.09	111.02
1	A	128	GLU	N-CA-C	5.63	120.60	111.37
1	F	53	LYS	N-CA-C	-5.58	101.39	110.20
1	E	119	ILE	CB-CA-C	-5.56	102.17	111.29
1	B	86	GLY	N-CA-C	-5.43	104.28	112.60
1	D	128	GLU	N-CA-C	5.42	117.89	111.33
1	E	128	GLU	N-CA-C	5.39	117.16	111.28
1	E	123	ASN	CA-C-N	5.35	126.53	119.84
1	E	123	ASN	C-N-CA	5.35	126.53	119.84
1	C	106	GLU	N-CA-C	-5.31	105.61	111.71
1	F	122	LEU	N-CA-C	5.30	117.71	110.24
1	B	166	LEU	N-CA-C	-5.26	106.92	113.55
1	E	27	LEU	N-CA-C	5.23	118.27	109.95
1	E	3	ILE	N-CA-C	5.15	116.49	110.62
1	A	53	LYS	N-CA-C	-5.08	101.43	109.96
1	E	86	GLY	N-CA-C	-5.06	104.85	112.60
1	C	53	LYS	N-CA-C	-5.06	101.46	109.96
1	E	51	ASP	N-CA-C	5.02	119.11	112.89

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	1311	0	1341	33	0
1	B	1210	0	1241	41	0
1	C	1311	0	1341	32	0
1	D	1210	0	1241	32	0
1	E	1311	0	1341	28	0
1	F	1187	0	1225	29	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	15	0	17	3	0
4	C	15	0	17	0	0
4	E	15	0	17	5	0
5	A	83	0	0	2	0
5	B	73	0	0	1	0
5	C	58	0	0	4	0
5	D	49	0	0	0	0
5	E	84	0	0	0	0
5	F	66	0	0	1	0
All	All	8010	0	7781	177	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 12.

All (177) 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:D:24:SER:HB2	1:D:25:PRO:HD3	1.44	0.97
1:A:118:SER:HA	1:A:122:LEU:HD23	1.50	0.94
1:C:8:ARG:O	1:C:11:GLN:HG2	1.70	0.90
1:E:2:ILE:HD12	1:E:3:ILE:HD12	1.58	0.85
1:C:73:ALA:HB1	1:C:79:ASP:OD1	1.76	0.85
1:A:24:SER:HB2	5:A:2266:HOH:O	1.77	0.84
1:C:24:SER:HB2	5:C:2226:HOH:O	1.76	0.84
1:A:73:ALA:HB1	1:A:79:ASP:OD1	1.77	0.83
1:B:29:ILE:HD11	1:B:47:ILE:HD13	1.61	0.83
1:D:47:ILE:HG23	1:D:51:ASP:HB2	1.59	0.81
1:B:4:LYS:CE	1:B:4:LYS:H	1.94	0.81
1:A:8:ARG:O	1:A:11:GLN:HG2	1.80	0.81
1:B:4:LYS:H	1:B:4:LYS:HE3	1.45	0.80
1:F:47:ILE:HG23	1:F:51:ASP:HB2	1.63	0.79
4:A:2201:EPE:O1S	1:B:25:PRO:HD2	1.85	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:27:LEU:HD23	1:E:28:CYS:N	2.02	0.75
1:A:152:HIS:HE1	1:A:170:GLU:HG3	1.51	0.73
1:B:29:ILE:HD11	1:B:47:ILE:CD1	2.18	0.73
1:F:34:ASP:OD1	1:F:36:ARG:HD3	1.88	0.73
1:F:25:PRO:HG3	1:F:50:GLY:O	1.88	0.73
1:B:73:ALA:O	1:B:79:ASP:HB2	1.89	0.72
1:C:64:ASP:O	1:C:68:ARG:HG2	1.89	0.72
1:E:92:MET:HG3	1:F:76:ALA:HB1	1.71	0.72
1:A:152:HIS:CE1	1:A:170:GLU:HG3	2.25	0.71
1:C:97:GLU:HG3	1:C:122:LEU:HD13	1.73	0.71
1:D:119:ILE:HA	1:D:123:ASN:ND2	2.06	0.69
1:E:29:ILE:HD11	1:E:47:ILE:CD1	2.23	0.69
1:C:68:ARG:HH11	1:C:68:ARG:HG3	1.58	0.68
1:A:130:GLU:HG2	1:E:147:GLU:OE2	1.93	0.68
1:D:25:PRO:HG3	1:D:50:GLY:O	1.94	0.68
1:B:2:ILE:N	1:B:4:LYS:HZ1	1.91	0.67
1:E:2:ILE:HD12	1:E:4:LYS:H	1.60	0.65
1:E:103:ARG:O	1:E:107:LEU:HB2	1.96	0.65
1:C:33:MET:CE	1:D:73:ALA:HB2	2.27	0.64
1:E:87:HIS:CE1	1:E:90:CYS:HB2	2.33	0.63
1:B:25:PRO:HG3	1:B:50:GLY:O	1.99	0.63
1:C:101:VAL:HG13	1:C:114:ILE:HG21	1.80	0.63
1:C:14:ARG:CG	1:C:14:ARG:HH11	2.14	0.61
1:D:29:ILE:HD11	1:D:47:ILE:HD13	1.84	0.60
1:D:73:ALA:O	1:D:79:ASP:HB2	2.01	0.59
1:E:27:LEU:HD23	1:E:28:CYS:H	1.66	0.59
1:C:117:PHE:CE1	1:C:121:VAL:HG21	2.37	0.59
1:B:43:ARG:HH11	1:B:43:ARG:HG3	1.68	0.59
1:A:33:MET:HE3	1:B:53:LYS:HB3	1.85	0.58
1:C:14:ARG:HH11	1:C:14:ARG:HG3	1.69	0.58
1:D:24:SER:CB	1:D:25:PRO:HD3	2.27	0.58
1:A:47:ILE:HG23	1:A:51:ASP:HB2	1.85	0.58
1:B:45:LEU:HD23	1:B:163:LEU:HD11	1.85	0.58
1:E:122:LEU:C	1:E:124:PRO:HD3	2.29	0.58
1:A:91:GLY:C	1:A:93:ALA:N	2.58	0.58
1:A:103:ARG:O	1:A:106:GLU:HB3	2.04	0.58
1:B:122:LEU:C	1:B:124:PRO:HD3	2.28	0.57
1:C:111:GLU:HB2	5:C:2260:HOH:O	2.04	0.57
1:F:144:LEU:O	1:F:146:PRO:HD3	2.05	0.57
1:C:112:GLU:N	5:C:2260:HOH:O	2.37	0.57
1:D:156:ILE:HD11	1:D:161:GLY:HA2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:2201:EPE:O2S	1:B:53:LYS:HE3	2.05	0.56
1:A:121:VAL:CG2	1:B:68:ARG:HD2	2.35	0.56
1:D:119:ILE:HA	1:D:123:ASN:HD21	1.69	0.56
1:B:10:ASN:C	1:B:12:ASP:H	2.12	0.56
1:C:2:ILE:O	1:C:2:ILE:HG13	2.04	0.55
1:B:123:ASN:N	1:B:124:PRO:HD3	2.21	0.55
1:F:87:HIS:O	1:F:128:GLU:HG2	2.06	0.55
1:B:118:SER:HA	1:B:122:LEU:HG	1.89	0.55
1:E:87:HIS:O	1:E:128:GLU:HG2	2.06	0.55
1:A:33:MET:CE	1:B:53:LYS:HB3	2.37	0.55
1:E:100:ILE:HG23	1:F:75:TYR:HB3	1.89	0.55
1:A:97:GLU:O	1:A:101:VAL:HG23	2.07	0.55
1:E:35:SER:OG	4:E:2203:EPE:O1S	2.23	0.54
1:F:10:ASN:ND2	1:F:163:LEU:HG	2.21	0.54
1:A:31:THR:C	1:A:60:ASN:HB3	2.33	0.54
1:E:91:GLY:HA3	1:E:125:VAL:HG11	1.90	0.54
1:A:96:ASP:CG	1:A:99:LEU:HB2	2.33	0.53
1:E:31:THR:C	1:E:60:ASN:HB3	2.34	0.53
1:E:127:ASP:HB2	1:E:130:GLU:HG2	1.89	0.53
1:A:33:MET:HE2	1:B:53:LYS:HG2	1.88	0.53
1:F:169:ASP:O	1:F:170:GLU:CB	2.56	0.53
1:B:10:ASN:C	1:B:12:ASP:N	2.66	0.53
1:C:31:THR:C	1:C:60:ASN:HB3	2.34	0.53
1:C:97:GLU:O	1:C:101:VAL:HG23	2.09	0.53
1:C:107:LEU:HD12	1:D:75:TYR:HE2	1.73	0.53
1:A:91:GLY:C	1:A:93:ALA:H	2.17	0.52
1:B:126:GLY:HA2	1:B:130:GLU:OE2	2.10	0.52
1:F:169:ASP:O	1:F:170:GLU:HB3	2.10	0.52
1:C:128:GLU:HB2	5:C:2234:HOH:O	2.09	0.52
1:E:27:LEU:HD22	1:E:29:ILE:HG13	1.92	0.52
1:A:127:ASP:H	1:A:130:GLU:CD	2.17	0.52
1:C:68:ARG:HG3	1:C:68:ARG:NH1	2.25	0.51
4:E:2203:EPE:O2S	1:F:53:LYS:HE3	2.09	0.51
1:F:151:VAL:O	1:F:169:ASP:HB2	2.10	0.51
1:D:64:ASP:O	1:D:68:ARG:HG3	2.11	0.51
1:F:169:ASP:OD2	1:F:170:GLU:N	2.40	0.50
1:C:47:ILE:HG23	1:C:51:ASP:HB2	1.92	0.50
1:F:97:GLU:O	1:F:101:VAL:HG23	2.11	0.50
1:D:68:ARG:O	1:D:72:VAL:HG23	2.11	0.50
1:E:107:LEU:HD21	1:F:149:ILE:HD11	1.93	0.50
1:D:31:THR:C	1:D:60:ASN:HB3	2.37	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:ILE:HD11	1:B:161:GLY:HA2	1.95	0.49
1:F:26:LYS:HG2	1:F:78:GLY:O	2.12	0.49
1:B:73:ALA:HA	1:B:77:LEU:HD12	1.95	0.49
1:A:33:MET:HE1	1:B:73:ALA:HB2	1.94	0.48
1:D:25:PRO:O	1:D:53:LYS:NZ	2.46	0.48
4:E:2203:EPE:O8	4:E:2203:EPE:H32	2.13	0.48
1:B:118:SER:HA	1:B:122:LEU:CG	2.43	0.48
1:C:108:GLY:O	1:C:109:VAL:C	2.57	0.48
1:B:87:HIS:CE1	1:B:90:CYS:HA	2.48	0.48
1:F:80:ASN:HA	1:F:149:ILE:HD12	1.95	0.48
1:B:4:LYS:HE3	1:B:4:LYS:N	2.22	0.48
1:B:74:ILE:HA	1:B:79:ASP:HB3	1.94	0.48
1:C:14:ARG:CG	1:C:14:ARG:NH1	2.73	0.48
1:D:47:ILE:HG23	1:D:51:ASP:CB	2.37	0.48
1:D:3:ILE:HD11	1:D:154:LEU:HD21	1.96	0.48
1:D:152:HIS:CE1	1:D:169:ASP:H	2.32	0.48
1:B:43:ARG:HG3	1:B:43:ARG:NH1	2.28	0.47
1:F:31:THR:C	1:F:60:ASN:HB3	2.39	0.47
1:E:29:ILE:HD11	1:E:47:ILE:HD12	1.97	0.47
1:D:87:HIS:CE1	1:D:90:CYS:HA	2.50	0.47
1:C:96:ASP:OD1	1:C:99:LEU:HB2	2.14	0.47
1:D:24:SER:HB2	1:D:25:PRO:CD	2.29	0.47
1:E:27:LEU:CD2	1:E:28:CYS:N	2.76	0.46
1:A:2:ILE:HB	1:C:81:GLU:OE1	2.16	0.46
1:C:96:ASP:CG	1:C:99:LEU:HB2	2.40	0.46
1:A:121:VAL:HG22	1:B:68:ARG:HD2	1.97	0.46
1:B:10:ASN:HB2	1:B:163:LEU:HD12	1.98	0.46
1:B:11:GLN:O	1:B:12:ASP:HB2	2.16	0.46
1:B:87:HIS:O	1:B:128:GLU:HG2	2.16	0.46
1:D:140:LYS:NZ	1:D:169:ASP:OD2	2.49	0.46
1:F:5:ASP:O	1:F:8:ARG:HB3	2.16	0.45
1:F:105:ARG:NH1	5:F:1043:HOH:O	2.46	0.45
1:B:47:ILE:HG23	1:B:51:ASP:HB2	1.98	0.45
4:A:2201:EPE:O1S	1:B:25:PRO:CD	2.62	0.44
1:A:156:ILE:HD11	1:A:161:GLY:HA2	1.99	0.44
1:C:33:MET:HE1	1:D:69:SER:O	2.17	0.44
1:C:143:PRO:HB2	1:D:113:VAL:HG21	2.00	0.44
1:F:102:SER:O	1:F:106:GLU:HG3	2.17	0.44
1:B:3:ILE:HG22	1:B:4:LYS:HE2	1.99	0.44
1:F:170:GLU:OXT	1:F:170:GLU:HG2	2.18	0.43
1:C:156:ILE:HD11	1:C:161:GLY:HA2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:29:ILE:HD11	1:D:47:ILE:CD1	2.48	0.43
1:F:7:LEU:HD12	1:F:7:LEU:HA	1.84	0.43
1:A:19:SER:HA	1:A:26:LYS:HD2	2.00	0.43
1:E:89:ASP:OD1	4:E:2203:EPE:H71	2.18	0.43
1:B:162:ARG:HG2	5:B:1073:HOH:O	2.17	0.43
1:A:33:MET:CE	1:B:73:ALA:HB2	2.48	0.43
4:E:2203:EPE:O8	4:E:2203:EPE:C3	2.65	0.43
1:F:5:ASP:O	1:F:8:ARG:CB	2.66	0.42
1:A:23:HIS:CE1	1:D:43:ARG:HH11	2.36	0.42
1:D:73:ALA:C	1:D:79:ASP:HB2	2.43	0.42
1:B:97:GLU:O	1:B:101:VAL:HG23	2.18	0.42
1:D:3:ILE:HG23	1:D:4:LYS:N	2.34	0.42
1:B:119:ILE:HA	1:B:123:ASN:ND2	2.34	0.42
1:E:123:ASN:N	1:E:124:PRO:HD3	2.35	0.42
1:D:100:ILE:O	1:D:104:MET:HG3	2.20	0.42
1:C:101:VAL:HG13	1:C:114:ILE:CG2	2.50	0.42
1:E:3:ILE:H	1:E:3:ILE:HG13	1.55	0.42
1:F:3:ILE:HD11	1:F:154:LEU:HD21	2.01	0.42
1:E:103:ARG:HG2	1:F:75:TYR:HA	2.02	0.41
1:C:3:ILE:HG23	1:C:4:LYS:N	2.35	0.41
1:E:53:LYS:HE3	1:E:77:LEU:HD13	2.02	0.41
1:C:87:HIS:O	1:C:128:GLU:HG2	2.20	0.41
1:A:103:ARG:O	1:A:107:LEU:HD23	2.20	0.41
1:A:107:LEU:HD22	1:A:107:LEU:N	2.35	0.41
1:F:80:ASN:HA	1:F:149:ILE:CD1	2.50	0.41
1:D:111:GLU:O	1:D:115:GLU:HG3	2.20	0.41
1:E:75:TYR:HE2	1:F:107:LEU:HD12	1.86	0.41
1:E:95:LEU:HD12	1:E:95:LEU:HA	1.84	0.41
1:E:4:LYS:O	1:E:8:ARG:HG3	2.20	0.41
1:A:22:LYS:HG2	1:D:43:ARG:HH12	1.87	0.40
1:A:87:HIS:CE1	1:A:90:CYS:HA	2.56	0.40
1:D:25:PRO:HD2	1:D:53:LYS:NZ	2.36	0.40
1:D:45:LEU:HD23	1:D:163:LEU:HD11	2.02	0.40
1:A:27:LEU:HD22	1:A:29:ILE:HD11	2.02	0.40
1:A:93:ALA:CA	5:A:2232:HOH:O	2.68	0.40
1:C:169:ASP:O	1:C:170:GLU:OXT	2.40	0.40
1:F:70:ALA:O	1:F:74:ILE:HG13	2.21	0.40
1:A:93:ALA:CB	1:A:127:ASP:HA	2.52	0.40
1:B:73:ALA:C	1:B:79:ASP:HB2	2.47	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	167/170 (98%)	157 (94%)	7 (4%)	3 (2%)	6	3
1	B	154/170 (91%)	152 (99%)	2 (1%)	0	100	100
1	C	167/170 (98%)	154 (92%)	10 (6%)	3 (2%)	6	3
1	D	154/170 (91%)	146 (95%)	8 (5%)	0	100	100
1	E	167/170 (98%)	158 (95%)	4 (2%)	5 (3%)	3	1
1	F	151/170 (89%)	142 (94%)	8 (5%)	1 (1%)	18	15
All	All	960/1020 (94%)	909 (95%)	39 (4%)	12 (1%)	9	6

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	125	VAL
1	C	109	VAL
1	C	123	ASN
1	E	121	VAL
1	A	94	ARG
1	E	119	ILE
1	E	120	ASP
1	A	122	LEU
1	F	125	VAL
1	C	124	PRO
1	E	107	LEU
1	E	124	PRO

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	147/148 (99%)	142 (97%)	5 (3%)	32	35
1	B	136/148 (92%)	132 (97%)	4 (3%)	37	42
1	C	147/148 (99%)	141 (96%)	6 (4%)	27	29
1	D	136/148 (92%)	133 (98%)	3 (2%)	45	53
1	E	147/148 (99%)	139 (95%)	8 (5%)	20	18
1	F	133/148 (90%)	126 (95%)	7 (5%)	20	19
All	All	846/888 (95%)	813 (96%)	33 (4%)	28	31

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ILE
1	A	27	LEU
1	A	43	ARG
1	A	99	LEU
1	A	112	GLU
1	B	4	LYS
1	B	24	SER
1	B	120	ASP
1	B	146	PRO
1	C	14	ARG
1	C	27	LEU
1	C	43	ARG
1	C	64	ASP
1	C	99	LEU
1	C	112	GLU
1	D	27	LEU
1	D	79	ASP
1	D	170	GLU
1	E	2	ILE
1	E	3	ILE
1	E	14	ARG
1	E	27	LEU
1	E	43	ARG
1	E	109	VAL
1	E	162	ARG
1	E	168	LEU
1	F	7	LEU
1	F	9	GLU

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Mol	Chain	Res	Type
1	F	27	LEU
1	F	36	ARG
1	F	40	LEU
1	F	43	ARG
1	F	77	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	11	GLN
1	B	123	ASN
1	D	123	ASN
1	E	123	ASN
1	F	116	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 12 are monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EPE	E	2203	-	15,15,15	1.79	4 (26%)	19,20,20	2.35	6 (31%)
4	EPE	C	2202	-	15,15,15	1.22	1 (6%)	19,20,20	1.09	1 (5%)
4	EPE	A	2201	-	15,15,15	1.49	4 (26%)	19,20,20	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
4	EPE	E	2203	-	-	3/9/19/19	0/1/1/1
4	EPE	C	2202	-	-	2/9/19/19	0/1/1/1
4	EPE	A	2201	-	-	2/9/19/19	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	2203	EPE	C6-N1	4.55	1.59	1.46
4	A	2201	EPE	C9-N1	2.94	1.54	1.47
4	E	2203	EPE	C7-C8	-2.82	1.40	1.51
4	E	2203	EPE	C2-N1	2.64	1.54	1.46
4	A	2201	EPE	C2-N1	2.53	1.53	1.46
4	C	2202	EPE	C6-N1	2.33	1.53	1.46
4	A	2201	EPE	C6-N1	2.30	1.53	1.46
4	E	2203	EPE	C10-S	2.23	1.80	1.77
4	A	2201	EPE	C10-S	2.11	1.80	1.77

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	2203	EPE	C5-N4-C3	5.92	121.59	108.84
4	E	2203	EPE	C3-C2-N1	-4.97	100.64	110.65
4	E	2203	EPE	O8-C8-C7	-3.01	98.83	111.22
4	E	2203	EPE	C7-N4-C3	2.64	118.27	111.24
4	E	2203	EPE	C7-N4-C5	-2.36	104.94	111.24
4	C	2202	EPE	O1S-S-C10	-2.35	103.18	106.73
4	E	2203	EPE	C2-C3-N4	2.27	115.23	110.65

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	2201	EPE	C10-C9-N1-C2
4	E	2203	EPE	C10-C9-N1-C6
4	E	2203	EPE	C8-C7-N4-C3
4	C	2202	EPE	C10-C9-N1-C2
4	C	2202	EPE	C10-C9-N1-C6
4	E	2203	EPE	C10-C9-N1-C2
4	A	2201	EPE	N4-C7-C8-O8

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	2203	EPE	5	0
4	A	2201	EPE	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.