



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 07:39 PM UTC

PDB ID : 3SIC / pdb_00003sic
Title : MOLECULAR RECOGNITION AT THE ACTIVE SITE OF SUBTILISIN BPN': CRYSTALLOGRAPHIC STUDIES USING GENETICALLY ENGINEERED PROTEINACEOUS INHIBITOR SSI (STREPTOMYCES SUBTILISIN INHIBITOR)
Authors : Mitsui, Y.; Takeuchi, Y.; Nakamura, K.T.
Deposited on : 1991-08-30
Resolution : 1.80 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
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

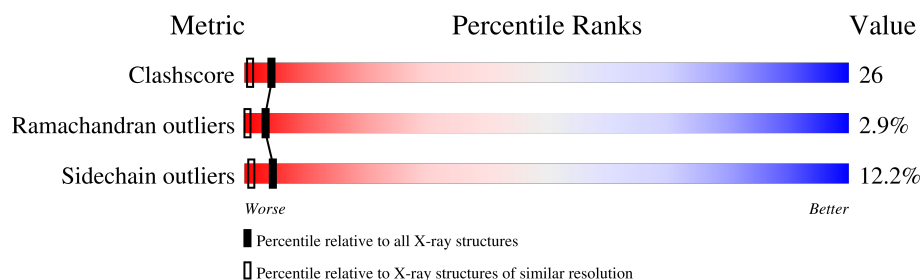
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)

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	E	275	
2	I	107	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2978 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 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 STREPTOMYCES SUBTILISIN INHIBITOR (SSI).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	107	Total	C	N	O	S	0	0	0
			765	477	131	151	6			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	73	LYS	MET	conflict	UNP P01006

- Molecule 3 is CALCIUM ION (CCD ID: 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	169	Total	O	0	0
			169	169		
4	I	104	Total	O	0	0
			104	104		

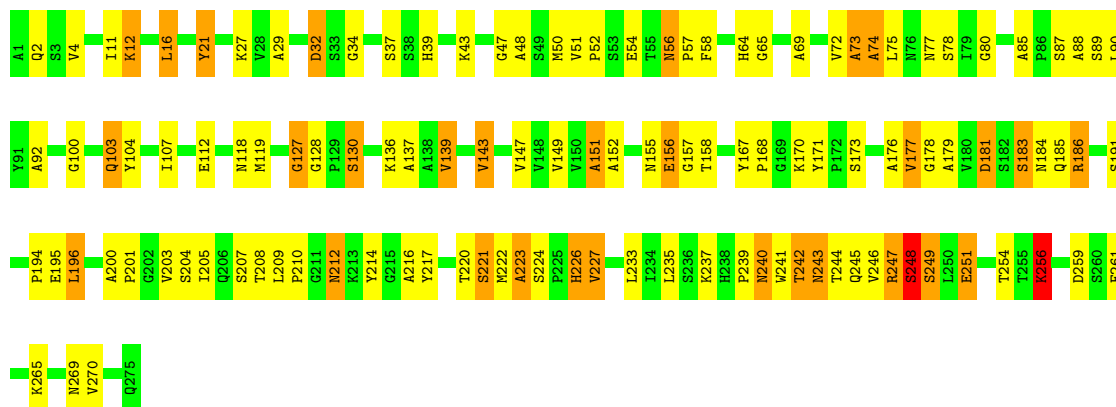
3 Residue-property plots

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.

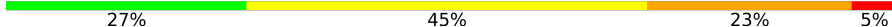
Note EDS was not executed.

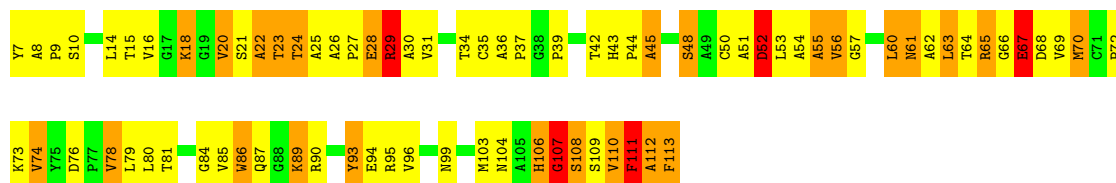
• Molecule 1: SUBTILISIN BPN'

Chain E: 



• Molecule 2: STREPTOMYCES SUBTILISIN INHIBITOR (SSI)

Chain I: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	77.20Å 185.90Å 69.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 1.80	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-1.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.178 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2978	wwPDB-VP
Average B, all atoms (Å ²)	22.0	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	1.39	1/1976 (0.1%)	2.24	97/2697 (3.6%)
2	I	1.17	3/781 (0.4%)	2.50	34/1066 (3.2%)
All	All	1.33	4/2757 (0.1%)	2.32	131/3763 (3.5%)

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	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	24	THR	N-CA	-7.03	1.37	1.46
1	E	178	GLY	N-CA	5.55	1.49	1.44
2	I	107	GLY	N-CA	5.03	1.52	1.45
2	I	23	THR	C-N	-5.00	1.26	1.33

All (131) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	23	THR	CA-C-N	27.45	173.97	121.54
2	I	23	THR	C-N-CA	27.45	173.97	121.54
2	I	112	ALA	CA-C-O	13.74	133.39	121.02
2	I	76	ASP	O-C-N	10.30	128.71	121.19
2	I	112	ALA	N-CA-C	-10.26	98.31	110.41
2	I	106	HIS	CA-CB-CG	-9.27	104.53	113.80
1	E	77	ASN	CB-CA-C	9.07	128.48	110.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	99	ASN	CA-CB-CG	8.98	121.58	112.60
1	E	2	GLN	CA-C-O	-8.78	110.81	120.38
2	I	52	ASP	CA-CB-CG	-8.70	103.90	112.60
1	E	240	ASN	CB-CA-C	8.69	126.39	111.45
1	E	2	GLN	O-C-N	8.54	133.37	123.29
1	E	155	ASN	CA-CB-CG	8.11	120.71	112.60
1	E	221	SER	CA-CB-OG	7.91	126.92	111.10
2	I	112	ALA	CA-C-N	7.89	135.90	121.70
2	I	112	ALA	C-N-CA	7.89	135.90	121.70
1	E	139	VAL	CB-CA-C	7.83	123.03	112.22
1	E	137	ALA	O-C-N	7.69	130.27	122.12
1	E	74	ALA	CA-C-O	-7.68	112.70	121.15
2	I	84	GLY	CA-C-O	7.62	126.17	120.91
2	I	23	THR	CA-C-O	7.59	130.55	120.15
1	E	112	GLU	CB-CG-CD	7.43	125.23	112.60
1	E	118	ASN	CA-CB-CG	-7.41	105.19	112.60
2	I	111	PHE	CA-C-N	7.36	132.79	121.53
2	I	111	PHE	C-N-CA	7.36	132.79	121.53
1	E	127	GLY	O-C-N	7.34	131.28	123.87
1	E	107	ILE	O-C-N	7.21	128.97	121.91
2	I	23	THR	O-C-N	-7.13	113.83	123.24
1	E	249	SER	CA-CB-OG	-7.04	97.02	111.10
1	E	184	ASN	CA-CB-CG	7.00	119.60	112.60
1	E	243	ASN	CA-C-N	6.96	129.60	120.28
1	E	243	ASN	C-N-CA	6.96	129.60	120.28
2	I	78	VAL	CB-CA-C	6.95	120.47	110.33
1	E	147	VAL	CA-C-O	-6.95	112.84	121.11
1	E	217	TYR	CA-CB-CG	6.93	126.38	113.90
1	E	127	GLY	CA-C-O	-6.91	114.86	121.49
1	E	227	VAL	CA-C-N	6.85	130.02	120.29
1	E	227	VAL	C-N-CA	6.85	130.02	120.29
2	I	78	VAL	N-CA-CB	-6.84	101.53	111.52
1	E	88	ALA	CA-C-O	-6.81	114.14	121.56
2	I	107	GLY	CA-C-N	6.81	134.55	121.54
2	I	107	GLY	C-N-CA	6.81	134.55	121.54
1	E	65	GLY	CA-C-O	-6.76	114.18	120.80
2	I	67	GLU	CA-CB-CG	6.73	127.56	114.10
1	E	259	ASP	CA-CB-CG	6.71	119.31	112.60
1	E	212	ASN	CA-C-O	-6.68	113.79	121.54
1	E	139	VAL	N-CA-CB	-6.67	100.57	110.58
1	E	248	SER	CA-C-O	6.66	128.03	120.90
1	E	254	THR	CA-CB-OG1	-6.62	99.67	109.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	34	GLY	CA-C-O	-6.60	117.69	122.45
1	E	176	ALA	CA-C-O	6.60	127.62	120.43
1	E	156	GLU	CB-CA-C	6.58	121.25	111.06
1	E	242	THR	CA-C-O	-6.55	114.23	121.89
2	I	94	GLU	CA-CB-CG	6.54	127.17	114.10
1	E	196	LEU	CA-CB-CG	6.50	139.04	116.30
1	E	259	ASP	CB-CA-C	6.43	121.36	109.54
1	E	269	ASN	CA-CB-CG	6.37	118.97	112.60
1	E	158	THR	CA-CB-OG1	-6.37	100.05	109.60
1	E	235	LEU	CA-C-O	-6.20	111.75	119.38
1	E	239	PRO	CA-C-N	-6.19	111.42	123.13
1	E	239	PRO	C-N-CA	-6.19	111.42	123.13
1	E	210	PRO	CB-CA-C	6.17	119.06	110.98
1	E	176	ALA	CB-CA-C	6.12	119.84	109.75
1	E	72	VAL	O-C-N	-6.10	115.41	121.94
1	E	207	SER	CA-C-N	6.10	130.52	120.94
1	E	207	SER	C-N-CA	6.10	130.52	120.94
1	E	186	ARG	CD-NE-CZ	-6.00	115.99	124.40
1	E	269	ASN	OD1-CG-ND2	-5.98	116.62	122.60
1	E	235	LEU	N-CA-C	-5.97	105.25	112.54
1	E	21	TYR	O-C-N	5.95	130.14	123.05
1	E	178	GLY	N-CA-C	-5.95	102.29	112.64
2	I	99	ASN	CA-C-O	-5.94	114.78	121.25
1	E	170	LYS	CA-C-N	5.93	128.91	120.49
1	E	170	LYS	C-N-CA	5.93	128.91	120.49
2	I	60	LEU	N-CA-C	-5.93	101.63	110.23
2	I	106	HIS	CA-C-O	-5.91	114.60	120.80
1	E	241	TRP	N-CA-C	-5.91	101.74	110.48
1	E	247	ARG	CA-C-O	5.88	127.00	120.82
1	E	12	LYS	CA-C-O	-5.88	113.52	120.57
1	E	235	LEU	N-CA-CB	5.85	120.09	110.39
1	E	103	GLN	OE1-CD-NE2	5.76	128.36	122.60
1	E	54	GLU	CG-CD-OE2	-5.76	105.16	118.40
2	I	60	LEU	CB-CA-C	5.76	119.28	109.72
1	E	48	ALA	CA-C-O	-5.75	115.08	121.23
1	E	203	VAL	N-CA-CB	-5.71	103.53	111.41
2	I	15	THR	CA-C-O	-5.70	114.77	121.44
1	E	56	ASN	O-C-N	5.69	127.61	121.12
1	E	4	VAL	O-C-N	5.69	126.15	120.92
1	E	151	ALA	O-C-N	5.66	129.73	123.33
2	I	20	VAL	N-CA-CB	-5.66	105.01	112.36
1	E	118	ASN	OD1-CG-ND2	5.65	128.25	122.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	77	ASN	CA-CB-CG	5.65	118.25	112.60
1	E	152	ALA	CA-C-N	5.64	127.84	120.28
1	E	152	ALA	C-N-CA	5.64	127.84	120.28
1	E	50	MET	N-CA-C	-5.64	105.99	112.92
1	E	256	LYS	O-C-N	5.61	129.74	122.89
1	E	149	VAL	O-C-N	5.60	129.13	123.20
1	E	214	TYR	CA-C-O	-5.59	114.57	121.06
1	E	240	ASN	CB-CG-ND2	-5.59	108.02	116.40
2	I	23	THR	CB-CA-C	5.57	118.53	110.79
1	E	107	ILE	N-CA-CB	5.57	117.06	110.55
1	E	73	ALA	N-CA-C	5.56	119.17	111.71
2	I	110	VAL	CA-C-O	5.52	127.02	121.17
1	E	208	THR	CA-C-O	-5.52	115.55	121.56
2	I	86	TRP	CA-C-O	-5.45	114.46	120.24
1	E	181	ASP	CB-CG-OD1	5.44	130.91	118.40
1	E	32	ASP	CA-CB-CG	5.42	118.02	112.60
1	E	168	PRO	CA-C-N	5.34	126.86	120.13
1	E	168	PRO	C-N-CA	5.34	126.86	120.13
1	E	251	GLU	CB-CG-CD	5.33	121.67	112.60
1	E	72	VAL	CA-C-O	5.33	127.37	121.18
1	E	261	PHE	N-CA-C	-5.32	105.53	112.23
1	E	220	THR	N-CA-C	-5.31	106.06	112.54
2	I	93	TYR	CA-CB-CG	5.30	123.45	113.90
2	I	29	ARG	NE-CZ-NH2	5.30	123.97	119.20
2	I	24	THR	N-CA-CB	5.25	119.37	110.49
1	E	203	VAL	CA-C-N	5.24	131.55	121.54
1	E	203	VAL	C-N-CA	5.24	131.55	121.54
1	E	143	VAL	CB-CA-C	5.24	119.21	112.14
1	E	75	LEU	N-CA-C	5.22	117.27	110.43
1	E	233	LEU	O-C-N	5.22	127.44	122.07
1	E	156	GLU	CG-CD-OE2	5.19	130.33	118.40
1	E	128	GLY	N-CA-C	-5.16	101.82	112.34
1	E	85	ALA	O-C-N	5.13	125.98	121.37
1	E	185	GLN	OE1-CD-NE2	5.13	127.73	122.60
2	I	73	LYS	CB-CA-C	5.07	118.19	111.14
1	E	89	SER	O-C-N	5.06	128.96	123.04
1	E	226	HIS	CA-CB-CG	5.05	118.85	113.80
1	E	235	LEU	O-C-N	5.05	129.19	122.43
1	E	223	ALA	N-CA-CB	-5.02	102.79	110.26
1	E	176	ALA	O-C-N	-5.01	117.60	123.27

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	186	ARG	Sidechain

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	E	1938	0	1899	53	1
2	I	765	0	742	97	1
3	E	2	0	0	0	0
4	E	169	0	0	12	1
4	I	104	0	0	12	2
All	All	2978	0	2641	140	4

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 26.

All (140) 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:177:VAL:HG22	4:E:623:HOH:O	1.33	1.29
2:I:28:GLU:HG3	2:I:29:ARG:HD3	1.42	1.01
4:E:660:HOH:O	2:I:74:VAL:HB	1.59	1.01
2:I:109:SER:HA	2:I:112:ALA:HB2	1.39	1.00
2:I:31:VAL:HB	2:I:42:THR:O	1.68	0.93
2:I:60:LEU:O	2:I:61:ASN:HB2	1.75	0.85
1:E:64:HIS:CD2	2:I:74:VAL:HG12	2.12	0.83
2:I:60:LEU:HD11	4:I:181:HOH:O	1.81	0.80
2:I:86:TRP:NE1	4:I:179:HOH:O	2.09	0.79
2:I:8:ALA:HB3	2:I:36:ALA:CB	2.13	0.78
4:E:600:HOH:O	2:I:74:VAL:HB	1.85	0.77
2:I:66:GLY:O	2:I:67:GLU:HB2	1.83	0.76
2:I:86:TRP:CD1	4:I:178:HOH:O	2.37	0.76
1:E:64:HIS:CD2	2:I:74:VAL:CG1	2.68	0.76
2:I:28:GLU:CG	2:I:29:ARG:HD3	2.16	0.76
1:E:64:HIS:HD2	2:I:74:VAL:HG12	1.53	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:29:ARG:HH11	2:I:29:ARG:HG2	1.54	0.72
2:I:20:VAL:HA	2:I:96:VAL:HG11	1.72	0.71
2:I:7:TYR:CE2	2:I:9:PRO:HG3	2.26	0.70
1:E:256:LYS:HD2	4:E:626:HOH:O	1.92	0.70
2:I:23:THR:O	4:I:203:HOH:O	2.10	0.69
2:I:21:SER:O	2:I:25:ALA:HB3	1.94	0.68
2:I:7:TYR:CG	2:I:7:TYR:O	2.47	0.67
2:I:79:LEU:HD12	2:I:96:VAL:HG13	1.75	0.66
2:I:64:THR:HG23	4:I:184:HOH:O	1.97	0.65
2:I:43:HIS:C	2:I:45:ALA:H	2.04	0.65
2:I:52:ASP:OD2	2:I:109:SER:OG	2.15	0.65
2:I:8:ALA:HB3	2:I:36:ALA:HB2	1.78	0.65
2:I:60:LEU:O	2:I:61:ASN:CB	2.45	0.63
2:I:60:LEU:CD1	4:I:181:HOH:O	2.41	0.63
2:I:103:MET:O	2:I:106:HIS:HB2	1.98	0.62
2:I:52:ASP:O	2:I:55:ALA:HB3	1.99	0.62
2:I:86:TRP:CE3	2:I:87:GLN:HB3	2.35	0.62
2:I:87:GLN:O	2:I:87:GLN:HG3	2.01	0.61
4:E:582:HOH:O	2:I:112:ALA:HB1	1.99	0.61
1:E:156:GLU:O	1:E:157:GLY:C	2.44	0.60
1:E:104:TYR:CZ	2:I:70:MET:HE2	2.36	0.60
2:I:48:SER:O	2:I:51:ALA:HB3	2.01	0.60
2:I:14:LEU:HD12	2:I:14:LEU:N	2.18	0.59
1:E:47:GLY:HA3	1:E:92:ALA:O	2.02	0.59
1:E:64:HIS:HD2	2:I:74:VAL:CG1	2.08	0.58
1:E:242:THR:OG1	1:E:245:GLN:HG3	2.03	0.58
2:I:8:ALA:HB3	2:I:36:ALA:HB1	1.84	0.57
2:I:37:PRO:HD3	4:I:128:HOH:O	2.03	0.57
2:I:53:LEU:CD2	4:I:181:HOH:O	2.51	0.57
2:I:66:GLY:O	2:I:67:GLU:CB	2.52	0.56
2:I:20:VAL:HG22	4:I:170:HOH:O	2.06	0.56
1:E:69:ALA:HB1	1:E:90:LEU:HD21	1.88	0.55
1:E:151:ALA:O	1:E:177:VAL:HG23	2.05	0.55
2:I:29:ARG:HH11	2:I:29:ARG:CG	2.20	0.55
1:E:191:SER:O	4:E:627:HOH:O	2.18	0.54
2:I:109:SER:O	2:I:112:ALA:HB3	2.07	0.54
2:I:14:LEU:O	2:I:30:ALA:HA	2.08	0.54
2:I:109:SER:HA	2:I:112:ALA:CB	2.27	0.54
2:I:85:VAL:HA	2:I:89:LYS:O	2.08	0.54
1:E:21:TYR:CZ	1:E:237:LYS:HG3	2.42	0.53
2:I:87:GLN:O	2:I:87:GLN:CG	2.57	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:104:TYR:CZ	2:I:70:MET:CE	2.92	0.52
1:E:100:GLY:O	2:I:72:PRO:HD3	2.10	0.52
2:I:7:TYR:O	2:I:9:PRO:HD3	2.10	0.52
1:E:212:ASN:CG	1:E:212:ASN:O	2.51	0.51
2:I:22:ALA:HA	2:I:79:LEU:HD21	1.92	0.51
1:E:127:GLY:HA2	1:E:167:TYR:O	2.10	0.51
2:I:43:HIS:CD2	2:I:44:PRO:HD2	2.45	0.51
2:I:53:LEU:HD21	4:I:181:HOH:O	2.10	0.51
2:I:48:SER:O	2:I:52:ASP:N	2.32	0.51
2:I:14:LEU:HA	2:I:81:THR:O	2.11	0.50
2:I:86:TRP:HE3	2:I:87:GLN:HB3	1.75	0.50
2:I:10:SER:O	2:I:34:THR:HG23	2.12	0.50
1:E:11:ILE:O	1:E:270:VAL:HG12	2.12	0.50
1:E:194:PRO:HD2	1:E:195:GLU:OE1	2.11	0.50
1:E:130:SER:CB	2:I:67:GLU:OE1	2.60	0.49
1:E:227:VAL:HG21	4:E:623:HOH:O	2.12	0.49
1:E:58:PHE:N	1:E:58:PHE:CD1	2.80	0.49
2:I:21:SER:O	2:I:25:ALA:CB	2.61	0.49
2:I:53:LEU:O	2:I:54:ALA:C	2.55	0.49
2:I:89:LYS:HB2	2:I:89:LYS:NZ	2.27	0.49
2:I:56:VAL:HG11	2:I:62:ALA:HB3	1.93	0.49
2:I:7:TYR:O	2:I:7:TYR:CD1	2.66	0.48
2:I:43:HIS:C	2:I:45:ALA:N	2.70	0.48
2:I:43:HIS:HD2	2:I:45:ALA:H	1.62	0.48
2:I:54:ALA:O	2:I:55:ALA:C	2.54	0.48
1:E:104:TYR:OH	2:I:70:MET:HE2	2.14	0.48
1:E:227:VAL:HG11	4:E:623:HOH:O	2.13	0.48
2:I:18:LYS:HB3	4:I:144:HOH:O	2.13	0.48
2:I:43:HIS:HD2	2:I:45:ALA:N	2.12	0.48
4:E:660:HOH:O	2:I:74:VAL:HA	2.13	0.48
4:E:660:HOH:O	2:I:74:VAL:CB	2.35	0.48
2:I:56:VAL:CG1	2:I:62:ALA:HB3	2.44	0.48
1:E:136:LYS:HG3	1:E:171:TYR:CE1	2.49	0.47
2:I:53:LEU:O	2:I:57:GLY:N	2.48	0.47
1:E:179:ALA:HA	1:E:200:ALA:O	2.15	0.47
1:E:181:ASP:C	1:E:183:SER:H	2.22	0.47
1:E:247:ARG:NE	1:E:251:GLU:OE2	2.45	0.47
1:E:136:LYS:HG3	1:E:171:TYR:CD1	2.50	0.47
1:E:195:GLU:OE1	1:E:195:GLU:N	2.47	0.47
1:E:205:ILE:O	1:E:216:ALA:HA	2.14	0.47
2:I:22:ALA:O	2:I:23:THR:OG1	2.32	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:16:VAL:HA	2:I:79:LEU:O	2.15	0.46
2:I:34:THR:O	2:I:39:PRO:HA	2.16	0.46
2:I:56:VAL:HG21	2:I:63:LEU:HD13	1.98	0.46
1:E:56:ASN:HA	1:E:57:PRO:HD2	1.82	0.46
1:E:73:ALA:O	1:E:74:ALA:C	2.58	0.46
2:I:43:HIS:HE1	2:I:110:VAL:O	2.00	0.45
1:E:130:SER:OG	2:I:67:GLU:OE1	2.30	0.45
2:I:80:LEU:HD21	2:I:111:PHE:CE1	2.51	0.45
2:I:66:GLY:C	2:I:68:ASP:H	2.24	0.45
1:E:177:VAL:HG21	1:E:224:SER:HA	1.99	0.45
2:I:63:LEU:HG	2:I:107:GLY:HA2	1.98	0.45
1:E:244:THR:O	1:E:248:SER:HB2	2.17	0.45
2:I:61:ASN:ND2	2:I:93:TYR:CE1	2.85	0.44
1:E:181:ASP:C	1:E:183:SER:N	2.75	0.44
1:E:181:ASP:OD1	1:E:183:SER:HB2	2.17	0.44
2:I:60:LEU:HD22	2:I:60:LEU:N	2.32	0.44
1:E:47:GLY:CA	1:E:92:ALA:O	2.66	0.43
1:E:29:ALA:HB2	1:E:119:MET:HG3	2.00	0.43
1:E:21:TYR:CE1	1:E:237:LYS:HG3	2.54	0.43
1:E:242:THR:O	1:E:246:VAL:HG23	2.18	0.43
4:E:660:HOH:O	2:I:74:VAL:CA	2.66	0.43
1:E:51:VAL:HA	1:E:52:PRO:HD3	1.90	0.43
2:I:48:SER:HA	2:I:51:ALA:HB3	2.00	0.43
2:I:63:LEU:O	2:I:64:THR:C	2.61	0.43
1:E:181:ASP:OD1	1:E:183:SER:CB	2.67	0.43
1:E:16:LEU:HD12	1:E:16:LEU:HA	1.79	0.42
2:I:48:SER:HB3	2:I:109:SER:CB	2.50	0.42
2:I:26:ALA:HA	2:I:27:PRO:HD3	1.78	0.42
2:I:104:ASN:C	2:I:106:HIS:H	2.25	0.42
1:E:200:ALA:HA	1:E:201:PRO:HD3	1.90	0.42
2:I:35:CYS:SG	2:I:50:CYS:CB	3.08	0.42
2:I:113:PHE:CB	4:I:189:HOH:O	2.66	0.42
2:I:113:PHE:CD1	2:I:113:PHE:C	2.98	0.42
1:E:243:ASN:OD1	1:E:243:ASN:N	2.52	0.41
2:I:111:PHE:CD1	2:I:111:PHE:N	2.87	0.41
2:I:65:ARG:HG2	2:I:66:GLY:N	2.35	0.41
1:E:143:VAL:HG21	1:E:173:SER:HB2	2.02	0.41
1:E:223:ALA:O	1:E:226:HIS:HB2	2.20	0.41
1:E:80:GLY:CA	4:E:513:HOH:O	2.69	0.41
1:E:39:HIS:CD2	1:E:209:LEU:O	2.74	0.41
1:E:37:SER:OG	1:E:58:PHE:HB3	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:23:THR:HA	2:I:25:ALA:H	1.85	0.40

All (4) 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:I:132:HOH:O	4:I:132:HOH:O[4_555]	1.39	0.81
2:I:23:THR:OG1	2:I:90:ARG:NE[2_555]	1.62	0.58
1:E:12:LYS:NZ	4:E:544:HOH:O[6_555]	2.03	0.17
4:I:122:HOH:O	4:I:122:HOH:O[3_555]	2.17	0.03

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	E	273/275 (99%)	260 (95%)	11 (4%)	2 (1%)	18	8
2	I	105/107 (98%)	79 (75%)	17 (16%)	9 (9%)	0	0
All	All	378/382 (99%)	339 (90%)	28 (7%)	11 (3%)	3	0

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	I	24	THR
2	I	65	ARG
2	I	61	ASN
2	I	108	SER
2	I	55	ALA
2	I	67	GLU
1	E	32	ASP
1	E	204	SER
2	I	22	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	I	107	GLY
2	I	45	ALA

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	199/205 (97%)	181 (91%)	18 (9%)	9	2
2	I	80/80 (100%)	64 (80%)	16 (20%)	1	0
All	All	279/285 (98%)	245 (88%)	34 (12%)	5	1

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	16	LEU
1	E	27	LYS
1	E	43	LYS
1	E	78	SER
1	E	87	SER
1	E	103	GLN
1	E	130	SER
1	E	139	VAL
1	E	177	VAL
1	E	183	SER
1	E	196	LEU
1	E	221	SER
1	E	222	MET
1	E	240	ASN
1	E	248	SER
1	E	249	SER
1	E	256	LYS
1	E	265	LYS
2	I	18	LYS
2	I	28	GLU
2	I	29	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	I	48	SER
2	I	52	ASP
2	I	56	VAL
2	I	63	LEU
2	I	69	VAL
2	I	70	MET
2	I	74	VAL
2	I	78	VAL
2	I	89	LYS
2	I	95	ARG
2	I	108	SER
2	I	111	PHE
2	I	113	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	59	GLN
1	E	103	GLN
1	E	123	ASN
1	E	271	GLN
2	I	43	HIS
2	I	61	ASN
2	I	106	HIS

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

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

There are no such residues in this entry.

5.8 Polymer linkage issues

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.