



Full wwPDB X-ray Structure Validation Report ⓘ

May 28, 2020 – 08:25 pm BST

PDB ID : 1SBN
Title : REFINED CRYSTAL STRUCTURES OF SUBTILISIN NOVO IN COM-
PLEX WITH WILD-TYPE AND TWO MUTANT EGLINS. COMPARISON
WITH OTHER SERINE PROTEINASE INHIBITOR COMPLEXES
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Deposited on : 1991-12-20
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

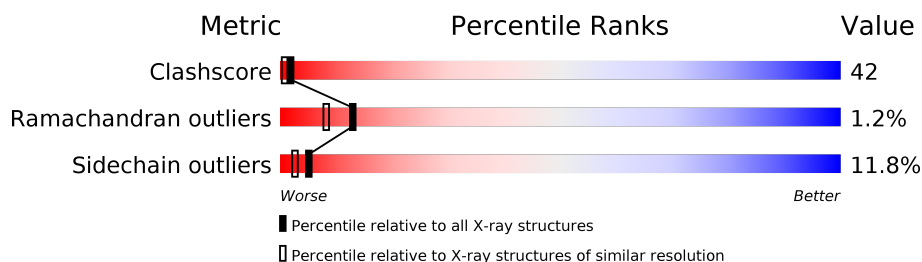
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (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 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	E	275	
2	I	70	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2781 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 SUBTILISIN NOVO BPN'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	275	Total	C	N	O	S	0	0	0
			1938	1204	335	394	5			

- 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
			525	339	93	93			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	33	ASN	ASP	CONFLICT	UNP P01051
I	45	ARG	LEU	CONFLICT	UNP P01051

- 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 water.

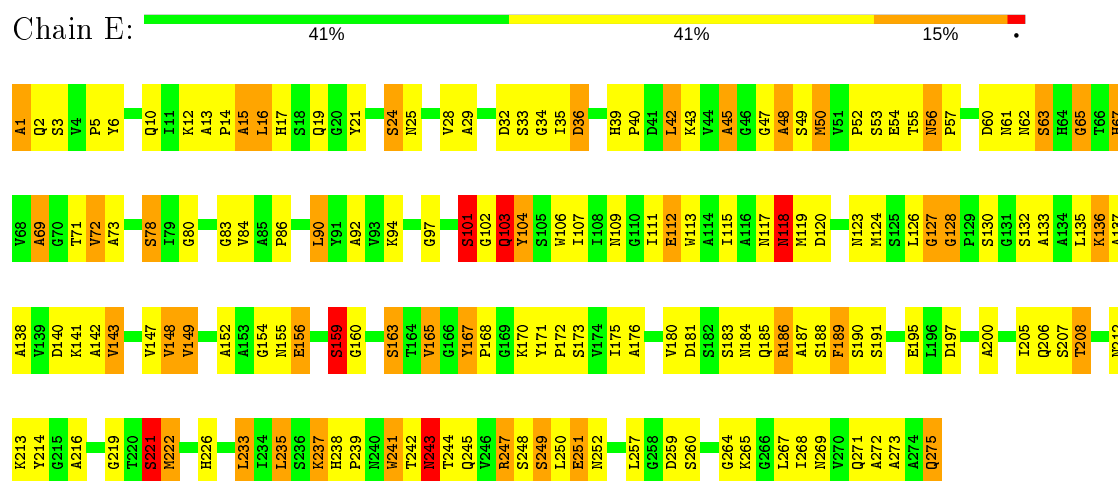
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	255	Total	O	0	0
			255	255		
4	I	61	Total	O	0	0
			61	61		

3 Residue-property plots

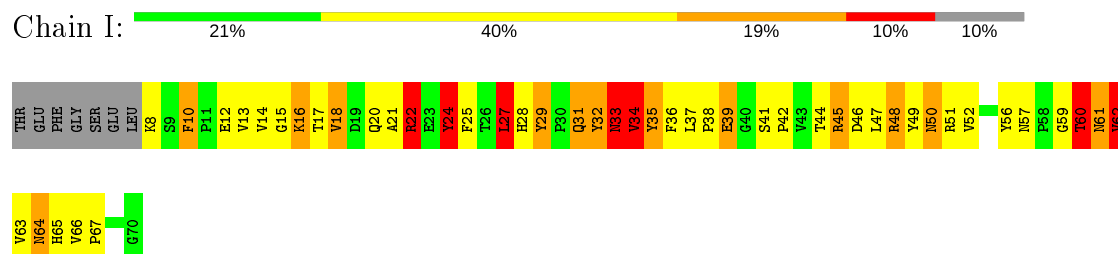
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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

Note EDS was not executed.

• Molecule 1: SUBTILISIN NOVO BPN'



• Molecule 2: EGLIN C



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	84.90 Å 84.90 Å 89.10 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	5.00 – 2.10	Depositor
% Data completeness (in resolution range)	(Not available) (5.00-2.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.186 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2781	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.95	1/1976 (0.1%)	2.22	79/2697 (2.9%)
2	I	0.89	0/543	2.48	35/741 (4.7%)
All	All	0.93	1/2519 (0.0%)	2.28	114/3438 (3.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	221	SER	CB-OG	-5.51	1.35	1.42

All (114) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	186	ARG	NE-CZ-NH2	18.97	129.78	120.30
2	I	48	ARG	NE-CZ-NH1	16.36	128.48	120.30
1	E	186	ARG	CD-NE-CZ	14.32	143.65	123.60
2	I	22	ARG	CD-NE-CZ	12.42	140.99	123.60
2	I	51	ARG	NE-CZ-NH1	-10.83	114.89	120.30
2	I	22	ARG	NE-CZ-NH1	10.71	125.66	120.30
1	E	221	SER	CA-CB-OG	10.09	138.43	111.20
1	E	73	ALA	N-CA-CB	-9.16	97.28	110.10
2	I	32	TYR	CB-CG-CD2	-8.99	115.61	121.00
1	E	156	GLU	CG-CD-OE2	-8.84	100.63	118.30
1	E	118	ASN	CA-CB-CG	8.53	132.17	113.40
1	E	48	ALA	N-CA-CB	-8.37	98.39	110.10
1	E	156	GLU	OE1-CD-OE2	8.29	133.25	123.30
1	E	24	SER	N-CA-CB	8.03	122.55	110.50
2	I	45	ARG	NE-CZ-NH2	-7.79	116.40	120.30
2	I	49	TYR	CB-CG-CD1	-7.79	116.33	121.00
2	I	46	ASP	CB-CG-OD2	-7.68	111.39	118.30
1	E	101	SER	O-C-N	7.49	135.93	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	49	TYR	CB-CG-CD2	7.33	125.40	121.00
1	E	152	ALA	N-CA-CB	-7.28	99.91	110.10
2	I	34	VAL	CB-CA-C	7.20	125.08	111.40
2	I	35	TYR	O-C-N	7.01	133.92	122.70
1	E	272	ALA	N-CA-CB	6.93	119.80	110.10
1	E	237	LYS	N-CA-CB	6.90	123.03	110.60
1	E	251	GLU	OE1-CD-OE2	6.85	131.52	123.30
1	E	32	ASP	CB-CG-OD1	6.83	124.44	118.30
1	E	101	SER	N-CA-CB	6.77	120.66	110.50
2	I	51	ARG	CD-NE-CZ	6.68	132.95	123.60
2	I	60	THR	CA-CB-CG2	6.50	121.50	112.40
2	I	16	LYS	CA-C-O	6.49	133.73	120.10
1	E	120	ASP	CB-CG-OD2	-6.39	112.55	118.30
2	I	62	VAL	CA-CB-CG1	-6.37	101.34	110.90
1	E	250	LEU	CA-CB-CG	6.36	129.92	115.30
1	E	167	TYR	CB-CG-CD2	6.33	124.80	121.00
1	E	42	LEU	CA-CB-CG	6.33	129.85	115.30
1	E	167	TYR	CB-CG-CD1	-6.26	117.24	121.00
1	E	233	LEU	O-C-N	6.26	132.71	122.70
1	E	159	SER	N-CA-CB	6.25	119.87	110.50
2	I	35	TYR	CB-CG-CD1	-6.22	117.27	121.00
2	I	27	LEU	O-C-N	6.17	132.57	122.70
1	E	186	ARG	NH1-CZ-NH2	-6.15	112.64	119.40
2	I	35	TYR	CB-CG-CD2	6.10	124.66	121.00
1	E	213	LYS	C-N-CA	6.10	136.94	121.70
1	E	176	ALA	CB-CA-C	6.07	119.20	110.10
2	I	44	THR	CA-CB-CG2	6.02	120.83	112.40
1	E	165	VAL	CG1-CB-CG2	-6.02	101.27	110.90
1	E	148	VAL	CA-CB-CG2	5.99	119.88	110.90
1	E	208	THR	CA-CB-OG1	-5.96	96.47	109.00
1	E	71	THR	CA-CB-OG1	-5.93	96.54	109.00
2	I	33	ASN	CB-CA-C	5.92	122.25	110.40
1	E	19	GLN	CA-CB-CG	5.92	126.42	113.40
1	E	25	ASN	CA-CB-CG	-5.92	100.39	113.40
2	I	35	TYR	CA-C-O	-5.91	107.68	120.10
1	E	128	GLY	O-C-N	5.90	132.31	121.10
2	I	29	TYR	CB-CG-CD1	-5.89	117.46	121.00
1	E	36	ASP	CB-CG-OD2	5.87	123.58	118.30
2	I	18	VAL	CG1-CB-CG2	5.86	120.27	110.90
2	I	32	TYR	CA-CB-CG	5.84	124.50	113.40
1	E	247	ARG	NE-CZ-NH2	5.78	123.19	120.30
1	E	132	SER	CB-CA-C	-5.74	99.20	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	140	ASP	CB-CG-OD1	-5.73	113.14	118.30
2	I	45	ARG	O-C-N	-5.72	113.55	122.70
2	I	48	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	E	249	SER	O-C-N	5.67	131.78	122.70
1	E	269	ASN	O-C-N	5.66	131.75	122.70
1	E	140	ASP	C-N-CA	5.64	135.81	121.70
1	E	33	SER	O-C-N	5.63	132.77	123.20
1	E	103	GLN	O-C-N	5.62	131.69	122.70
2	I	48	ARG	N-CA-CB	5.62	120.71	110.60
1	E	190	SER	CB-CA-C	5.60	120.73	110.10
1	E	42	LEU	O-C-N	5.58	131.62	122.70
1	E	45	ALA	CB-CA-C	-5.58	101.73	110.10
2	I	32	TYR	CB-CG-CD1	5.57	124.34	121.00
2	I	24	TYR	CB-CG-CD1	-5.57	117.66	121.00
1	E	163	SER	N-CA-CB	5.55	118.83	110.50
1	E	15	ALA	O-C-N	5.47	131.45	122.70
1	E	186	ARG	NE-CZ-NH1	-5.45	117.58	120.30
2	I	22	ARG	CB-CG-CD	5.43	125.72	111.60
1	E	90	LEU	N-CA-CB	-5.42	99.55	110.40
1	E	243	ASN	CA-C-O	-5.42	108.72	120.10
1	E	219	GLY	O-C-N	5.41	131.36	122.70
1	E	200	ALA	O-C-N	5.40	131.36	121.10
1	E	69	ALA	N-CA-CB	5.40	117.66	110.10
1	E	175	ILE	CA-CB-CG2	5.39	121.69	110.90
1	E	104	TYR	CB-CG-CD1	5.39	124.23	121.00
1	E	72	VAL	CG1-CB-CG2	-5.35	102.34	110.90
1	E	259	ASP	C-N-CA	5.33	135.01	121.70
1	E	127	GLY	O-C-N	5.32	132.24	123.20
1	E	103	GLN	N-CA-CB	5.29	120.12	110.60
2	I	33	ASN	CA-CB-CG	5.27	124.99	113.40
1	E	112	GLU	CA-CB-CG	5.26	124.98	113.40
1	E	67	HIS	O-C-N	-5.26	114.28	122.70
1	E	251	GLU	CG-CD-OE1	-5.26	107.78	118.30
1	E	65	GLY	C-N-CA	5.26	134.84	121.70
1	E	136	LYS	CA-C-O	-5.24	109.10	120.10
2	I	48	ARG	CD-NE-CZ	5.24	130.93	123.60
1	E	123	ASN	CA-C-O	-5.22	109.14	120.10
1	E	73	ALA	N-CA-C	5.21	125.08	111.00
1	E	149	VAL	O-C-N	5.19	131.00	122.70
1	E	19	GLN	N-CA-CB	5.18	119.93	110.60
1	E	235	LEU	CA-CB-CG	5.18	127.22	115.30
1	E	188	SER	CB-CA-C	5.17	119.92	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	51	ARG	NE-CZ-NH2	5.17	122.89	120.30
1	E	104	TYR	CB-CG-CD2	-5.16	117.90	121.00
1	E	268	ILE	CG1-CB-CG2	5.15	122.73	111.40
1	E	73	ALA	CA-C-N	5.14	128.50	117.20
1	E	78	SER	N-CA-CB	-5.12	102.82	110.50
1	E	208	THR	CA-CB-CG2	5.11	119.56	112.40
2	I	62	VAL	CA-CB-CG2	5.11	118.57	110.90
2	I	37	LEU	CA-CB-CG	5.06	126.93	115.30
1	E	189	PHE	O-C-N	-5.04	114.63	122.70
1	E	247	ARG	CG-CD-NE	-5.04	101.21	111.80
1	E	143	VAL	CA-C-O	-5.02	109.56	120.10
1	E	1	ALA	O-C-N	5.01	130.72	122.70

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	E	1938	0	1899	147	1
2	I	525	0	502	62	0
3	E	2	0	0	0	0
4	E	255	0	0	33	5
4	I	61	0	0	7	0
All	All	2781	0	2401	205	5

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 42.

All (205) 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:130:SER:HB3	4:E:523:HOH:O	1.31	1.25
1:E:103:GLN:HG3	4:E:395:HOH:O	1.51	1.09
1:E:133:ALA:HA	4:E:416:HOH:O	1.68	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:52:PRO:HD2	4:E:457:HOH:O	1.68	0.92
2:I:27:LEU:HD23	4:I:587:HOH:O	1.69	0.91
1:E:165:VAL:O	1:E:170:LYS:HD2	1.71	0.91
1:E:1:ALA:HA	1:E:78:SER:O	1.72	0.89
1:E:40:PRO:HD3	1:E:212:ASN:OD1	1.74	0.87
1:E:138:ALA:HA	1:E:141:LYS:HE2	1.55	0.86
1:E:13:ALA:N	1:E:14:PRO:HD2	1.89	0.86
1:E:62:ASN:O	1:E:63:SER:HB3	1.75	0.84
1:E:136:LYS:HG3	1:E:136:LYS:O	1.78	0.83
2:I:31:GLN:H	2:I:31:GLN:NE2	1.77	0.82
1:E:136:LYS:O	1:E:136:LYS:CG	2.27	0.82
2:I:8:LYS:N	4:I:325:HOH:O	2.13	0.80
2:I:60:THR:O	2:I:62:VAL:HG22	1.82	0.80
1:E:242:THR:H	1:E:245:GLN:HE21	1.29	0.78
2:I:29:TYR:HD1	2:I:31:GLN:OE1	1.66	0.78
1:E:12:LYS:C	1:E:14:PRO:HD2	2.03	0.77
1:E:13:ALA:N	1:E:14:PRO:CD	2.45	0.77
1:E:242:THR:H	1:E:245:GLN:NE2	1.84	0.75
1:E:275:GLN:HE21	1:E:275:GLN:N	1.83	0.75
1:E:10:GLN:HE21	1:E:184:ASN:ND2	1.84	0.74
2:I:16:LYS:HB3	2:I:20:GLN:HB2	1.69	0.74
1:E:133:ALA:CA	4:E:416:HOH:O	2.32	0.72
1:E:62:ASN:O	1:E:63:SER:CB	2.39	0.71
1:E:15:ALA:CB	1:E:271:GLN:HG3	2.22	0.70
2:I:39:GLU:OE1	2:I:64:ASN:OD1	2.11	0.69
1:E:238:HIS:HD2	1:E:241:TRP:CZ3	2.11	0.68
1:E:271:GLN:NE2	4:E:407:HOH:O	2.27	0.67
1:E:10:GLN:HE21	1:E:184:ASN:HD21	1.40	0.67
1:E:102:GLY:O	2:I:42:PRO:HD2	1.95	0.66
1:E:248:SER:O	1:E:252:ASN:N	2.29	0.66
1:E:239:PRO:HG2	4:E:555:HOH:O	1.97	0.64
1:E:275:GLN:CA	1:E:275:GLN:HE21	2.10	0.64
1:E:16:LEU:HD13	1:E:21:TYR:HB2	1.80	0.64
1:E:195:GLU:OE2	4:E:441:HOH:O	2.15	0.64
1:E:16:LEU:HD13	1:E:21:TYR:CB	2.27	0.64
1:E:83:GLY:O	1:E:86:PRO:HD3	1.98	0.63
1:E:181:ASP:OD2	4:E:359:HOH:O	2.16	0.63
2:I:60:THR:HB	2:I:62:VAL:HG23	1.81	0.62
2:I:16:LYS:HB3	2:I:20:GLN:CB	2.28	0.62
2:I:48:ARG:HD3	4:I:410:HOH:O	2.00	0.62
1:E:103:GLN:HA	4:E:436:HOH:O	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:10:GLN:NE2	1:E:184:ASN:ND2	2.47	0.62
2:I:50:ASN:H	2:I:50:ASN:HD22	1.46	0.62
1:E:243:ASN:HD22	1:E:244:THR:N	1.99	0.61
1:E:54:GLU:HB2	1:E:94:LYS:HE2	1.83	0.61
1:E:29:ALA:HB2	1:E:119:MET:HG3	1.82	0.60
1:E:43:LYS:HG2	4:E:482:HOH:O	2.01	0.60
2:I:60:THR:C	2:I:62:VAL:N	2.54	0.60
1:E:195:GLU:OE2	4:E:439:HOH:O	2.16	0.60
1:E:103:GLN:HG2	1:E:106:TRP:CE2	2.37	0.60
1:E:43:LYS:NZ	4:E:496:HOH:O	2.35	0.59
1:E:127:GLY:HA2	1:E:167:TYR:O	2.03	0.59
1:E:247:ARG:HD3	4:E:564:HOH:O	2.03	0.59
1:E:221:SER:HB2	2:I:45:ARG:O	2.03	0.59
1:E:102:GLY:HA2	1:E:106:TRP:CZ3	2.38	0.58
1:E:137:ALA:O	1:E:141:LYS:HB2	2.04	0.58
2:I:60:THR:C	2:I:62:VAL:H	2.08	0.57
2:I:60:THR:O	2:I:62:VAL:N	2.36	0.57
1:E:148:VAL:HG22	1:E:243:ASN:HB2	1.87	0.57
2:I:60:THR:HG22	2:I:62:VAL:CG2	2.34	0.57
2:I:60:THR:CB	2:I:62:VAL:HG23	2.36	0.56
2:I:59:GLY:C	2:I:61:ASN:N	2.57	0.56
1:E:130:SER:CB	4:E:523:HOH:O	2.11	0.56
2:I:59:GLY:HA2	4:I:593:HOH:O	2.05	0.55
2:I:64:ASN:ND2	2:I:65:HIS:ND1	2.54	0.55
1:E:136:LYS:HB2	1:E:171:TYR:CZ	2.42	0.55
1:E:112:GLU:HG3	4:E:540:HOH:O	2.06	0.54
1:E:205:ILE:O	1:E:216:ALA:HA	2.07	0.54
1:E:238:HIS:CD2	1:E:241:TRP:CZ3	2.96	0.54
2:I:12:GLU:OE1	2:I:24:TYR:OH	2.16	0.54
2:I:31:GLN:H	2:I:31:GLN:HE21	1.54	0.54
2:I:60:THR:O	2:I:62:VAL:CG2	2.54	0.54
1:E:103:GLN:NE2	4:E:481:HOH:O	2.40	0.54
1:E:138:ALA:CA	1:E:141:LYS:HE2	2.36	0.54
1:E:239:PRO:HD2	4:E:555:HOH:O	2.07	0.54
1:E:15:ALA:HB3	1:E:271:GLN:HG3	1.90	0.54
2:I:57:ASN:O	2:I:61:ASN:HA	2.07	0.54
1:E:40:PRO:CD	1:E:212:ASN:OD1	2.52	0.53
1:E:55:THR:O	1:E:57:PRO:HD3	2.08	0.53
1:E:97:GLY:HA3	4:E:332:HOH:O	2.07	0.53
1:E:186:ARG:HG2	1:E:187:ALA:O	2.09	0.53
1:E:17:HIS:NE2	1:E:84:VAL:O	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:107:ILE:O	1:E:111:ILE:HG13	2.10	0.52
1:E:5:PRO:HA	4:E:342:HOH:O	2.10	0.52
2:I:31:GLN:N	2:I:31:GLN:NE2	2.55	0.52
1:E:238:HIS:HD2	1:E:241:TRP:CE3	2.27	0.52
1:E:170:LYS:HE3	4:E:439:HOH:O	2.10	0.52
1:E:28:VAL:HG11	1:E:72:VAL:HG11	1.91	0.52
1:E:170:LYS:NZ	4:E:430:HOH:O	2.43	0.52
1:E:275:GLN:OXT	1:E:275:GLN:NE2	2.43	0.52
1:E:56:ASN:HD22	1:E:56:ASN:C	2.13	0.51
1:E:21:TYR:CZ	1:E:237:LYS:HG3	2.46	0.51
1:E:155:ASN:HA	1:E:189:PHE:O	2.11	0.51
2:I:33:ASN:ND2	4:I:445:HOH:O	2.44	0.51
1:E:60:ASP:OD2	1:E:63:SER:HA	2.11	0.51
1:E:1:ALA:CA	1:E:78:SER:O	2.54	0.50
1:E:128:GLY:N	1:E:167:TYR:O	2.40	0.50
1:E:56:ASN:ND2	1:E:56:ASN:C	2.64	0.50
1:E:124:MET:HE3	1:E:149:VAL:HG13	1.94	0.49
1:E:124:MET:CE	1:E:149:VAL:CG1	2.90	0.49
2:I:17:THR:HG22	2:I:62:VAL:HG13	1.93	0.49
1:E:247:ARG:O	1:E:251:GLU:HG3	2.12	0.49
2:I:59:GLY:C	2:I:61:ASN:H	2.14	0.49
2:I:57:ASN:O	2:I:61:ASN:N	2.46	0.48
1:E:35:ILE:HD13	1:E:69:ALA:HB2	1.96	0.48
1:E:69:ALA:HB1	1:E:90:LEU:HD21	1.95	0.48
1:E:184:ASN:HD21	1:E:267:LEU:HD22	1.79	0.48
1:E:34:GLY:O	1:E:65:GLY:HA3	2.13	0.48
2:I:17:THR:HA	2:I:62:VAL:HA	1.94	0.48
1:E:136:LYS:O	1:E:136:LYS:HG2	2.13	0.48
1:E:21:TYR:O	1:E:233:LEU:HD22	2.13	0.48
2:I:24:TYR:O	2:I:27:LEU:N	2.46	0.48
1:E:133:ALA:CB	4:E:416:HOH:O	2.60	0.48
2:I:22:ARG:HH11	2:I:36:PHE:HE1	1.61	0.48
1:E:141:LYS:HG2	4:E:545:HOH:O	2.13	0.47
2:I:34:VAL:HG12	2:I:52:VAL:HB	1.96	0.47
1:E:2:GLN:HA	1:E:80:GLY:O	2.14	0.47
2:I:21:ALA:O	2:I:22:ARG:C	2.53	0.47
1:E:36:ASP:OD1	1:E:36:ASP:C	2.53	0.47
1:E:111:ILE:O	1:E:115:ILE:N	2.41	0.47
1:E:184:ASN:ND2	1:E:267:LEU:HD22	2.30	0.47
2:I:59:GLY:O	2:I:61:ASN:N	2.48	0.47
1:E:107:ILE:HD13	1:E:126:LEU:CD1	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:48:ALA:C	1:E:57:PRO:HG3	2.36	0.46
1:E:118:ASN:O	4:E:417:HOH:O	2.21	0.46
1:E:12:LYS:CA	1:E:14:PRO:HD2	2.45	0.46
1:E:183:SER:HB2	1:E:185:GLN:HG2	1.98	0.46
2:I:17:THR:HA	2:I:61:ASN:O	2.15	0.46
1:E:165:VAL:O	1:E:170:LYS:CD	2.56	0.46
1:E:35:ILE:HG13	1:E:92:ALA:HB2	1.98	0.46
2:I:50:ASN:H	2:I:50:ASN:ND2	2.11	0.46
1:E:104:TYR:CE1	2:I:42:PRO:HG3	2.50	0.46
2:I:57:ASN:O	2:I:61:ASN:CA	2.64	0.45
1:E:15:ALA:HB1	1:E:271:GLN:HG3	1.99	0.45
2:I:60:THR:HG22	2:I:62:VAL:HG23	1.97	0.45
1:E:35:ILE:HG13	1:E:92:ALA:CB	2.47	0.45
2:I:33:ASN:ND2	2:I:35:TYR:CZ	2.85	0.45
2:I:32:TYR:O	2:I:34:VAL:HG22	2.17	0.45
1:E:275:GLN:CD	1:E:275:GLN:OXT	2.56	0.44
2:I:31:GLN:N	2:I:31:GLN:HE21	2.13	0.44
1:E:101:SER:HB3	2:I:42:PRO:O	2.17	0.44
2:I:59:GLY:O	2:I:60:THR:C	2.56	0.44
1:E:135:LEU:O	1:E:138:ALA:HB3	2.17	0.44
1:E:124:MET:CE	1:E:149:VAL:HG13	2.48	0.44
1:E:60:ASP:OD2	1:E:63:SER:CA	2.66	0.44
1:E:275:GLN:CA	1:E:275:GLN:NE2	2.76	0.44
1:E:127:GLY:CA	1:E:167:TYR:O	2.66	0.44
1:E:163:SER:HB3	4:E:547:HOH:O	2.17	0.44
2:I:20:GLN:NE2	4:I:495:HOH:O	2.51	0.44
2:I:14:VAL:HG23	2:I:66:VAL:HA	2.00	0.44
2:I:57:ASN:ND2	2:I:60:THR:OG1	2.51	0.43
2:I:66:VAL:HA	2:I:67:PRO:HD3	1.82	0.43
1:E:207:SER:O	1:E:214:TYR:HA	2.18	0.43
1:E:249:SER:OG	1:E:273:ALA:O	2.36	0.43
1:E:163:SER:CB	4:E:547:HOH:O	2.66	0.43
2:I:39:GLU:HG2	2:I:39:GLU:O	2.18	0.43
1:E:248:SER:O	1:E:252:ASN:HB2	2.19	0.43
2:I:13:VAL:HG12	2:I:63:VAL:HG11	2.01	0.43
1:E:124:MET:HE3	1:E:149:VAL:CG1	2.49	0.43
1:E:67:HIS:CD2	1:E:207:SER:HB3	2.53	0.43
1:E:238:HIS:CD2	1:E:241:TRP:CE3	3.06	0.43
1:E:115:ILE:HG12	1:E:142:ALA:HA	2.01	0.43
1:E:113:TRP:O	1:E:117:ASN:ND2	2.49	0.42
1:E:207:SER:OG	1:E:208:THR:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:195:GLU:OE2	4:E:501:HOH:O	2.20	0.42
1:E:205:ILE:HG13	1:E:222:MET:HB3	2.00	0.42
1:E:6:TYR:CD1	1:E:6:TYR:C	2.93	0.42
1:E:154:GLY:HA3	4:E:550:HOH:O	2.19	0.42
1:E:61:ASN:CG	4:E:345:HOH:O	2.57	0.42
1:E:156:GLU:HB2	1:E:191:SER:OG	2.19	0.42
1:E:107:ILE:HD13	1:E:126:LEU:HD11	2.01	0.42
1:E:260:SER:HA	1:E:264:GLY:O	2.19	0.42
2:I:10:PHE:CD1	2:I:10:PHE:N	2.87	0.42
1:E:117:ASN:O	1:E:118:ASN:CB	2.67	0.42
2:I:38:PRO:O	2:I:39:GLU:C	2.58	0.42
1:E:197:ASP:O	1:E:265:LYS:HG2	2.20	0.42
1:E:257:LEU:HD11	1:E:267:LEU:HB2	2.02	0.42
1:E:45:ALA:HA	4:E:541:HOH:O	2.19	0.42
1:E:49:SER:C	1:E:50:MET:HG2	2.41	0.42
2:I:60:THR:CG2	2:I:62:VAL:HG23	2.49	0.42
2:I:64:ASN:H	2:I:64:ASN:HD22	1.67	0.41
1:E:54:GLU:OE2	1:E:97:GLY:HA2	2.19	0.41
1:E:273:ALA:C	1:E:275:GLN:H	2.21	0.41
1:E:39:HIS:HA	1:E:40:PRO:HD3	1.83	0.41
1:E:275:GLN:HB3	4:E:344:HOH:O	2.20	0.41
1:E:243:ASN:HD22	1:E:244:THR:H	1.66	0.41
1:E:86:PRO:HG2	4:E:565:HOH:O	2.21	0.41
1:E:248:SER:O	1:E:252:ASN:CB	2.68	0.41
2:I:24:TYR:CE1	2:I:28:HIS:ND1	2.89	0.41
1:E:84:VAL:HG21	1:E:226:HIS:HA	2.02	0.41
2:I:24:TYR:HB3	2:I:25:PHE:H	1.64	0.41
2:I:47:LEU:O	4:I:561:HOH:O	2.21	0.41
2:I:18:VAL:CG2	2:I:56:TYR:CD2	3.03	0.41
1:E:143:VAL:HG22	1:E:147:VAL:O	2.20	0.41
1:E:171:TYR:HA	1:E:172:PRO:HD3	1.93	0.41
1:E:238:HIS:CD2	1:E:241:TRP:CH2	3.09	0.41
1:E:235:LEU:O	1:E:239:PRO:HA	2.20	0.40
2:I:10:PHE:O	2:I:67:PRO:HD2	2.20	0.40
1:E:167:TYR:HB3	1:E:168:PRO:HA	2.04	0.40
1:E:159:SER:C	1:E:160:GLY:O	2.57	0.40
1:E:47:GLY:HA3	1:E:92:ALA:O	2.21	0.40
2:I:41:SER:HA	2:I:42:PRO:HD3	1.88	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:351:HOH:O	4:E:351:HOH:O[4_556]	1.75	0.45
4:E:415:HOH:O	4:E:415:HOH:O[5_556]	1.95	0.25
1:E:160:GLY:N	4:E:351:HOH:O[4_556]	1.97	0.23
4:E:359:HOH:O	4:E:578:HOH:O[4_556]	2.06	0.14
4:E:446:HOH:O	4:E:511:HOH:O[3_664]	2.15	0.05

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	273/275 (99%)	255 (93%)	17 (6%)	1 (0%)	34	32
2	I	61/70 (87%)	51 (84%)	7 (12%)	3 (5%)	2	0
All	All	334/345 (97%)	306 (92%)	24 (7%)	4 (1%)	13	8

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	I	61	ASN
1	E	63	SER
2	I	24	TYR
2	I	15	GLY

5.3.2 Protein sidechains [i](#)

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	205/205 (100%)	185 (90%)	20 (10%)	8	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	I	58/64 (91%)	47 (81%)	11 (19%)	1	0
All	All	263/269 (98%)	232 (88%)	31 (12%)	5	2

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	3	SER
1	E	16	LEU
1	E	24	SER
1	E	42	LEU
1	E	50	MET
1	E	53	SER
1	E	56	ASN
1	E	101	SER
1	E	103	GLN
1	E	109	ASN
1	E	118	ASN
1	E	159	SER
1	E	173	SER
1	E	180	VAL
1	E	206	GLN
1	E	221	SER
1	E	222	MET
1	E	241	TRP
1	E	243	ASN
1	E	275	GLN
2	I	10	PHE
2	I	22	ARG
2	I	27	LEU
2	I	31	GLN
2	I	33	ASN
2	I	34	VAL
2	I	39	GLU
2	I	50	ASN
2	I	60	THR
2	I	62	VAL
2	I	64	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	56	ASN
1	E	59	GLN
1	E	76	ASN
1	E	118	ASN
1	E	184	ASN
1	E	185	GLN
1	E	238	HIS
1	E	243	ASN
1	E	245	GLN
1	E	271	GLN
1	E	275	GLN
2	I	31	GLN
2	I	33	ASN
2	I	50	ASN
2	I	57	ASN
2	I	64	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 2 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 ⓘ

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.