



Full wwPDB X-ray Structure Validation Report ⓘ

May 28, 2020 – 08:31 pm BST

PDB ID : 1TEC
Title : CRYSTALLOGRAPHIC REFINEMENT BY INCORPORATION OF
MOLECULAR DYNAMICS. THE THERMOSTABLE SERINE PROTEASE
THERMITASE COMPLEXED WITH EGLIN-C
Authors : Gros, P.; Dijkstra, B.W.; Hol, W.G.J.
Deposited on : 1989-05-24
Resolution : 2.20 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

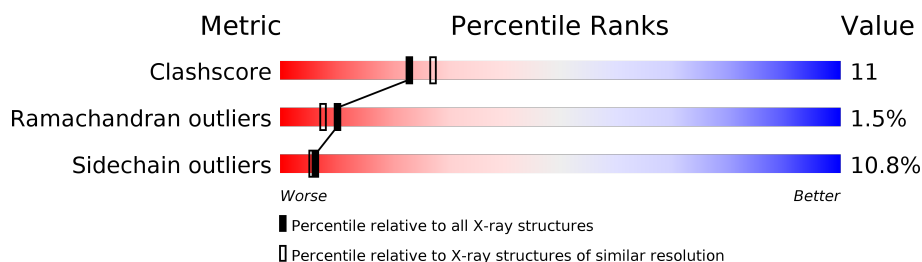
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)

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 on 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	E	279	
2	I	70	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 2737 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 THERMITASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	279	Total	C	N	O	S	0	0	0
			2004	1242	351	409	2			

- Molecule 2 is a protein called EGLIN C.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	I	63	Total	C	N	O	0	0	0
			522	339	89	94			

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	2	Total	Ca	0	0
			2	2		

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	1	Total	Na	0	0
			1	1		

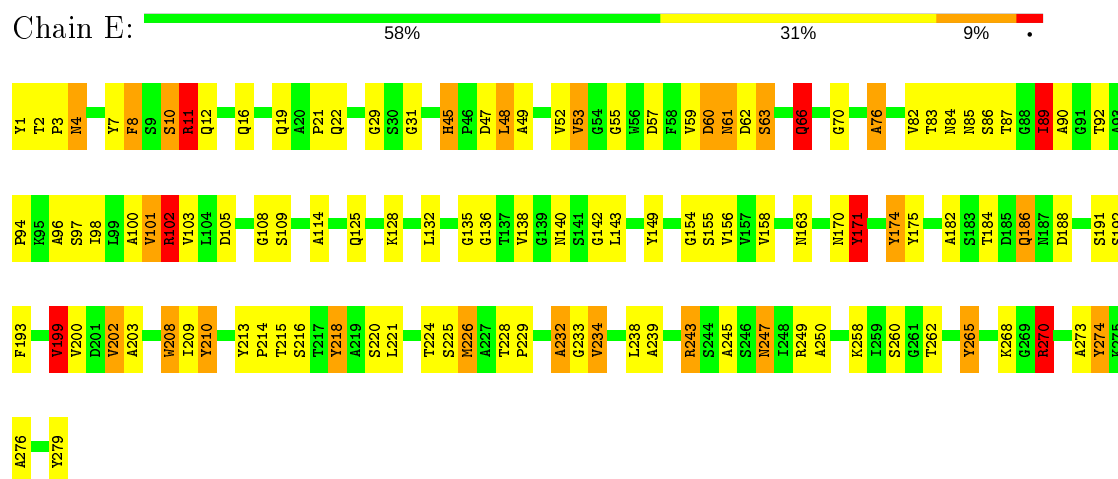
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	166	Total	O	0	0
			166	166		
5	I	42	Total	O	0	0
			42	42		

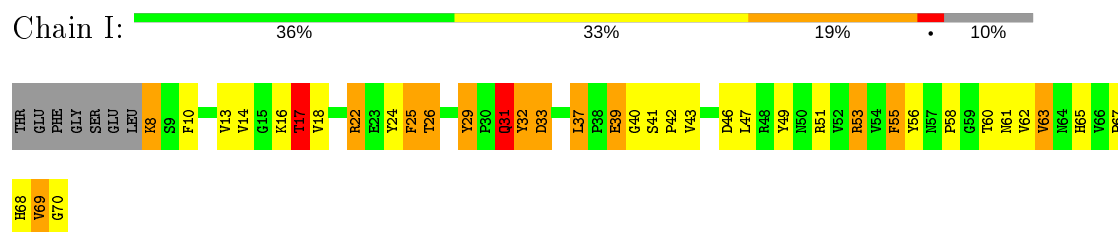
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

• Molecule 1: THERMITASE



• Molecule 2: EGLIN C



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	63.25Å 72.10Å 89.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.20 56.09 – 2.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-2.20) 76.2 (56.09-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.64 (at 2.20Å)	Xtriage
Refinement program	GROMOS	Depositor
R, R_{free}	(Not available) , (Not available) 0.174 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	24.0	Xtriage
Anisotropy	0.902	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 71.3	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	0.95	EDS
Total number of atoms	2737	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 4.98% 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: NA, CA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	E	0.98	0/2049	1.65	27/2805 (1.0%)
2	I	0.99	0/540	1.75	14/738 (1.9%)
All	All	0.98	0/2589	1.67	41/3543 (1.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	43
2	I	0	19
All	All	0	62

There are no bond length outliers.

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	218	TYR	CB-CG-CD1	-10.44	114.74	121.00
1	E	213	TYR	CB-CG-CD2	-10.01	114.99	121.00
1	E	274	TYR	CB-CG-CD1	-8.76	115.75	121.00
1	E	270	ARG	NE-CZ-NH2	-8.61	115.99	120.30
1	E	265	TYR	CB-CG-CD2	-8.29	116.03	121.00
1	E	249	ARG	NE-CZ-NH1	7.66	124.13	120.30
1	E	102	ARG	NE-CZ-NH2	7.07	123.84	120.30
1	E	270	ARG	NE-CZ-NH1	6.94	123.77	120.30
2	I	33	ASP	CB-CG-OD2	-6.68	112.29	118.30
2	I	46	ASP	CB-CG-OD1	-6.43	112.51	118.30
1	E	174	TYR	CB-CG-CD2	-6.38	117.17	121.00
1	E	202	VAL	CA-CB-CG2	6.36	120.44	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	171	TYR	CB-CG-CD1	-6.32	117.20	121.00
2	I	17	THR	N-CA-CB	-6.32	98.29	110.30
2	I	32	TYR	CB-CG-CD2	-6.32	117.21	121.00
1	E	60	ASP	CB-CG-OD2	-6.29	112.64	118.30
1	E	89	ILE	CA-CB-CG2	6.27	123.44	110.90
2	I	56	TYR	CB-CG-CD2	-6.21	117.28	121.00
2	I	37	LEU	N-CA-CB	-6.17	98.07	110.40
2	I	13	VAL	CA-CB-CG2	6.07	120.00	110.90
1	E	213	TYR	CD1-CG-CD2	5.90	124.39	117.90
2	I	53	ARG	NE-CZ-NH2	-5.83	117.39	120.30
1	E	226	MET	CG-SD-CE	5.78	109.45	100.20
2	I	31	GLN	CB-CA-C	-5.71	98.98	110.40
1	E	1	TYR	CB-CG-CD2	-5.70	117.58	121.00
1	E	7	TYR	CB-CG-CD2	-5.63	117.62	121.00
1	E	279	TYR	CB-CG-CD2	-5.52	117.69	121.00
1	E	11	ARG	NH1-CZ-NH2	-5.50	113.35	119.40
1	E	249	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	E	143	LEU	CB-CG-CD2	-5.43	101.78	111.00
1	E	62	ASP	CB-CG-OD2	-5.38	113.45	118.30
2	I	33	ASP	CB-CG-OD1	5.33	123.10	118.30
1	E	210	TYR	CZ-CE2-CD2	-5.32	115.01	119.80
1	E	199	VAL	CG1-CB-CG2	-5.31	102.41	110.90
1	E	213	TYR	CG-CD1-CE1	-5.27	117.09	121.30
2	I	24	TYR	CB-CG-CD2	-5.19	117.89	121.00
2	I	14	VAL	CG1-CB-CG2	-5.18	102.62	110.90
2	I	29	TYR	CB-CG-CD1	-5.17	117.90	121.00
2	I	22	ARG	CG-CD-NE	-5.12	101.04	111.80
1	E	208	TRP	CB-CG-CD1	-5.05	120.44	127.00
1	E	234	VAL	CG1-CB-CG2	-5.01	102.88	110.90

There are no chirality outliers.

All (62) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	101	VAL	Mainchain
1	E	102	ARG	Mainchain
1	E	105	ASP	Mainchain
1	E	108	GLY	Mainchain
1	E	11	ARG	Sidechain
1	E	114	ALA	Mainchain
1	E	132	LEU	Mainchain
1	E	136	GLY	Mainchain

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Mol	Chain	Res	Type	Group
1	E	142	GLY	Mainchain
1	E	149	TYR	Sidechain
1	E	155	SER	Mainchain
1	E	16	GLN	Mainchain
1	E	171	TYR	Sidechain
1	E	174	TYR	Sidechain,Mainchain
1	E	175	TYR	Sidechain
1	E	191	SER	Mainchain
1	E	192	SER	Mainchain
1	E	193	PHE	Sidechain
1	E	209	ILE	Mainchain
1	E	21	PRO	Mainchain
1	E	216	SER	Mainchain
1	E	218	TYR	Sidechain
1	E	232	ALA	Mainchain
1	E	243	ARG	Sidechain
1	E	250	ALA	Mainchain
1	E	258	LYS	Mainchain
1	E	262	THR	Mainchain
1	E	265	TYR	Sidechain
1	E	270	ARG	Mainchain
1	E	3	PRO	Mainchain
1	E	31	GLY	Mainchain
1	E	45	HIS	Sidechain
1	E	52	VAL	Mainchain
1	E	60	ASP	Mainchain
1	E	61	ASN	Mainchain
1	E	63	SER	Mainchain
1	E	66	GLN	Mainchain
1	E	70	GLY	Mainchain
1	E	76	ALA	Mainchain
1	E	8	PHE	Sidechain
1	E	84	ASN	Mainchain
1	E	87	THR	Mainchain
2	I	16	LYS	Mainchain
2	I	18	VAL	Mainchain
2	I	25	PHE	Sidechain
2	I	26	THR	Mainchain
2	I	29	TYR	Sidechain
2	I	31	GLN	Mainchain
2	I	32	TYR	Sidechain
2	I	39	GLU	Mainchain

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Mol	Chain	Res	Type	Group
2	I	42	PRO	Mainchain
2	I	43	VAL	Mainchain
2	I	49	TYR	Sidechain
2	I	53	ARG	Sidechain
2	I	55	PHE	Mainchain
2	I	58	PRO	Mainchain
2	I	63	VAL	Mainchain
2	I	65	HIS	Sidechain,Mainchain
2	I	69	VAL	Mainchain
2	I	8	LYS	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	E	2004	0	1909	47	0
2	I	522	0	498	12	1
3	E	2	0	0	0	0
4	E	1	0	0	0	0
5	E	166	0	0	2	2
5	I	42	0	0	2	0
All	All	2737	0	2407	56	2

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 11.

All (56) 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:E:186:GLN:NE2	1:E:186:GLN:H	1.63	0.96
1:E:243:ARG:HD3	1:E:247:ASN:HD22	1.52	0.75
1:E:243:ARG:HD3	1:E:247:ASN:ND2	2.01	0.75
1:E:4:ASN:ND2	1:E:86:SER:H	1.86	0.73
1:E:163:ASN:HD21	1:E:224:THR:H	1.38	0.72
1:E:59:VAL:HG22	1:E:102:ARG:NH1	2.04	0.71
1:E:19:GLN:HE21	1:E:22:GLN:NE2	1.89	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:66:GLN:HE21	1:E:66:GLN:H	1.39	0.70
1:E:138:VAL:HG12	2:I:40:GLY:HA3	1.73	0.70
1:E:208:TRP:HE3	1:E:220:SER:HG	1.44	0.65
1:E:186:GLN:H	1:E:186:GLN:HE21	1.44	0.65
2:I:10:PHE:HB2	2:I:67:PRO:HG2	1.79	0.65
1:E:182:ALA:HB2	1:E:200:VAL:HG11	1.79	0.65
1:E:8:PHE:HA	1:E:12:GLN:HE21	1.62	0.63
1:E:128:LYS:HB2	5:E:473:HOH:O	2.01	0.60
1:E:184:THR:HG23	1:E:203:ALA:HB1	1.84	0.60
1:E:186:GLN:CD	1:E:186:GLN:H	2.07	0.58
2:I:25:PHE:HB3	5:I:78:HOH:O	2.02	0.58
1:E:225:SER:O	1:E:229:PRO:HD3	2.04	0.58
1:E:229:PRO:HA	1:E:232:ALA:HB3	1.85	0.58
1:E:138:VAL:HG12	2:I:40:GLY:CA	2.34	0.56
1:E:220:SER:O	1:E:221:LEU:HD23	2.05	0.56
1:E:76:ALA:HB1	1:E:98:ILE:HD13	1.91	0.53
2:I:60:THR:OG1	2:I:62:VAL:HG22	2.09	0.52
2:I:8:LYS:O	2:I:68:HIS:HB2	2.09	0.52
1:E:47:ASP:O	1:E:82:VAL:HG23	2.09	0.52
1:E:101:VAL:HG12	1:E:103:VAL:HG13	1.92	0.50
1:E:158:VAL:HG12	1:E:228:THR:HG23	1.94	0.50
2:I:22:ARG:O	2:I:26:THR:HG23	2.11	0.50
1:E:199:VAL:HG11	5:E:430:HOH:O	2.14	0.48
1:E:45:HIS:HB3	1:E:48:LEU:HB2	1.96	0.48
1:E:29:GLY:O	1:E:96:ALA:HB2	2.13	0.48
2:I:70:GLY:HA3	5:I:107:HOH:O	2.14	0.47
1:E:186:GLN:N	1:E:186:GLN:NE2	2.47	0.47
1:E:83:THR:HB	1:E:94:PRO:HB3	1.96	0.47
1:E:234:VAL:HG22	1:E:273:ALA:HB2	1.97	0.47
1:E:66:GLN:H	1:E:66:GLN:NE2	2.09	0.46
1:E:238:LEU:HD11	1:E:276:ALA:HB1	1.99	0.45
1:E:55:GLY:HA3	1:E:100:ALA:O	2.17	0.45
1:E:19:GLN:O	1:E:274:TYR:HB2	2.16	0.45
1:E:186:GLN:N	1:E:186:GLN:HE21	2.12	0.44
1:E:128:LYS:HG2	1:E:239:ALA:HB1	2.00	0.44
1:E:208:TRP:HE3	1:E:220:SER:OG	1.97	0.43
2:I:17:THR:HA	2:I:61:ASN:O	2.19	0.43
1:E:92:THR:HB	1:E:233:GLY:HA3	1.99	0.43
1:E:89:ILE:HG23	1:E:90:ALA:O	2.19	0.43
2:I:37:LEU:O	2:I:55:PHE:HA	2.19	0.42
1:E:135:GLY:HA2	1:E:171:TYR:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:154:GLY:O	1:E:245:ALA:HB2	2.19	0.42
2:I:51:ARG:O	2:I:69:VAL:HA	2.20	0.41
1:E:10:SER:O	1:E:11:ARG:HG3	2.20	0.41
1:E:214:PRO:HA	1:E:215:THR:HA	1.75	0.41
1:E:57:ASP:C	1:E:57:ASP:OD1	2.60	0.41
1:E:53:VAL:HG13	1:E:97:SER:HB2	2.03	0.40
1:E:4:ASN:C	1:E:4:ASN:HD22	2.24	0.40
1:E:138:VAL:CG1	2:I:40:GLY:HA3	2.48	0.40

All (2) 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)
2:I:62:VAL:CG2	5:E:399:HOH:O[2_455]	2.15	0.05
5:E:429:HOH:O	5:E:459:HOH:O[3_544]	2.19	0.01

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	277/279 (99%)	254 (92%)	18 (6%)	5 (2%)	8	5
2	I	61/70 (87%)	58 (95%)	3 (5%)	0	100	100
All	All	338/349 (97%)	312 (92%)	21 (6%)	5 (2%)	10	8

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	49	ALA
1	E	53	VAL
1	E	61	ASN
1	E	125	GLN

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Mol	Chain	Res	Type
1	E	140	ASN

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	E	202/202 (100%)	181 (90%)	21 (10%)	7	6
2	I	58/64 (91%)	51 (88%)	7 (12%)	5	4
All	All	260/266 (98%)	232 (89%)	28 (11%)	6	6

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	2	THR
1	E	4	ASN
1	E	10	SER
1	E	48	LEU
1	E	63	SER
1	E	66	GLN
1	E	85	ASN
1	E	89	ILE
1	E	109	SER
1	E	156	VAL
1	E	170	ASN
1	E	186	GLN
1	E	188	ASP
1	E	199	VAL
1	E	202	VAL
1	E	210	TYR
1	E	226	MET
1	E	247	ASN
1	E	260	SER
1	E	268	LYS
1	E	270	ARG
2	I	17	THR

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Mol	Chain	Res	Type
2	I	31	GLN
2	I	33	ASP
2	I	39	GLU
2	I	41	SER
2	I	47	LEU
2	I	63	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	4	ASN
1	E	12	GLN
1	E	22	GLN
1	E	66	GLN
1	E	85	ASN
1	E	125	GLN
1	E	144	GLN
1	E	148	ASN
1	E	152	ASN
1	E	163	ASN
1	E	177	ASN
1	E	186	GLN
1	E	247	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 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 [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 ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.