



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 05:23 AM UTC

PDB ID : 1SUA / pdb_00001sua
Title : SUBTILISIN BPN'
Authors : Almog, O.; Gilliland, G.L.
Deposited on : 1997-01-14
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

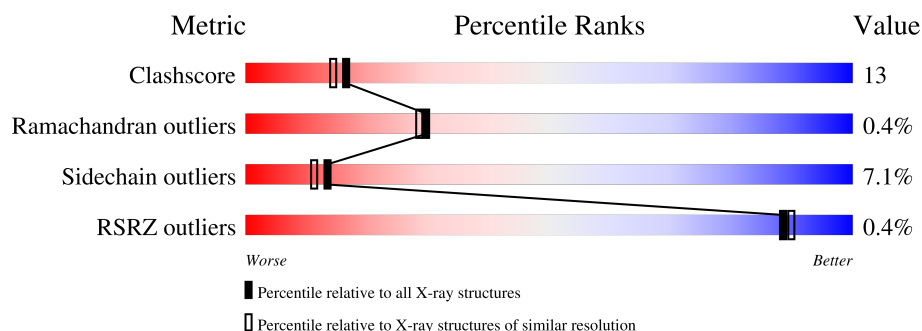
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

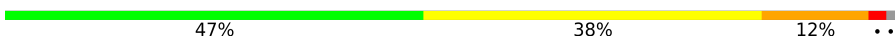
The reported resolution of this entry is 2.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	266	
2	C	4	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2018 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	A	263	Total	C	N	O	S	0	1	0
			1852	1153	318	377	4			

There are 17 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	43	ASN	LYS	engineered mutation	UNP P00782
A	50	PHE	MET	engineered mutation	UNP P00782
A	73	LEU	ALA	engineered mutation	UNP P00782
A	?	-	LEU	deletion	UNP P00782
A	?	-	ASN	deletion	UNP P00782
A	?	-	ASN	deletion	UNP P00782
A	?	-	SER	deletion	UNP P00782
A	?	-	ILE	deletion	UNP P00782
A	?	-	GLY	deletion	UNP P00782
A	?	-	VAL	deletion	UNP P00782
A	?	-	LEU	deletion	UNP P00782
A	?	-	GLY	deletion	UNP P00782
A	206	VAL	GLN	engineered mutation	UNP P00782
A	217	LYS	TYR	engineered mutation	UNP P00782
A	218	SER	ASN	engineered mutation	UNP P00782
A	221	ALA	SER	engineered mutation	UNP P00782
A	271	GLU	GLN	engineered mutation	UNP P00782

- Molecule 2 is a protein called TETRAPEPTIDE ALA-LEU-ALA-LEU.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	4	Total	C	N	O	0	0	0
			27	18	4	5			

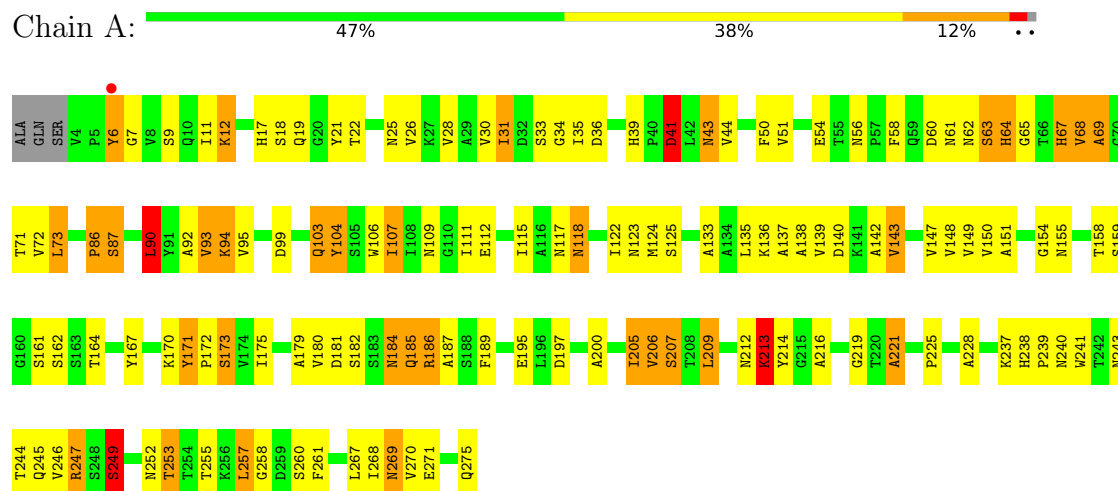
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	137	Total 137	O 137	0	0
3	C	2	Total 2	O 2	0	0

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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: SUBTILISIN BPN'



• Molecule 2: TETRAPEPTIDE ALA-LEU-ALA-LEU



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	53.53Å 60.33Å 83.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.10 8.00 – 2.14	Depositor EDS
% Data completeness (in resolution range)	82.0 (8.00-2.10) 65.8 (8.00-2.14)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	PROLSQ	Depositor
R, R_{free}	0.180 , (Not available) 0.161 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	11.4	Xtriage
Anisotropy	1.096	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 61.4	EDS
L-test for twinning ¹	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	2018	wwPDB-VP
Average B, all atoms (Å ²)	10.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.05% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Theoretical 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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.47	4/1895 (0.2%)	2.74	172/2587 (6.6%)
2	C	1.15	0/26	2.42	1/33 (3.0%)
All	All	1.47	4/1921 (0.2%)	2.73	173/2620 (6.6%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	257	LEU	CA-C	-8.97	1.48	1.53
1	A	257	LEU	N-CA	7.52	1.50	1.46
1	A	200	ALA	C-O	5.93	1.29	1.24
1	A	22	THR	CA-CB	5.73	1.63	1.53

All (173) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	41	ASP	CA-CB-CG	18.55	131.15	112.60
1	A	43	ASN	CA-CB-CG	15.76	128.36	112.60
1	A	50	PHE	CA-C-N	13.06	131.48	122.60
1	A	50	PHE	C-N-CA	13.06	131.48	122.60
1	A	118	ASN	CA-CB-CG	12.44	125.03	112.60
1	A	239	PRO	CA-C-N	12.13	141.30	120.68
1	A	239	PRO	C-N-CA	12.13	141.30	120.68
1	A	99	ASP	CA-CB-CG	11.76	124.36	112.60
1	A	243	ASN	CA-CB-CG	11.35	123.95	112.60
1	A	228	ALA	CA-C-N	10.36	131.39	120.00
1	A	228	ALA	C-N-CA	10.36	131.39	120.00
1	A	62	ASN	CA-C-N	10.12	140.86	121.54
1	A	62	ASN	C-N-CA	10.12	140.86	121.54
1	A	56	ASN	CB-CA-C	9.84	121.06	109.85
1	A	212	ASN	CA-CB-CG	9.71	122.31	112.60
1	A	155	ASN	CA-CB-CG	9.61	122.21	112.60
1	A	56	ASN	CA-CB-CG	9.19	121.79	112.60
1	A	103	GLN	CB-CG-CD	8.96	127.83	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	17	HIS	CA-CB-CG	8.78	122.58	113.80
1	A	184	ASN	CA-CB-CG	8.69	121.29	112.60
1	A	106	TRP	CA-C-N	8.65	131.46	120.56
1	A	106	TRP	C-N-CA	8.65	131.46	120.56
1	A	60	ASP	CA-CB-CG	8.61	121.21	112.60
1	A	109	ASN	CA-C-N	8.59	129.45	120.00
1	A	109	ASN	C-N-CA	8.59	129.45	120.00
1	A	185	GLN	CB-CG-CD	8.46	126.98	112.60
1	A	207	SER	CA-C-N	8.41	132.67	120.82
1	A	207	SER	C-N-CA	8.41	132.67	120.82
1	A	180	VAL	CA-CB-CG2	8.35	124.59	110.40
1	A	181	ASP	CA-CB-CG	8.24	120.84	112.60
1	A	206	VAL	CB-CA-C	8.19	120.86	110.96
1	A	164	THR	CA-C-N	8.16	136.66	121.97
1	A	164	THR	C-N-CA	8.16	136.66	121.97
1	A	186	ARG	CD-NE-CZ	8.00	135.60	124.40
1	A	240	ASN	CA-C-N	7.65	131.73	120.87
1	A	240	ASN	C-N-CA	7.65	131.73	120.87
2	C	677	LEU	CB-CA-C	7.59	124.52	110.10
1	A	212	ASN	CB-CA-C	7.48	122.51	111.89
1	A	269	ASN	CA-CB-CG	7.46	120.06	112.60
1	A	221	ALA	CA-C-N	7.45	133.32	120.58
1	A	221	ALA	C-N-CA	7.45	133.32	120.58
1	A	9	SER	CA-C-N	7.32	130.41	120.38
1	A	9	SER	C-N-CA	7.32	130.41	120.38
1	A	137	ALA	CA-C-N	7.23	129.84	120.44
1	A	137	ALA	C-N-CA	7.23	129.84	120.44
1	A	31	ILE	CB-CA-C	7.20	120.89	112.68
1	A	107	ILE	N-CA-CB	7.19	118.96	110.55
1	A	133	ALA	CA-C-N	7.18	129.90	120.28
1	A	133	ALA	C-N-CA	7.18	129.90	120.28
1	A	28	VAL	CA-CB-CG2	7.13	122.52	110.40
1	A	58	PHE	CA-CB-CG	7.06	120.86	113.80
1	A	61	ASN	CA-CB-CG	7.02	119.62	112.60
1	A	111	ILE	CA-C-N	6.93	129.57	120.28
1	A	111	ILE	C-N-CA	6.93	129.57	120.28
1	A	139	VAL	N-CA-CB	6.91	118.64	110.55
1	A	41	ASP	N-CA-CB	6.91	120.09	110.07
1	A	54	GLU	CB-CG-CD	6.89	124.32	112.60
1	A	109	ASN	CA-CB-CG	6.86	119.46	112.60
1	A	206	VAL	N-CA-CB	6.78	118.72	111.00
1	A	161	SER	CA-C-N	6.74	132.58	121.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	161	SER	C-N-CA	6.74	132.58	121.39
1	A	12	LYS	CA-C-N	6.73	130.93	120.97
1	A	12	LYS	C-N-CA	6.73	130.93	120.97
1	A	257	LEU	CB-CA-C	6.72	126.74	117.07
1	A	179	ALA	N-CA-C	6.71	119.87	109.07
1	A	26	VAL	CA-C-N	6.65	131.48	122.84
1	A	26	VAL	C-N-CA	6.65	131.48	122.84
1	A	69	ALA	CA-C-N	6.60	127.31	119.98
1	A	69	ALA	C-N-CA	6.60	127.31	119.98
1	A	60	ASP	CB-CA-C	6.58	122.53	111.22
1	A	6	TYR	N-CA-C	6.57	119.28	111.33
1	A	25	ASN	CA-CB-CG	6.51	119.11	112.60
1	A	197	ASP	CA-CB-CG	6.46	119.06	112.60
1	A	252	ASN	CA-CB-CG	6.44	119.04	112.60
1	A	36	ASP	CA-CB-CG	6.42	119.02	112.60
1	A	125	SER	CA-C-N	6.37	132.53	122.21
1	A	125	SER	C-N-CA	6.37	132.53	122.21
1	A	150	VAL	CB-CA-C	6.37	120.12	110.62
1	A	64	HIS	CA-C-N	6.35	127.03	119.98
1	A	64	HIS	C-N-CA	6.35	127.03	119.98
1	A	261	PHE	CA-CB-CG	6.33	120.13	113.80
1	A	106	TRP	CA-CB-CG	6.24	125.45	113.60
1	A	213	LYS	CA-C-N	6.18	132.49	122.29
1	A	213	LYS	C-N-CA	6.18	132.49	122.29
1	A	249	SER	CA-C-N	6.18	128.84	120.44
1	A	249	SER	C-N-CA	6.18	128.84	120.44
1	A	270	VAL	CB-CA-C	6.14	121.67	112.16
1	A	173	SER	CA-C-N	6.10	130.70	122.90
1	A	173	SER	C-N-CA	6.10	130.70	122.90
1	A	171	TYR	CA-C-N	6.08	125.80	119.05
1	A	171	TYR	C-N-CA	6.08	125.80	119.05
1	A	106	TRP	CB-CA-C	6.05	120.38	110.88
1	A	244	THR	CB-CA-C	6.02	120.79	110.79
1	A	72	VAL	CA-C-N	6.00	128.32	120.28
1	A	72	VAL	C-N-CA	6.00	128.32	120.28
1	A	244	THR	CA-C-N	5.98	128.30	120.28
1	A	244	THR	C-N-CA	5.98	128.30	120.28
1	A	25	ASN	CB-CA-C	5.94	121.93	111.06
1	A	261	PHE	CA-C-N	5.94	133.93	122.53
1	A	261	PHE	C-N-CA	5.94	133.93	122.53
1	A	73	LEU	CB-CA-C	5.92	120.62	110.79
1	A	112	GLU	CA-C-N	5.89	128.09	120.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	112	GLU	C-N-CA	5.89	128.09	120.44
1	A	143	VAL	N-CA-CB	5.86	117.41	110.55
1	A	158	THR	CA-CB-CG2	5.86	120.46	110.50
1	A	258	GLY	CA-C-N	5.84	129.00	120.71
1	A	258	GLY	C-N-CA	5.84	129.00	120.71
1	A	103	GLN	CA-CB-CG	5.82	125.74	114.10
1	A	30	VAL	CB-CA-C	5.81	119.08	111.53
1	A	93	VAL	CB-CA-C	5.77	119.03	111.53
1	A	140	ASP	CA-CB-CG	5.76	118.36	112.60
1	A	7	GLY	CA-C-N	5.72	127.77	120.56
1	A	7	GLY	C-N-CA	5.72	127.77	120.56
1	A	90	LEU	CB-CA-C	5.70	118.94	109.53
1	A	87	SER	CA-CB-OG	5.70	122.50	111.10
1	A	255	THR	N-CA-CB	5.61	119.14	110.21
1	A	117	ASN	O-C-N	-5.60	115.16	122.39
1	A	43	ASN	OD1-CG-ND2	-5.59	117.01	122.60
1	A	44	VAL	CA-CB-CG2	5.53	119.81	110.40
1	A	18	SER	CA-C-N	5.51	129.92	120.72
1	A	18	SER	C-N-CA	5.51	129.92	120.72
1	A	104	TYR	CB-CA-C	5.51	119.93	110.79
1	A	246	VAL	CB-CA-C	5.50	119.00	111.97
1	A	270	VAL	CA-C-N	5.48	128.08	120.29
1	A	270	VAL	C-N-CA	5.48	128.08	120.29
1	A	117	ASN	CA-C-N	5.47	129.90	122.19
1	A	117	ASN	C-N-CA	5.47	129.90	122.19
1	A	63	SER	N-CA-CB	5.47	119.73	110.49
1	A	170	LYS	CA-C-N	5.46	128.07	120.65
1	A	170	LYS	C-N-CA	5.46	128.07	120.65
1	A	44	VAL	CB-CA-C	5.43	118.89	110.96
1	A	185	GLN	CA-CB-CG	5.42	124.94	114.10
1	A	123	ASN	N-CA-CB	5.41	119.77	110.68
1	A	238	HIS	CA-C-N	5.41	125.23	119.28
1	A	238	HIS	C-N-CA	5.41	125.23	119.28
1	A	164	THR	CB-CA-C	5.41	119.06	109.65
1	A	205	ILE	CB-CA-C	5.40	117.50	110.96
1	A	71	THR	CA-C-N	5.36	127.32	120.56
1	A	71	THR	C-N-CA	5.36	127.32	120.56
1	A	155	ASN	CA-C-O	5.34	128.15	120.51
1	A	184	ASN	CA-C-N	5.33	129.99	122.09
1	A	184	ASN	C-N-CA	5.33	129.99	122.09
1	A	71	THR	CB-CA-C	5.32	119.89	110.85
1	A	271	GLU	CA-CB-CG	5.31	124.72	114.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	28	VAL	CA-CB-CG1	5.26	119.35	110.40
1	A	67	HIS	CA-C-N	5.25	127.17	120.56
1	A	67	HIS	C-N-CA	5.25	127.17	120.56
1	A	148	VAL	CA-CB-CG2	5.24	119.30	110.40
1	A	68	VAL	CB-CA-C	5.22	118.65	111.97
1	A	73	LEU	N-CA-CB	5.21	117.78	110.12
1	A	138	ALA	CA-C-N	5.21	127.12	120.56
1	A	138	ALA	C-N-CA	5.21	127.12	120.56
1	A	149	VAL	CB-CA-C	5.21	118.56	110.96
1	A	253	THR	CA-CB-CG2	5.20	119.35	110.50
1	A	247	ARG	NE-CZ-NH1	5.19	126.69	121.50
1	A	195	GLU	CA-C-N	5.16	128.67	121.24
1	A	195	GLU	C-N-CA	5.16	128.67	121.24
1	A	187	ALA	CA-C-N	5.14	127.89	120.38
1	A	187	ALA	C-N-CA	5.14	127.89	120.38
1	A	241	TRP	CA-CB-CG	5.11	123.31	113.60
1	A	205	ILE	CA-CB-CG2	5.10	119.18	110.50
1	A	86	PRO	CB-CA-C	5.10	120.17	112.21
1	A	39	HIS	CA-C-N	5.09	125.13	119.32
1	A	39	HIS	C-N-CA	5.09	125.13	119.32
1	A	73	LEU	N-CA-C	5.09	116.83	111.28
1	A	51	VAL	CA-C-O	5.09	121.97	119.12
1	A	209	LEU	CB-CA-C	5.08	117.28	109.15
1	A	142	ALA	CA-C-N	5.07	126.95	120.56
1	A	142	ALA	C-N-CA	5.07	126.95	120.56
1	A	143	VAL	CB-CA-C	5.05	118.43	111.97
1	A	115	ILE	O-C-N	5.01	127.31	121.94
1	A	171	TYR	CA-CB-CG	5.01	122.92	113.90
1	A	260	SER	N-CA-C	5.01	117.47	111.71

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	A	1852	0	1807	48	0
2	C	27	0	31	6	0
3	A	137	0	0	5	0
3	C	2	0	0	0	0
All	All	2018	0	1838	48	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (48) 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:A:103:GLN:HG3	3:A:409:HOH:O	1.70	0.92
1:A:175:ILE:HD11	1:A:247:ARG:HG3	1.56	0.88
1:A:68:VAL:HG13	1:A:225:PRO:HG3	1.66	0.77
1:A:69:ALA:HB1	1:A:90:LEU:HD21	1.72	0.72
1:A:122:ILE:HD12	1:A:147:VAL:HG11	1.71	0.71
1:A:33:SER:O	1:A:94:LYS:HE3	1.91	0.70
1:A:206:VAL:HG13	1:A:216:ALA:HB2	1.83	0.61
1:A:34:GLY:O	1:A:65:GLY:HA3	2.03	0.59
1:A:189:PHE:CE1	1:A:219:GLY:HA2	2.38	0.59
1:A:221:ALA:HB2	2:C:677:LEU:C	2.30	0.57
1:A:143:VAL:HG21	1:A:173:SER:HB2	1.87	0.56
1:A:35:ILE:HD12	1:A:92:ALA:HB2	1.87	0.56
1:A:86:PRO:HB3	3:A:422:HOH:O	2.05	0.56
1:A:175:ILE:CD1	1:A:247:ARG:HG3	2.32	0.56
1:A:257:LEU:HD11	1:A:267:LEU:HB2	1.87	0.56
1:A:31:ILE:HD12	1:A:122:ILE:HG23	1.89	0.55
1:A:122:ILE:CD1	1:A:147:VAL:HG11	2.36	0.55
1:A:107:ILE:CD1	2:C:674:ALA:HB3	2.38	0.53
1:A:41:ASP:OD2	1:A:214:TYR:OH	2.23	0.53
1:A:12:LYS:HD2	1:A:269:ASN:ND2	2.24	0.52
1:A:206:VAL:CG1	1:A:216:ALA:HB2	2.38	0.52
1:A:21:TYR:CZ	1:A:237:LYS:HG3	2.46	0.50
1:A:73:LEU:HG	1:A:90:LEU:HD13	1.93	0.50
1:A:31:ILE:CG2	1:A:95:VAL:HG21	2.42	0.49
1:A:206:VAL:HG22	3:A:369:HOH:O	2.12	0.49
1:A:159:SER:O	1:A:162:SER:HB2	2.12	0.49
1:A:167:TYR:HD2	1:A:171:TYR:CZ	2.31	0.49
1:A:107:ILE:HD11	2:C:674:ALA:HB3	1.95	0.48
1:A:209:LEU:HB2	1:A:213:LYS:HB3	1.96	0.46
1:A:171:TYR:HA	1:A:172:PRO:HD3	1.81	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:MET:O	1:A:151:ALA:HA	2.16	0.46
1:A:154:GLY:HA2	2:C:677:LEU:HD13	1.97	0.46
1:A:245:GLN:HG3	3:A:348:HOH:O	2.15	0.46
1:A:31:ILE:HG23	1:A:95:VAL:HG21	1.97	0.45
1:A:205:ILE:O	1:A:216:ALA:HA	2.16	0.45
1:A:249:SER:O	1:A:253:THR:OG1	2.33	0.44
1:A:104:TYR:CE1	2:C:674:ALA:HB2	2.52	0.44
1:A:67:HIS:CD2	1:A:207:SER:HB3	2.54	0.43
1:A:31:ILE:HG12	1:A:93:VAL:CG1	2.48	0.42
1:A:21:TYR:CE2	1:A:237:LYS:HG3	2.53	0.42
1:A:6:TYR:CE2	1:A:182:SER:HB2	2.55	0.42
1:A:136:LYS:HG2	3:A:337:HOH:O	2.19	0.42
1:A:41:ASP:CG	1:A:214:TYR:HH	2.25	0.41
1:A:64:HIS:O	1:A:68:VAL:HG23	2.20	0.41
1:A:104:TYR:CE2	1:A:135:LEU:HD22	2.55	0.41
1:A:184:ASN:HB3	1:A:257:LEU:HD22	2.03	0.41
1:A:104:TYR:HE1	2:C:674:ALA:HB2	1.85	0.41
1:A:31:ILE:HG12	1:A:93:VAL:HG11	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	262/266 (98%)	249 (95%)	12 (5%)	1 (0%)	30	28
2	C	2/4 (50%)	2 (100%)	0	0	100	100
All	All	264/270 (98%)	251 (95%)	12 (4%)	1 (0%)	30	28

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	63	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	A	196/198 (99%)	182 (93%)	14 (7%)	13	11
2	C	2/2 (100%)	2 (100%)	0	100	100
All	All	198/200 (99%)	184 (93%)	14 (7%)	13	11

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ILE
1	A	19	GLN
1	A	41	ASP
1	A	43	ASN
1	A	87	SER
1	A	90	LEU
1	A	94	LYS
1	A	118	ASN
1	A	185	GLN
1	A	186	ARG
1	A	213	LYS
1	A	249	SER
1	A	268	ILE
1	A	275	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	GLN
1	A	61	ASN
1	A	117	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	263/266 (98%)	-0.68	1 (0%) 88 90	2, 9, 19, 28	1 (0%)
2	C	4/4 (100%)	-0.16	0 100 100	9, 9, 10, 11	4 (100%)
All	All	267/270 (98%)	-0.67	1 (0%) 88 90	2, 9, 19, 28	5 (1%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	6	TYR	2.7

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.