



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:38 PM UTC

PDB ID : 5SIC / pdb_00005sic
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 : 1991-11-18
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 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

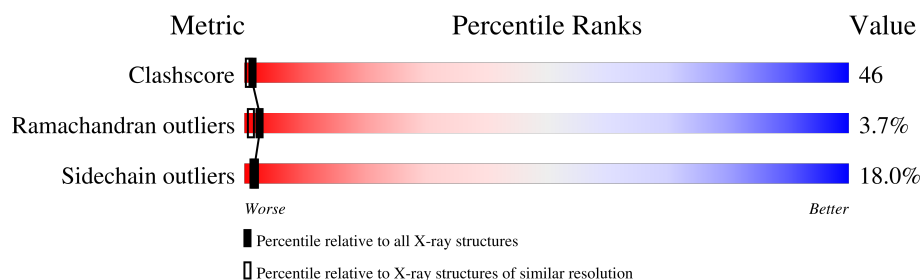
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

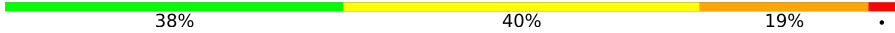
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (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 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

There are 4 unique types of molecules in this entry. The entry contains 2989 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 SUBTILISIN INHIBITOR (SSI).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	107	Total	C	N	O	S	0	0	0
			761	474	131	151	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	70	GLY	MET	conflict	UNP P01006
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.

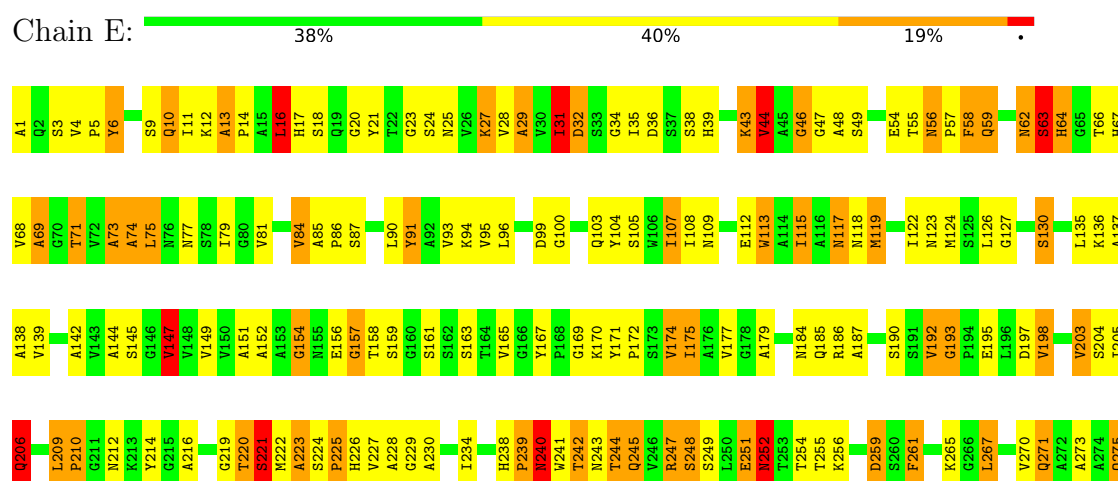
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	172	Total	O	0	0
			172	172		
4	I	116	Total	O	0	0
			116	116		

3 Residue-property plots [i](#)

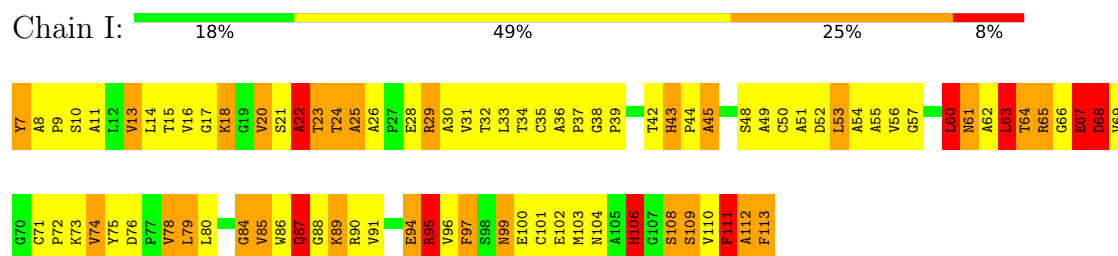
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



• Molecule 2: SUBTILISIN INHIBITOR (SSI)



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) – 2.20	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.176 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2989	wwPDB-VP
Average B, all atoms (Å ²)	15.0	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:
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	1.47	11/1976 (0.6%)	2.46	138/2697 (5.1%)
2	I	1.21	0/777	2.41	34/1061 (3.2%)
All	All	1.40	11/2753 (0.4%)	2.44	172/3758 (4.6%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	242	THR	N-CA	6.97	1.54	1.45
1	E	46	GLY	N-CA	6.46	1.52	1.45
1	E	154	GLY	N-CA	6.27	1.51	1.45
1	E	59	GLN	N-CA	5.51	1.53	1.46
1	E	47	GLY	N-CA	5.34	1.50	1.45
1	E	244	THR	CB-OG1	5.34	1.52	1.43
1	E	245	GLN	N-CA	5.26	1.52	1.46
1	E	34	GLY	N-CA	5.17	1.53	1.45
1	E	74	ALA	N-CA	5.12	1.52	1.46
1	E	24	SER	C-N	-5.09	1.27	1.33
1	E	58	PHE	N-CA	5.05	1.51	1.46

All (172) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	23	THR	CA-C-N	17.66	155.28	121.54
2	I	23	THR	C-N-CA	17.66	155.28	121.54
2	I	106	HIS	CA-CB-CG	-16.06	97.74	113.80
2	I	112	ALA	CA-C-O	13.54	132.70	119.97
2	I	112	ALA	N-CA-C	-12.44	95.74	112.03
1	E	10	GLN	OE1-CD-NE2	12.24	134.84	122.60
2	I	111	PHE	CA-C-N	11.68	140.24	121.08
2	I	111	PHE	C-N-CA	11.68	140.24	121.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	23	THR	CA-C-O	11.38	134.59	120.25
1	E	99	ASP	CA-CB-CG	10.49	123.09	112.60
1	E	64	HIS	CA-C-N	10.49	131.62	119.98
1	E	64	HIS	C-N-CA	10.49	131.62	119.98
1	E	214	TYR	CA-C-O	-10.26	108.86	120.66
1	E	252	ASN	CA-CB-CG	9.55	122.15	112.60
1	E	240	ASN	CA-C-N	9.53	135.04	121.42
1	E	240	ASN	C-N-CA	9.53	135.04	121.42
1	E	6	TYR	CA-C-N	9.52	130.75	119.99
1	E	6	TYR	C-N-CA	9.52	130.75	119.99
1	E	198	VAL	N-CA-CB	-9.34	98.44	112.35
1	E	56	ASN	CA-C-O	9.30	127.17	119.36
2	I	68	ASP	CA-CB-CG	9.06	121.66	112.60
1	E	261	PHE	CA-CB-CG	9.06	122.86	113.80
1	E	216	ALA	CA-C-O	-8.99	111.19	120.71
1	E	17	HIS	CA-CB-CG	8.98	122.78	113.80
1	E	240	ASN	OD1-CG-ND2	8.91	131.51	122.60
1	E	69	ALA	CA-C-O	-8.68	111.35	120.55
1	E	251	GLU	CB-CG-CD	8.59	127.21	112.60
1	E	252	ASN	OD1-CG-ND2	-8.59	114.01	122.60
1	E	69	ALA	O-C-N	8.45	131.07	122.12
2	I	99	ASN	CA-CB-CG	8.12	120.72	112.60
2	I	110	VAL	CA-C-O	8.09	129.68	121.27
1	E	55	THR	CA-C-O	-7.83	110.40	119.56
2	I	76	ASP	O-C-N	7.80	128.39	121.37
2	I	84	GLY	CA-C-O	7.73	126.24	120.91
1	E	123	ASN	CA-CB-CG	7.70	120.30	112.60
1	E	25	ASN	CA-CB-CG	7.63	120.23	112.60
1	E	107	ILE	N-CA-CB	7.52	118.51	110.62
1	E	221	SER	CA-CB-OG	7.43	125.97	111.10
1	E	271	GLN	CA-C-N	7.37	133.21	120.68
1	E	271	GLN	C-N-CA	7.37	133.21	120.68
1	E	137	ALA	CA-C-N	7.17	130.12	120.65
1	E	137	ALA	C-N-CA	7.17	130.12	120.65
1	E	197	ASP	CA-CB-CG	-7.16	105.44	112.60
1	E	255	THR	CA-C-O	-7.04	112.54	120.43
1	E	21	TYR	O-C-N	7.00	131.95	123.13
1	E	62	ASN	OD1-CG-ND2	6.99	129.59	122.60
1	E	154	GLY	N-CA-C	-6.96	104.48	111.85
1	E	245	GLN	OE1-CD-NE2	6.95	129.54	122.60
1	E	203	VAL	CA-C-N	6.86	133.21	122.78
1	E	203	VAL	C-N-CA	6.86	133.21	122.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	161	SER	N-CA-C	-6.84	102.22	112.54
1	E	32	ASP	CA-CB-CG	6.78	119.38	112.60
1	E	206	GLN	OE1-CD-NE2	6.74	129.34	122.60
1	E	10	GLN	O-C-N	6.74	129.26	122.12
1	E	214	TYR	O-C-N	6.70	131.44	123.27
1	E	69	ALA	N-CA-CB	6.70	119.97	110.12
2	I	28	GLU	CA-CB-CG	6.70	127.50	114.10
1	E	244	THR	CA-CB-CG2	6.67	121.84	110.50
1	E	122	ILE	CA-C-O	-6.65	113.22	120.67
2	I	87	GLN	N-CA-C	-6.65	102.21	111.52
1	E	244	THR	CA-CB-OG1	-6.65	99.63	109.60
1	E	4	VAL	O-C-N	6.62	127.01	120.92
1	E	220	THR	N-CA-C	-6.54	104.40	112.38
2	I	79	LEU	CA-C-O	6.54	127.51	120.38
1	E	147	VAL	CA-C-O	-6.49	113.64	121.04
1	E	31	ILE	N-CA-CB	6.49	117.60	110.53
1	E	21	TYR	CA-C-O	-6.47	113.54	120.46
1	E	240	ASN	CB-CA-C	6.42	122.49	111.45
1	E	13	ALA	CA-C-N	6.36	126.85	119.47
1	E	13	ALA	C-N-CA	6.36	126.85	119.47
1	E	48	ALA	CA-C-O	-6.35	114.44	121.23
1	E	247	ARG	NE-CZ-NH2	6.32	124.88	119.20
1	E	244	THR	CA-C-O	6.31	127.24	120.55
1	E	118	ASN	CA-C-O	-6.20	114.65	121.84
2	I	75	TYR	CA-C-O	6.20	127.76	120.70
1	E	240	ASN	CA-CB-CG	-6.19	106.41	112.60
2	I	63	LEU	CB-CA-C	6.18	121.86	111.22
1	E	229	GLY	N-CA-C	-6.18	104.86	112.77
1	E	20	GLY	CA-C-N	-6.15	114.37	123.11
1	E	20	GLY	C-N-CA	-6.15	114.37	123.11
1	E	275	GLN	OE1-CD-NE2	6.15	128.75	122.60
1	E	193	GLY	O-C-N	6.15	127.92	121.77
1	E	85	ALA	CA-C-N	6.11	126.00	119.28
1	E	85	ALA	C-N-CA	6.11	126.00	119.28
1	E	107	ILE	N-CA-C	-6.07	103.92	110.23
1	E	29	ALA	CA-C-N	-5.99	115.52	122.95
1	E	29	ALA	C-N-CA	-5.99	115.52	122.95
1	E	115	ILE	N-CA-CB	5.97	117.53	110.55
1	E	109	ASN	CA-C-N	5.97	126.44	119.94
1	E	109	ASN	C-N-CA	5.97	126.44	119.94
1	E	119	MET	O-C-N	5.97	129.70	122.96
1	E	112	GLU	CB-CG-CD	5.96	122.74	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	209	LEU	O-C-N	5.95	126.19	121.55
1	E	91	TYR	CA-C-O	5.94	127.49	120.66
1	E	68	VAL	O-C-N	5.88	127.68	121.91
2	I	64	THR	N-CA-CB	5.88	118.34	109.34
1	E	117	ASN	O-C-N	5.85	129.45	122.26
1	E	179	ALA	CA-C-O	5.84	127.38	120.66
1	E	261	PHE	N-CA-C	-5.83	105.66	112.89
1	E	28	VAL	O-C-N	5.83	129.30	123.18
2	I	79	LEU	CB-CA-C	5.79	119.74	109.72
1	E	16	LEU	CB-CA-C	5.79	120.04	110.90
1	E	163	SER	CB-CA-C	5.78	119.39	109.51
1	E	119	MET	CA-C-O	-5.77	114.83	121.47
2	I	20	VAL	N-CA-CB	-5.76	104.83	112.26
1	E	99	ASP	CB-CG-OD1	5.74	131.60	118.40
1	E	254	THR	CA-CB-CG2	5.73	120.25	110.50
2	I	106	HIS	CA-C-O	-5.72	114.79	120.80
1	E	17	HIS	N-CA-CB	5.72	119.18	110.14
1	E	154	GLY	CA-C-O	-5.69	117.72	122.33
1	E	223	ALA	CA-C-O	5.68	126.25	119.60
1	E	48	ALA	O-C-N	5.62	129.43	123.42
1	E	210	PRO	CA-C-O	-5.62	115.05	121.56
2	I	111	PHE	CA-C-O	5.61	127.68	121.39
1	E	259	ASP	CA-CB-CG	5.60	118.20	112.60
2	I	60	LEU	N-CA-C	-5.58	102.02	110.28
1	E	71	THR	N-CA-CB	5.58	119.49	110.40
1	E	94	LYS	CA-CB-CG	5.57	125.25	114.10
1	E	64	HIS	CA-CB-CG	-5.57	108.23	113.80
1	E	206	GLN	CB-CG-CD	-5.55	103.16	112.60
1	E	11	ILE	CA-C-O	-5.53	112.52	119.48
1	E	175	ILE	CA-C-O	-5.52	114.75	121.04
1	E	255	THR	N-CA-C	-5.48	100.24	108.96
2	I	95	ARG	CG-CD-NE	5.47	124.05	112.00
1	E	240	ASN	CB-CG-ND2	-5.47	108.19	116.40
1	E	62	ASN	CB-CA-C	5.47	118.83	109.65
1	E	239	PRO	CA-C-N	-5.46	112.81	123.13
1	E	239	PRO	C-N-CA	-5.46	112.81	123.13
1	E	225	PRO	CB-CA-C	5.44	119.57	111.62
1	E	249	SER	CA-CB-OG	-5.44	100.22	111.10
2	I	63	LEU	N-CA-CB	-5.43	101.28	110.46
1	E	220	THR	N-CA-CB	5.42	119.54	110.32
1	E	59	GLN	CG-CD-NE2	-5.41	108.28	116.40
1	E	242	THR	CA-C-N	5.39	127.50	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	242	THR	C-N-CA	5.39	127.50	120.28
2	I	97	PHE	CA-C-N	5.38	128.24	120.38
2	I	97	PHE	C-N-CA	5.38	128.24	120.38
1	E	241	TRP	CA-C-O	-5.37	114.92	121.05
1	E	198	VAL	CA-CB-CG2	-5.37	101.27	110.40
1	E	38	SER	CA-C-N	5.37	128.11	120.49
1	E	38	SER	C-N-CA	5.37	128.11	120.49
1	E	144	ALA	N-CA-C	-5.36	105.44	111.28
1	E	238	HIS	CB-CA-C	-5.36	101.15	111.12
2	I	43	HIS	O-C-N	5.34	127.47	121.32
1	E	66	THR	N-CA-CB	5.34	117.97	110.12
1	E	49	SER	N-CA-C	5.34	117.66	109.07
1	E	247	ARG	NE-CZ-NH1	-5.33	116.17	121.50
1	E	46	GLY	CA-C-O	-5.33	116.35	121.41
1	E	73	ALA	CA-C-O	-5.33	115.05	121.34
1	E	219	GLY	CA-C-N	5.32	129.12	120.60
1	E	219	GLY	C-N-CA	5.32	129.12	120.60
1	E	228	ALA	O-C-N	5.30	128.19	122.15
1	E	238	HIS	O-C-N	5.28	126.17	121.36
1	E	239	PRO	O-C-N	5.28	129.60	122.37
2	I	110	VAL	N-CA-C	-5.25	104.85	110.36
1	E	77	ASN	OD1-CG-ND2	5.23	127.83	122.60
1	E	158	THR	CA-CB-OG1	-5.23	101.76	109.60
1	E	18	SER	N-CA-CB	5.21	118.24	110.22
1	E	54	GLU	O-C-N	5.18	130.11	123.06
1	E	10	GLN	CB-CG-CD	-5.15	103.84	112.60
1	E	238	HIS	CA-C-O	-5.13	113.61	120.64
2	I	22	ALA	CA-C-N	-5.11	115.03	122.44
2	I	22	ALA	C-N-CA	-5.11	115.03	122.44
1	E	247	ARG	CD-NE-CZ	-5.11	117.25	124.40
1	E	113	TRP	N-CA-C	-5.08	105.82	111.36
1	E	119	MET	N-CA-C	-5.08	102.97	110.48
1	E	130	SER	O-C-N	5.07	129.55	123.16
1	E	44	VAL	N-CA-C	5.06	115.05	107.51
1	E	23	GLY	CA-C-O	5.06	124.88	119.06
1	E	24	SER	CA-CB-OG	-5.04	101.01	111.10
2	I	74	VAL	O-C-N	5.04	128.27	122.93
2	I	85	VAL	CB-CA-C	5.02	119.69	110.71

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	111	1
2	I	761	0	736	146	1
3	E	2	0	0	0	0
4	E	172	0	0	15	1
4	I	116	0	0	31	1
All	All	2989	0	2635	245	3

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 46.

All (245) 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)
2:I:44:PRO:CB	4:I:132:HOH:O	1.96	1.13
1:E:139:VAL:HG11	1:E:174:VAL:HG23	1.32	1.07
1:E:139:VAL:HG11	1:E:174:VAL:CG2	1.96	0.96
2:I:31:VAL:HB	2:I:42:THR:O	1.67	0.92
1:E:242:THR:OG1	1:E:245:GLN:HG3	1.70	0.91
2:I:66:GLY:O	2:I:67:GLU:HB2	1.69	0.91
2:I:53:LEU:HD23	4:I:181:HOH:O	1.72	0.89
2:I:109:SER:HA	2:I:112:ALA:HB2	1.53	0.87
2:I:86:TRP:CE3	2:I:87:GLN:HB2	2.13	0.84
2:I:43:HIS:C	2:I:45:ALA:H	1.88	0.82
2:I:44:PRO:HB2	4:I:132:HOH:O	1.69	0.81
2:I:18:LYS:HE3	2:I:78:VAL:HG23	1.63	0.81
1:E:240:ASN:OD1	4:E:592:HOH:O	2.00	0.80
2:I:68:ASP:HB2	4:I:190:HOH:O	1.83	0.78
4:E:601:HOH:O	2:I:74:VAL:HB	1.83	0.77
2:I:48:SER:O	2:I:51:ALA:HB3	1.86	0.76
1:E:100:GLY:O	2:I:72:PRO:HD3	1.85	0.76
2:I:80:LEU:O	2:I:94:GLU:HA	1.87	0.75
2:I:111:PHE:HA	2:I:113:PHE:O	1.86	0.75
2:I:13:VAL:HG12	2:I:32:THR:HG22	1.69	0.75
2:I:14:LEU:O	2:I:30:ALA:HA	1.87	0.75
2:I:65:ARG:NH1	2:I:66:GLY:HA3	2.02	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:152:ALA:O	4:E:551:HOH:O	2.07	0.72
2:I:22:ALA:HB2	4:I:219:HOH:O	1.89	0.72
1:E:69:ALA:HB1	1:E:90:LEU:HD21	1.71	0.72
1:E:239:PRO:O	4:E:591:HOH:O	2.06	0.72
1:E:165:VAL:O	1:E:170:LYS:NZ	2.23	0.71
2:I:53:LEU:O	2:I:57:GLY:N	2.24	0.70
2:I:7:TYR:O	2:I:7:TYR:CG	2.45	0.69
1:E:117:ASN:O	1:E:119:MET:HE2	1.92	0.69
2:I:104:ASN:HB3	4:I:185:HOH:O	1.91	0.69
2:I:60:LEU:HD11	4:I:181:HOH:O	1.93	0.69
1:E:104:TYR:O	1:E:108:ILE:HG13	1.92	0.68
2:I:23:THR:N	4:I:211:HOH:O	2.21	0.68
2:I:86:TRP:O	2:I:89:LYS:HB3	1.93	0.68
1:E:13:ALA:HB3	1:E:14:PRO:HD3	1.74	0.67
1:E:156:GLU:O	1:E:157:GLY:C	2.36	0.67
2:I:87:GLN:HG2	4:I:207:HOH:O	1.95	0.67
2:I:48:SER:O	2:I:52:ASP:N	2.28	0.65
2:I:10:SER:O	2:I:34:THR:HG23	1.96	0.65
1:E:64:HIS:CD2	2:I:74:VAL:CG1	2.79	0.65
1:E:31:ILE:HG23	1:E:93:VAL:CG1	2.27	0.65
2:I:44:PRO:HB3	4:I:132:HOH:O	1.81	0.64
2:I:29:ARG:HG2	2:I:29:ARG:HH11	1.62	0.64
2:I:56:VAL:HG21	2:I:63:LEU:HD13	1.79	0.64
2:I:86:TRP:HE3	2:I:87:GLN:HB2	1.63	0.64
2:I:86:TRP:CD1	4:I:177:HOH:O	2.52	0.63
2:I:35:CYS:CB	2:I:50:CYS:SG	2.86	0.63
2:I:18:LYS:O	4:I:167:HOH:O	2.15	0.62
2:I:56:VAL:HG12	2:I:56:VAL:O	1.98	0.62
1:E:16:LEU:HD22	1:E:270:VAL:HG13	1.81	0.62
1:E:71:THR:HG21	1:E:226:HIS:CE1	2.35	0.62
1:E:195:GLU:N	1:E:195:GLU:OE1	2.33	0.61
2:I:60:LEU:CD1	4:I:181:HOH:O	2.49	0.60
1:E:192:VAL:HG23	1:E:261:PHE:CE1	2.37	0.60
2:I:8:ALA:HB3	2:I:36:ALA:CB	2.32	0.60
2:I:73:LYS:HA	2:I:73:LYS:HE2	1.84	0.60
1:E:135:LEU:O	1:E:138:ALA:HB3	2.02	0.60
2:I:8:ALA:HB3	2:I:36:ALA:HB1	1.84	0.60
2:I:43:HIS:C	2:I:45:ALA:N	2.58	0.60
2:I:60:LEU:O	2:I:61:ASN:HB2	2.02	0.59
1:E:74:ALA:CB	1:E:81:VAL:HG23	2.32	0.59
1:E:64:HIS:CE1	2:I:72:PRO:HB3	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:192:VAL:HB	1:E:261:PHE:O	2.03	0.59
2:I:85:VAL:HA	2:I:89:LYS:O	2.02	0.59
2:I:63:LEU:O	2:I:64:THR:C	2.46	0.59
1:E:96:LEU:HD13	2:I:72:PRO:HG3	1.85	0.58
1:E:44:VAL:HG12	1:E:44:VAL:O	2.03	0.58
2:I:49:ALA:O	2:I:52:ASP:N	2.37	0.58
1:E:139:VAL:CG1	1:E:174:VAL:HG23	2.21	0.58
2:I:52:ASP:O	2:I:55:ALA:HB3	2.04	0.58
2:I:18:LYS:C	4:I:167:HOH:O	2.46	0.57
1:E:1:ALA:CB	4:E:513:HOH:O	2.52	0.57
1:E:74:ALA:HB1	1:E:81:VAL:HG23	1.86	0.57
2:I:7:TYR:O	2:I:9:PRO:HD3	2.05	0.57
1:E:130:SER:OG	2:I:67:GLU:HA	2.04	0.56
2:I:21:SER:O	2:I:25:ALA:HB3	2.05	0.56
1:E:10:GLN:HG2	1:E:267:LEU:HD11	1.87	0.56
1:E:221:SER:HB2	2:I:73:LYS:O	2.06	0.56
1:E:56:ASN:OD1	1:E:57:PRO:HD2	2.05	0.56
1:E:1:ALA:HB2	4:E:513:HOH:O	2.06	0.56
1:E:256:LYS:HD2	4:E:626:HOH:O	2.05	0.56
2:I:111:PHE:CA	2:I:113:PHE:O	2.52	0.56
1:E:136:LYS:HG3	1:E:171:TYR:CD1	2.42	0.55
1:E:10:GLN:NE2	1:E:184:ASN:OD1	2.38	0.55
1:E:62:ASN:OD1	1:E:64:HIS:HB2	2.07	0.54
1:E:244:THR:O	1:E:248:SER:HB2	2.08	0.54
1:E:63:SER:HB2	1:E:210:PRO:CD	2.38	0.54
1:E:270:VAL:O	1:E:270:VAL:HG22	2.07	0.54
1:E:29:ALA:HB2	1:E:119:MET:HG3	1.90	0.54
2:I:68:ASP:CB	4:I:190:HOH:O	2.49	0.53
2:I:60:LEU:O	2:I:61:ASN:CB	2.56	0.53
2:I:73:LYS:HA	2:I:73:LYS:CE	2.39	0.53
1:E:27:LYS:HD3	4:E:542:HOH:O	2.08	0.53
1:E:64:HIS:CD2	2:I:74:VAL:HG13	2.43	0.53
2:I:60:LEU:N	2:I:60:LEU:HD22	2.23	0.53
2:I:85:VAL:HG12	2:I:90:ARG:HA	1.89	0.53
1:E:127:GLY:HA2	1:E:167:TYR:O	2.08	0.53
2:I:79:LEU:HD12	2:I:96:VAL:CG1	2.39	0.53
1:E:130:SER:CB	2:I:67:GLU:OE1	2.56	0.53
2:I:99:ASN:ND2	4:I:117:HOH:O	2.42	0.53
2:I:50:CYS:HA	2:I:53:LEU:HD12	1.90	0.52
2:I:87:GLN:O	2:I:88:GLY:C	2.52	0.52
1:E:44:VAL:HG11	1:E:58:PHE:CE1	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:86:TRP:CZ3	2:I:87:GLN:HB2	2.45	0.52
2:I:44:PRO:CA	4:I:132:HOH:O	2.44	0.52
2:I:102:GLU:OE2	4:I:116:HOH:O	2.19	0.52
2:I:49:ALA:O	2:I:50:CYS:C	2.53	0.52
2:I:14:LEU:HB3	2:I:113:PHE:CE1	2.45	0.51
1:E:64:HIS:CD2	2:I:74:VAL:HG11	2.46	0.51
2:I:97:PHE:HA	4:I:138:HOH:O	2.09	0.51
2:I:35:CYS:HB3	2:I:50:CYS:HB3	1.93	0.51
2:I:35:CYS:SG	2:I:50:CYS:CB	2.99	0.51
1:E:224:SER:N	1:E:225:PRO:HD2	2.26	0.51
1:E:142:ALA:O	1:E:145:SER:HB2	2.11	0.51
1:E:64:HIS:HD2	2:I:74:VAL:HG11	1.76	0.50
2:I:35:CYS:CB	2:I:50:CYS:HG	2.15	0.50
2:I:65:ARG:HH12	2:I:66:GLY:HA3	1.75	0.50
1:E:142:ALA:O	1:E:147:VAL:HG23	2.11	0.50
1:E:31:ILE:HG23	1:E:93:VAL:HB	1.93	0.50
2:I:79:LEU:HD12	2:I:96:VAL:HG12	1.94	0.50
1:E:64:HIS:NE2	2:I:74:VAL:HG13	2.27	0.50
1:E:136:LYS:HB2	1:E:171:TYR:CZ	2.47	0.50
2:I:7:TYR:CE2	2:I:9:PRO:HG3	2.47	0.49
1:E:172:PRO:HD2	4:E:634:HOH:O	2.12	0.49
2:I:60:LEU:HD21	4:I:181:HOH:O	2.11	0.49
2:I:64:THR:HG23	4:I:183:HOH:O	2.13	0.49
1:E:124:MET:O	1:E:151:ALA:HA	2.12	0.49
2:I:84:GLY:O	2:I:91:VAL:N	2.46	0.49
1:E:252:ASN:HA	4:E:653:HOH:O	2.12	0.48
2:I:44:PRO:HA	4:I:132:HOH:O	2.10	0.48
1:E:154:GLY:O	1:E:220:THR:HG21	2.13	0.48
1:E:175:ILE:HG12	1:E:247:ARG:HD2	1.96	0.48
1:E:35:ILE:HD13	1:E:69:ALA:CB	2.44	0.48
1:E:187:ALA:HB2	1:E:203:VAL:CG2	2.43	0.48
2:I:113:PHE:HA	4:I:192:HOH:O	2.14	0.47
2:I:97:PHE:CE1	2:I:103:MET:HG3	2.49	0.47
2:I:18:LYS:HE3	2:I:78:VAL:CG2	2.41	0.47
1:E:139:VAL:HG13	1:E:149:VAL:HG11	1.97	0.47
2:I:91:VAL:HA	4:I:145:HOH:O	2.14	0.47
2:I:95:ARG:HD2	2:I:97:PHE:CZ	2.50	0.47
1:E:212:ASN:N	4:E:521:HOH:O	2.41	0.47
1:E:3:SER:O	1:E:81:VAL:HA	2.15	0.46
1:E:12:LYS:HB3	1:E:271:GLN:HB2	1.97	0.46
1:E:67:HIS:CE1	1:E:205:ILE:O	2.68	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:222:MET:O	1:E:226:HIS:ND1	2.49	0.46
2:I:90:ARG:C	2:I:91:VAL:HG23	2.41	0.46
1:E:157:GLY:HA2	1:E:190:SER:O	2.15	0.46
1:E:184:ASN:OD1	1:E:267:LEU:HD22	2.14	0.46
2:I:112:ALA:HB1	4:I:195:HOH:O	2.16	0.46
1:E:31:ILE:HG22	1:E:95:VAL:HG13	1.97	0.46
2:I:21:SER:HA	2:I:79:LEU:HD13	1.97	0.46
2:I:100:GLU:N	4:I:137:HOH:O	2.48	0.46
1:E:35:ILE:HD13	1:E:69:ALA:HB2	1.96	0.46
2:I:52:ASP:OD2	2:I:108:SER:OG	2.27	0.46
2:I:54:ALA:O	2:I:57:GLY:N	2.44	0.46
1:E:193:GLY:HA2	1:E:261:PHE:CE2	2.51	0.46
2:I:60:LEU:N	4:I:146:HOH:O	2.41	0.46
2:I:86:TRP:CH2	4:I:207:HOH:O	2.67	0.46
1:E:115:ILE:HG12	1:E:142:ALA:HA	1.98	0.45
1:E:247:ARG:NE	1:E:251:GLU:OE2	2.48	0.45
2:I:56:VAL:CG1	2:I:62:ALA:HB3	2.46	0.45
2:I:31:VAL:CB	2:I:42:THR:O	2.52	0.45
1:E:156:GLU:O	1:E:157:GLY:O	2.33	0.45
1:E:46:GLY:O	1:E:91:TYR:HA	2.16	0.45
1:E:9:SER:O	1:E:10:GLN:C	2.60	0.45
2:I:53:LEU:O	2:I:54:ALA:C	2.60	0.45
2:I:60:LEU:N	2:I:60:LEU:CD2	2.80	0.45
2:I:109:SER:O	2:I:112:ALA:HB3	2.17	0.45
2:I:65:ARG:HH11	2:I:66:GLY:N	2.15	0.45
2:I:60:LEU:CD2	2:I:60:LEU:H	2.30	0.44
1:E:227:VAL:O	1:E:230:ALA:HB3	2.17	0.44
2:I:60:LEU:C	2:I:61:ASN:HD22	2.26	0.44
2:I:65:ARG:HH11	2:I:66:GLY:H	1.65	0.44
1:E:6:TYR:O	1:E:9:SER:HB2	2.17	0.44
1:E:242:THR:H	1:E:245:GLN:HG3	1.83	0.44
1:E:139:VAL:CG1	1:E:174:VAL:CG2	2.83	0.44
1:E:169:GLY:HA2	1:E:174:VAL:HG11	2.00	0.44
2:I:21:SER:CA	2:I:79:LEU:HD13	2.47	0.44
2:I:109:SER:CA	2:I:112:ALA:HB2	2.37	0.44
2:I:60:LEU:CD2	4:I:181:HOH:O	2.65	0.43
1:E:169:GLY:HA2	1:E:174:VAL:CG1	2.49	0.43
1:E:252:ASN:CG	4:E:653:HOH:O	2.61	0.43
2:I:22:ALA:CB	4:I:219:HOH:O	2.60	0.43
2:I:56:VAL:O	2:I:56:VAL:CG1	2.66	0.43
2:I:37:PRO:CD	2:I:38:GLY:H	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:108:SER:OG	2:I:109:SER:N	2.50	0.43
2:I:87:GLN:O	2:I:89:LYS:N	2.51	0.43
1:E:206:GLN:HE21	1:E:206:GLN:HB3	1.09	0.43
2:I:16:VAL:HA	2:I:79:LEU:O	2.17	0.43
2:I:60:LEU:O	2:I:61:ASN:ND2	2.52	0.43
1:E:67:HIS:NE2	1:E:205:ILE:O	2.52	0.43
2:I:64:THR:O	2:I:106:HIS:O	2.35	0.43
2:I:90:ARG:O	2:I:91:VAL:HG23	2.18	0.43
2:I:103:MET:O	2:I:106:HIS:HB2	2.19	0.43
1:E:31:ILE:HG23	1:E:93:VAL:CB	2.49	0.43
1:E:84:VAL:C	1:E:86:PRO:HD3	2.43	0.43
1:E:247:ARG:O	1:E:248:SER:C	2.60	0.43
2:I:80:LEU:HD21	2:I:111:PHE:CZ	2.54	0.43
1:E:192:VAL:CG2	1:E:261:PHE:CE1	3.02	0.42
2:I:38:GLY:HA2	2:I:39:PRO:HD3	1.84	0.42
1:E:154:GLY:HA2	2:I:73:LYS:HD3	2.01	0.42
2:I:65:ARG:NH1	2:I:66:GLY:CA	2.76	0.42
1:E:3:SER:O	1:E:5:PRO:HD3	2.20	0.42
2:I:7:TYR:O	2:I:7:TYR:CD2	2.72	0.42
2:I:15:THR:HA	2:I:29:ARG:O	2.20	0.42
2:I:16:VAL:HG21	2:I:103:MET:HE1	2.01	0.42
2:I:111:PHE:HB3	2:I:113:PHE:O	2.20	0.42
1:E:63:SER:O	1:E:64:HIS:C	2.63	0.42
1:E:177:VAL:HG12	1:E:223:ALA:HB1	2.02	0.42
1:E:245:GLN:HE21	1:E:245:GLN:HB3	1.65	0.42
2:I:8:ALA:HB3	2:I:36:ALA:HB2	2.01	0.42
1:E:31:ILE:CG2	1:E:93:VAL:HG12	2.50	0.41
1:E:39:HIS:CD2	1:E:209:LEU:O	2.73	0.41
1:E:234:ILE:HD11	1:E:273:ALA:CB	2.50	0.41
1:E:195:GLU:HG3	4:E:633:HOH:O	2.19	0.41
1:E:44:VAL:CG1	1:E:58:PHE:CE1	3.04	0.41
1:E:73:ALA:O	1:E:74:ALA:C	2.60	0.41
1:E:63:SER:HB2	1:E:210:PRO:HD2	2.02	0.41
2:I:18:LYS:HB3	4:I:144:HOH:O	2.20	0.41
2:I:13:VAL:HA	2:I:31:VAL:O	2.20	0.41
2:I:64:THR:O	2:I:65:ARG:O	2.38	0.41
2:I:96:VAL:HG23	2:I:96:VAL:O	2.21	0.41
1:E:170:LYS:HG2	1:E:195:GLU:HG2	2.01	0.41
1:E:177:VAL:HG22	1:E:227:VAL:HG21	2.03	0.41
2:I:35:CYS:SG	2:I:50:CYS:HA	2.61	0.41
1:E:43:LYS:O	4:E:524:HOH:O	2.22	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:107:ILE:O	1:E:108:ILE:C	2.64	0.41
1:E:243:ASN:N	1:E:243:ASN:OD1	2.53	0.41
2:I:11:ALA:O	2:I:84:GLY:HA3	2.20	0.41
2:I:17:GLY:HA3	2:I:26:ALA:O	2.21	0.41
2:I:54:ALA:O	2:I:55:ALA:C	2.63	0.41
1:E:165:VAL:HG11	1:E:195:GLU:HB2	2.01	0.41
2:I:37:PRO:HD2	2:I:38:GLY:H	1.86	0.41
2:I:67:GLU:HA	2:I:67:GLU:OE1	2.21	0.41
2:I:71:CYS:HB3	2:I:101:CYS:HB3	1.94	0.40
1:E:71:THR:O	1:E:71:THR:HG22	2.20	0.40
2:I:50:CYS:CA	2:I:53:LEU:HD12	2.51	0.40
1:E:113:TRP:CE3	1:E:113:TRP:C	3.00	0.40
4:E:601:HOH:O	2:I:74:VAL:CB	2.57	0.40
2:I:7:TYR:O	2:I:7:TYR:CD1	2.74	0.40
2:I:34:THR:O	2:I:39:PRO:HA	2.21	0.40
1:E:31:ILE:HG23	1:E:93:VAL:HG12	2.03	0.40
2:I:52:ASP:O	2:I:53:LEU:C	2.64	0.40
2:I:97:PHE:CE2	2:I:106:HIS:CD2	3.10	0.40

All (3) 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:133:HOH:O	4:I:133:HOH:O[4_555]	1.93	0.27
1:E:275:GLN:O	4:E:532:HOH:O[6_555]	2.04	0.16
2:I:23:THR:OG1	2:I:90:ARG:NE[2_555]	2.04	0.16

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%)	247 (90%)	20 (7%)	6 (2%)	5 3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	I	105/107 (98%)	72 (69%)	25 (24%)	8 (8%)	1	0
All	All	378/382 (99%)	319 (84%)	45 (12%)	14 (4%)	2	1

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	I	24	THR
2	I	25	ALA
2	I	45	ALA
2	I	65	ARG
1	E	63	SER
2	I	61	ASN
1	E	32	ASP
1	E	36	ASP
1	E	157	GLY
2	I	22	ALA
2	I	67	GLU
2	I	108	SER
1	E	75	LEU
1	E	159	SER

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	205/205 (100%)	176 (86%)	29 (14%)	3	3
2	I	79/79 (100%)	57 (72%)	22 (28%)	0	0
All	All	284/284 (100%)	233 (82%)	51 (18%)	2	1

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	16	LEU
1	E	27	LYS

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Mol	Chain	Res	Type
1	E	31	ILE
1	E	43	LYS
1	E	44	VAL
1	E	59	GLN
1	E	63	SER
1	E	75	LEU
1	E	79	ILE
1	E	84	VAL
1	E	87	SER
1	E	103	GLN
1	E	105	SER
1	E	126	LEU
1	E	147	VAL
1	E	174	VAL
1	E	185	GLN
1	E	186	ARG
1	E	192	VAL
1	E	198	VAL
1	E	204	SER
1	E	206	GLN
1	E	221	SER
1	E	240	ASN
1	E	248	SER
1	E	252	ASN
1	E	259	ASP
1	E	265	LYS
1	E	267	LEU
2	I	7	TYR
2	I	13	VAL
2	I	18	LYS
2	I	20	VAL
2	I	24	THR
2	I	29	ARG
2	I	33	LEU
2	I	53	LEU
2	I	60	LEU
2	I	63	LEU
2	I	67	GLU
2	I	68	ASP
2	I	69	VAL
2	I	78	VAL
2	I	87	GLN

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Mol	Chain	Res	Type
2	I	89	LYS
2	I	94	GLU
2	I	95	ARG
2	I	106	HIS
2	I	109	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	206	GLN
1	E	240	ASN
1	E	245	GLN
1	E	271	GLN
2	I	43	HIS
2	I	61	ASN
2	I	106	HIS

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 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.