



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:54 PM UTC

PDB ID : 1BRS / pdb_00001brs
Title : PROTEIN-PROTEIN RECOGNITION: CRYSTAL STRUCTURAL ANALYSIS OF A BARNASE-BARSTAR COMPLEX AT 2.0-Å RESOLUTION
Authors : Buckle, A.M.; Schreiber, G.; Fersht, A.R.
Deposited on : 1994-03-11
Resolution : 2.00 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

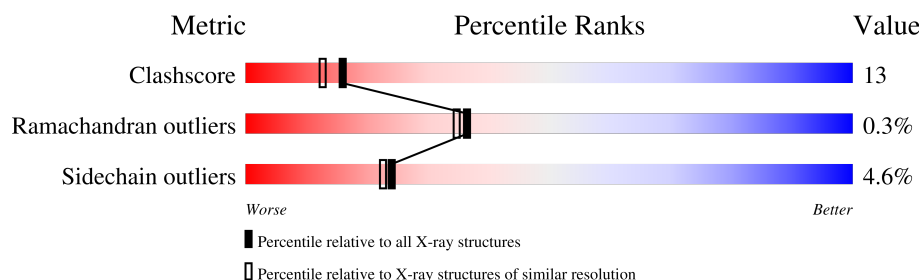
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)

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	A	110	65% 27% 5% .
1	B	110	69% 26% 5%
1	C	110	44% 45% 9% . .
2	D	89	56% 34% 8% .
2	E	89	65% 21% 8% . .
2	F	89	48% 43% 8% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5153 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 BARNASE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	108	Total	C	N	O	0	0	0
			864	547	150	167			
1	B	110	Total	C	N	O	0	0	0
			878	555	153	170			
1	C	108	Total	C	N	O	0	0	0
			839	533	146	160			

- Molecule 2 is a protein called BARSTAR.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	87	Total	C	N	O	0	1	0
			695	449	112	134			
2	E	86	Total	C	N	O	0	0	0
			665	430	103	132			
2	F	89	Total	C	N	O	0	0	0
			699	450	116	133			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	40	ALA	CYS	conflict	UNP P11540
D	82	ALA	CYS	conflict	UNP P11540
E	40	ALA	CYS	conflict	UNP P11540
E	82	ALA	CYS	conflict	UNP P11540
F	40	ALA	CYS	conflict	UNP P11540
F	82	ALA	CYS	conflict	UNP P11540

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	145	Total	O	0	0
			145	145		

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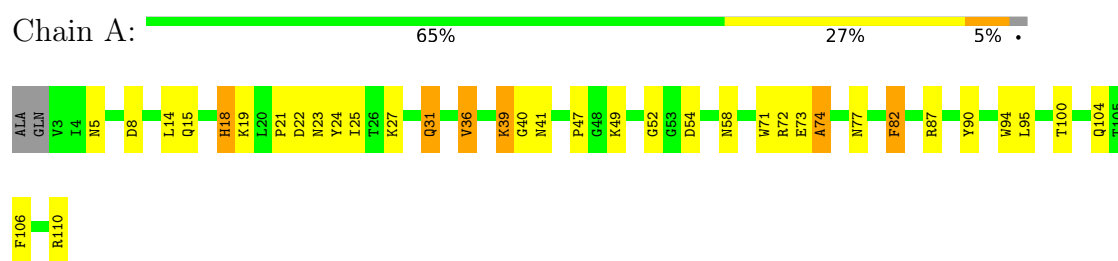
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	137	Total 137	O 137	0	0
3	C	50	Total 50	O 50	0	0
3	D	77	Total 77	O 77	0	0
3	E	64	Total 64	O 64	0	0
3	F	40	Total 40	O 40	0	0

3 Residue-property plots

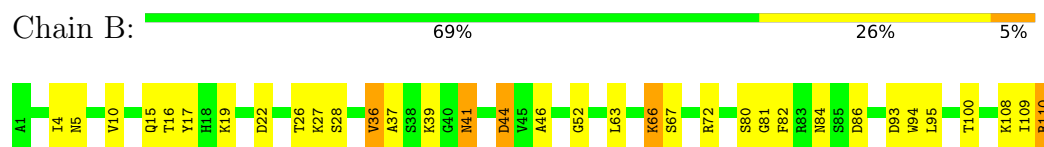
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

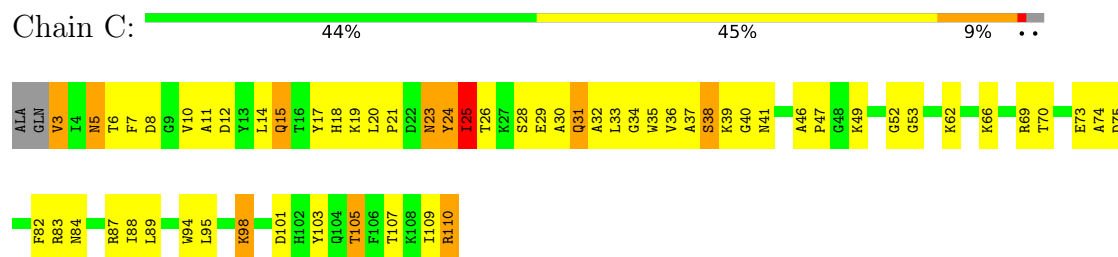
• Molecule 1: BARNASE



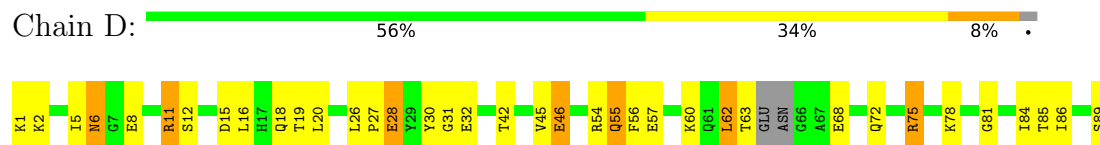
• Molecule 1: BARNASE



• Molecule 1: BARNASE



• Molecule 2: BARSTAR

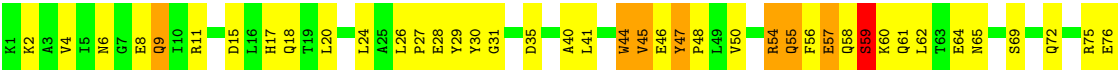


• Molecule 2: BARSTAR





● Molecule 2: BARSTAR



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	207.25Å 43.86Å 84.71Å 90.00° 107.76° 90.00°	Depositor
Resolution (Å)	7.00 – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) (7.00-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.172 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5153	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

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	1.12	1/885 (0.1%)	2.19	40/1197 (3.3%)
1	B	1.02	1/899 (0.1%)	2.15	33/1216 (2.7%)
1	C	0.82	0/860	2.20	45/1168 (3.9%)
2	D	0.93	0/711	2.13	30/962 (3.1%)
2	E	0.95	1/677 (0.1%)	2.39	26/919 (2.8%)
2	F	0.90	0/712	2.32	47/966 (4.9%)
All	All	0.97	3/4744 (0.1%)	2.22	221/6428 (3.4%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	110	ARG	C-O	15.50	1.54	1.23
1	B	110	ARG	C-O	10.73	1.45	1.23
2	E	89	SER	C-O	-8.42	1.06	1.23

All (221) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	75	ARG	CD-NE-CZ	33.72	171.60	124.40
2	E	75	ARG	NE-CZ-NH2	13.18	131.06	119.20
2	D	75	ARG	CD-NE-CZ	11.54	140.56	124.40
1	B	82	PHE	CA-CB-CG	-10.47	103.33	113.80
2	E	15	ASP	CA-CB-CG	-9.89	102.71	112.60
2	F	11	ARG	CD-NE-CZ	9.85	138.19	124.40
1	A	18	HIS	CA-CB-CG	-9.26	104.54	113.80
2	F	61	GLN	CA-CB-CG	8.94	131.98	114.10
2	F	61	GLN	N-CA-CB	8.89	122.90	110.01
1	C	24	TYR	CA-CB-CG	-8.83	98.00	113.90
2	F	47	TYR	O-C-N	8.76	128.79	121.35
2	F	31	GLY	N-CA-C	8.68	124.22	114.67
1	B	17	TYR	CA-C-O	-8.57	109.37	119.15
2	E	75	ARG	NE-CZ-NH1	-8.55	112.95	121.50
2	F	59	SER	CA-C-N	8.48	131.64	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	59	SER	C-N-CA	8.48	131.64	120.28
1	B	94	TRP	N-CA-C	8.30	122.82	111.54
1	C	95	LEU	N-CA-C	-8.29	95.72	109.07
1	A	87	ARG	NE-CZ-NH2	8.12	126.50	119.20
2	E	53	TRP	CA-C-O	-8.09	112.10	120.84
2	D	30	TYR	CA-C-O	8.01	128.41	120.88
2	F	54	ARG	CD-NE-CZ	7.92	135.49	124.40
1	A	31	GLN	O-C-N	7.91	130.51	122.12
2	D	46	GLU	CB-CG-CD	-7.75	99.43	112.60
1	B	15	GLN	CA-CB-CG	7.74	129.59	114.10
1	A	73	GLU	CA-C-O	-7.74	112.66	121.40
2	F	75	ARG	CD-NE-CZ	7.71	135.19	124.40
1	C	25	ILE	O-C-N	7.68	131.58	123.05
1	C	94	TRP	N-CA-C	7.65	121.79	111.24
2	F	77	ALA	CA-C-O	7.63	128.64	120.55
1	A	74	ALA	CA-C-O	-7.59	112.48	120.99
1	C	14	LEU	CA-C-N	7.59	130.78	120.54
1	C	14	LEU	C-N-CA	7.59	130.78	120.54
2	D	63	THR	CA-C-O	-7.58	107.92	120.80
2	E	80	GLU	CB-CG-CD	-7.55	99.77	112.60
1	A	94	TRP	N-CA-C	7.54	121.92	111.74
2	F	15	ASP	O-C-N	7.49	130.05	122.12
1	A	22	ASP	CA-CB-CG	-7.47	105.13	112.60
2	E	75	ARG	CG-CD-NE	7.47	128.44	112.00
2	F	81	GLY	CA-C-O	-7.41	110.77	119.07
1	A	58	ASN	CB-CG-ND2	7.38	127.47	116.40
2	F	58	GLN	CG-CD-NE2	7.34	127.41	116.40
1	B	41	ASN	N-CA-C	7.11	121.67	112.92
2	F	75	ARG	NE-CZ-NH2	-7.11	112.80	119.20
1	C	83	ARG	CD-NE-CZ	7.10	134.34	124.40
1	B	63	LEU	CA-C-O	-7.04	113.38	120.63
1	C	40	GLY	N-CA-C	-7.02	104.51	115.67
1	A	36	VAL	O-C-N	7.01	129.51	122.71
2	D	81	GLY	N-CA-C	6.97	124.40	114.64
1	C	31	GLN	O-C-N	6.93	129.30	122.09
1	C	15	GLN	CB-CA-C	-6.86	99.84	110.81
1	C	15	GLN	OE1-CD-NE2	6.82	129.42	122.60
1	B	46	ALA	CA-C-O	6.81	128.13	121.32
2	F	60	LYS	CA-C-N	6.80	129.28	120.44
2	F	60	LYS	C-N-CA	6.80	129.28	120.44
2	E	80	GLU	CA-C-O	-6.77	111.64	119.56
2	D	16	LEU	CA-C-O	-6.74	113.74	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2	LYS	CA-C-N	6.71	132.45	122.99
2	D	2	LYS	C-N-CA	6.71	132.45	122.99
1	C	40	GLY	O-C-N	6.69	129.89	122.47
1	B	37	ALA	O-C-N	6.67	129.02	122.09
2	F	47	TYR	CA-CB-CG	-6.67	101.90	113.90
1	A	110	ARG	N-CA-CB	6.66	121.83	110.50
1	B	22	ASP	CA-CB-CG	-6.64	105.96	112.60
2	F	61	GLN	CB-CG-CD	6.63	123.88	112.60
2	D	72	GLN	OE1-CD-NE2	-6.63	115.97	122.60
1	A	74	ALA	O-C-N	6.63	130.82	123.33
1	A	25	ILE	CA-C-O	-6.59	114.30	121.28
1	B	41	ASN	CA-CB-CG	6.57	119.17	112.60
2	E	83	ASP	CA-CB-CG	-6.52	106.08	112.60
1	C	69	ARG	CD-NE-CZ	6.50	133.50	124.40
2	D	19	THR	CA-CB-OG1	-6.49	99.87	109.60
1	B	52	GLY	CA-C-N	-6.44	112.45	122.69
1	B	52	GLY	C-N-CA	-6.44	112.45	122.69
2	F	61	GLN	CB-CA-C	-6.44	100.77	110.88
1	C	18	HIS	CA-CB-CG	-6.42	107.38	113.80
2	E	85	THR	O-C-N	6.37	130.88	123.30
1	C	10	VAL	CA-C-O	-6.36	114.33	120.95
1	A	106	PHE	CA-C-O	-6.31	113.98	121.11
2	D	2	LYS	CA-C-O	-6.28	113.57	120.36
2	F	59	SER	N-CA-CB	-6.28	100.59	109.94
1	A	54	ASP	CA-CB-CG	-6.25	106.34	112.60
2	F	57	GLU	O-C-N	6.25	128.75	122.12
1	C	5	ASN	CA-CB-CG	-6.25	106.35	112.60
1	A	58	ASN	CA-CB-CG	6.25	118.85	112.60
1	C	94	TRP	CA-C-N	6.24	131.60	123.00
1	C	94	TRP	C-N-CA	6.24	131.60	123.00
1	C	47	PRO	CB-CA-C	6.14	119.38	111.21
2	D	42	THR	CA-C-O	-6.14	111.88	119.18
1	A	24	TYR	CA-C-O	-6.12	114.01	120.80
1	A	47	PRO	CB-CA-C	6.09	119.32	111.46
1	A	41	ASN	CA-CB-CG	-6.09	106.51	112.60
2	D	20	LEU	O-C-N	6.07	128.32	122.07
1	C	19	LYS	CA-C-O	-6.04	114.77	121.23
2	E	31	GLY	N-CA-C	6.04	121.31	114.67
2	E	15	ASP	CA-C-O	6.03	127.15	120.82
1	C	53	GLY	N-CA-C	6.01	123.02	115.21
1	C	82	PHE	CA-CB-CG	-6.00	107.81	113.80
1	C	62	LYS	CA-C-O	-5.97	112.75	119.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	58	GLN	CA-C-O	5.97	127.09	120.82
1	A	36	VAL	CA-C-O	-5.96	114.25	120.51
1	C	38	SER	CA-C-O	5.96	126.64	119.61
2	E	55	GLN	O-C-N	5.94	130.37	122.41
1	B	16	THR	CA-CB-OG1	-5.94	100.69	109.60
2	F	17	HIS	O-C-N	5.93	128.41	122.12
2	F	58	GLN	CA-C-N	5.93	128.54	120.54
2	F	58	GLN	C-N-CA	5.93	128.54	120.54
1	A	90	TYR	CA-C-O	-5.92	113.50	120.60
2	E	77	ALA	CA-C-O	5.91	126.81	120.55
2	F	17	HIS	CA-CB-CG	-5.91	107.89	113.80
2	F	35	ASP	O-C-N	5.90	128.38	122.12
2	D	31	GLY	N-CA-C	5.89	121.15	114.67
1	C	46	ALA	O-C-N	5.83	128.02	121.32
1	A	77	ASN	OD1-CG-ND2	-5.79	116.81	122.60
2	F	55	GLN	CA-C-O	-5.77	115.14	121.84
2	D	28	GLU	CB-CG-CD	5.77	122.41	112.60
1	C	6	THR	CA-C-O	-5.77	114.58	121.56
1	B	44	ASP	CB-CA-C	-5.77	101.10	110.79
1	C	17	TYR	N-CA-C	5.76	120.31	113.28
1	C	37	ALA	CA-C-N	5.75	129.89	120.63
1	C	37	ALA	C-N-CA	5.75	129.89	120.63
1	A	5	ASN	OD1-CG-ND2	-5.74	116.86	122.60
1	B	94	TRP	CA-CB-CG	-5.74	102.69	113.60
1	A	95	LEU	N-CA-C	-5.72	101.16	110.20
1	A	90	TYR	O-C-N	5.72	130.25	123.33
1	B	80	SER	CA-C-N	-5.70	112.58	121.42
1	B	80	SER	C-N-CA	-5.70	112.58	121.42
1	B	93	ASP	CA-C-N	5.69	130.21	122.07
1	B	93	ASP	C-N-CA	5.69	130.21	122.07
1	B	36	VAL	N-CA-CB	5.69	119.38	112.10
2	F	45	VAL	CA-C-N	5.68	130.50	122.09
2	F	45	VAL	C-N-CA	5.68	130.50	122.09
1	B	66	LYS	CA-C-O	5.64	128.57	120.51
1	B	10	VAL	CA-C-O	-5.62	114.69	120.71
2	F	69	SER	CA-CB-OG	-5.61	99.88	111.10
1	C	15	GLN	CA-C-O	5.61	126.90	120.90
1	C	24	TYR	O-C-N	5.60	129.60	123.22
2	D	57	GLU	CB-CG-CD	-5.58	103.11	112.60
1	A	31	GLN	CG-CD-NE2	5.58	124.77	116.40
1	C	5	ASN	N-CA-C	5.57	119.18	111.71
1	B	72	ARG	O-C-N	5.54	129.70	123.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	8	ASP	CA-CB-CG	-5.54	107.06	112.60
2	E	39	ASP	CA-CB-CG	-5.53	107.08	112.60
2	D	55	GLN	OE1-CD-NE2	5.52	128.12	122.60
2	E	3	ALA	CB-CA-C	5.49	118.58	109.53
2	E	26	LEU	CA-C-O	-5.48	114.74	120.88
2	F	28	GLU	CA-C-O	-5.46	113.92	120.10
2	E	57	GLU	CA-C-O	-5.45	114.82	120.92
2	E	19	THR	O-C-N	5.45	127.97	122.09
1	C	8	ASP	CA-CB-CG	-5.43	107.17	112.60
1	A	95	LEU	N-CA-CB	5.43	118.26	110.06
1	B	16	THR	N-CA-C	5.43	118.02	111.40
2	F	4	VAL	O-C-N	-5.42	117.48	123.18
1	A	87	ARG	NE-CZ-NH1	-5.42	116.08	121.50
2	D	5	ILE	CA-C-O	-5.39	114.76	120.53
2	F	58	GLN	OE1-CD-NE2	-5.39	117.21	122.60
2	D	11	ARG	NE-CZ-NH1	-5.38	116.12	121.50
1	A	8	ASP	CB-CA-C	-5.37	101.71	110.85
2	E	72	GLN	CA-CB-CG	5.35	124.81	114.10
2	F	2	LYS	CA-C-O	5.35	126.14	120.36
1	C	25	ILE	CA-C-O	-5.33	114.90	120.76
1	B	81	GLY	O-C-N	5.32	127.30	122.88
2	D	45	VAL	CA-C-O	5.32	126.90	121.58
1	C	6	THR	N-CA-CB	5.31	119.03	110.85
2	F	15	ASP	CB-CA-C	-5.31	101.98	110.79
2	D	11	ARG	CD-NE-CZ	5.30	131.82	124.40
2	D	15	ASP	CB-CA-C	-5.30	102.56	110.88
2	D	6	ASN	OD1-CG-ND2	-5.30	117.30	122.60
2	D	1	LYS	CA-CB-CG	5.29	124.69	114.10
2	E	3	ALA	O-C-N	-5.29	117.02	123.16
1	C	107	THR	CA-C-O	-5.29	114.45	120.32
2	F	50	VAL	N-CA-CB	5.29	118.12	111.46
1	A	15	GLN	CB-CG-CD	-5.27	103.64	112.60
2	E	15	ASP	CB-CG-OD2	-5.26	106.30	118.40
1	C	95	LEU	N-CA-CB	5.25	118.81	110.57
1	C	88	ILE	O-C-N	5.25	128.49	123.14
1	A	71	TRP	CA-C-O	5.25	127.04	121.11
1	A	82	PHE	CA-CB-CG	-5.25	108.56	113.80
2	F	75	ARG	NE-CZ-NH1	5.24	126.74	121.50
1	A	58	ASN	N-CA-CB	-5.24	103.38	111.65
2	F	2	LYS	CA-C-N	5.24	130.38	123.05
2	F	2	LYS	C-N-CA	5.24	130.38	123.05
2	D	55	GLN	CB-CA-C	-5.23	104.46	111.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	40	GLY	N-CA-C	-5.22	105.81	114.48
2	F	46	GLU	O-C-N	5.21	129.21	123.16
1	A	100	THR	CA-C-O	5.21	125.33	119.18
2	E	14	SER	CA-C-N	5.21	127.21	120.44
2	E	14	SER	C-N-CA	5.21	127.21	120.44
2	F	59	SER	CA-C-O	5.21	126.47	120.90
1	C	110	ARG	CA-CB-CG	5.20	124.50	114.10
1	C	103	TYR	N-CA-C	5.20	120.78	113.56
1	B	95	LEU	CA-C-O	-5.20	115.13	121.05
2	E	25	ALA	O-C-N	5.17	128.78	122.58
1	C	69	ARG	NE-CZ-NH1	5.16	126.66	121.50
2	F	57	GLU	CA-C-O	-5.15	115.09	120.55
1	A	24	TYR	CA-CB-CG	-5.15	104.63	113.90
1	C	75	ASP	CA-C-O	-5.13	115.97	121.56
1	B	5	ASN	OD1-CG-ND2	-5.13	117.47	122.60
1	B	95	LEU	N-CA-C	-5.13	102.10	110.20
1	B	19	LYS	O-C-N	5.13	128.53	123.46
1	A	110	ARG	CD-NE-CZ	5.12	131.57	124.40
1	C	26	THR	CA-CB-OG1	-5.11	101.93	109.60
2	D	12	SER	O-C-N	5.11	128.63	123.26
1	B	100	THR	N-CA-CB	5.11	118.41	110.80
2	D	75	ARG	CA-CB-CG	-5.11	103.89	114.10
2	D	68	GLU	CA-C-N	5.09	127.10	120.28
2	D	68	GLU	C-N-CA	5.09	127.10	120.28
2	F	9	GLN	CB-CG-CD	-5.09	103.95	112.60
1	A	100	THR	N-CA-C	-5.08	105.99	113.61
1	A	72	ARG	CD-NE-CZ	-5.07	117.31	124.40
2	F	85	THR	CA-CB-OG1	-5.06	102.01	109.60
1	B	26	THR	CA-C-O	-5.06	116.12	121.94
1	C	10	VAL	O-C-N	5.06	126.78	121.87
2	D	85	THR	CA-CB-OG1	-5.06	102.02	109.60
1	B	86	ASP	CB-CA-C	-5.05	101.42	109.75
1	A	8	ASP	N-CA-C	5.04	116.86	111.36
2	E	4	VAL	CB-CA-C	-5.04	103.62	110.42
1	B	4	ILE	N-CA-CB	5.02	119.51	111.23
2	F	75	ARG	CA-C-O	-5.01	115.11	120.42
1	C	88	ILE	CA-C-O	-5.01	115.00	120.72
2	F	24	LEU	CA-C-O	-5.01	113.49	119.35

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	864	0	833	29	0
1	B	878	0	849	9	0
1	C	839	0	782	31	0
2	D	695	0	689	18	0
2	E	665	0	633	13	0
2	F	699	0	689	20	0
3	A	145	0	0	3	1
3	B	137	0	0	2	1
3	C	50	0	0	3	0
3	D	77	0	0	3	0
3	E	64	0	0	1	0
3	F	40	0	0	2	0
All	All	5153	0	4475	120	1

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 (120) 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:36:VAL:HB	1:A:39:LYS:CG	1.62	1.30
1:A:39:LYS:NZ	1:A:39:LYS:CB	2.10	1.14
1:A:39:LYS:CB	1:A:39:LYS:HZ2	1.63	1.10
1:A:36:VAL:HB	1:A:39:LYS:HG3	1.32	1.08
2:E:55:GLN:HE21	2:E:55:GLN:HA	1.16	1.07
1:A:39:LYS:HZ2	1:A:39:LYS:HB3	0.89	1.05
1:A:39:LYS:NZ	1:A:39:LYS:HB3	1.57	1.00
1:C:21:PRO:HB2	1:C:23:ASN:OD1	1.66	0.94
1:A:36:VAL:HB	1:A:39:LYS:HG2	1.50	0.93
1:A:36:VAL:HG21	1:A:39:LYS:HD2	1.55	0.89
2:E:72:GLN:O	2:E:76:GLU:HG3	1.73	0.89
2:E:55:GLN:HE21	2:E:55:GLN:CA	1.86	0.88
2:F:72:GLN:O	2:F:76:GLU:HG3	1.80	0.81
1:B:36:VAL:HB	1:B:39:LYS:HE2	1.65	0.79
2:D:11:ARG:HA	2:D:62:LEU:HD12	1.63	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:78:LYS:HE2	2:F:84:ILE:O	1.82	0.78
2:E:55:GLN:HA	2:E:55:GLN:NE2	1.96	0.77
2:F:6:ASN:HD21	2:F:54:ARG:HH11	1.31	0.77
1:A:39:LYS:CB	1:A:39:LYS:HZ3	1.99	0.76
1:A:36:VAL:CG2	1:A:39:LYS:HD2	2.15	0.75
1:C:101:ASP:OD2	1:C:105:THR:HG22	1.86	0.74
1:A:36:VAL:CB	1:A:39:LYS:CG	2.56	0.72
2:D:75:ARG:HD2	3:D:115:HOH:O	1.89	0.72
1:A:27:LYS:O	1:A:31:GLN:HG3	1.91	0.71
1:C:109:ILE:O	1:C:110:ARG:HD3	1.93	0.69
2:D:6:ASN:HD21	2:D:54:ARG:HH11	1.39	0.68
1:C:32:ALA:C	1:C:34:GLY:H	2.00	0.68
1:C:101:ASP:CG	1:C:105:THR:HG22	2.19	0.68
2:F:47:TYR:HB3	2:F:48:PRO:HA	1.74	0.68
2:F:56:PHE:O	2:F:59:SER:HB3	1.97	0.64
1:B:36:VAL:HB	1:B:39:LYS:CE	2.25	0.64
1:C:29:GLU:O	1:C:32:ALA:HB3	1.97	0.64
2:D:62:LEU:HD23	2:D:62:LEU:N	2.13	0.64
1:A:104:GLN:HG2	3:D:126:HOH:O	1.97	0.63
1:A:36:VAL:CB	1:A:39:LYS:HG2	2.25	0.63
1:C:36:VAL:HG12	1:C:39:LYS:CG	2.28	0.62
1:B:109:ILE:O	1:B:110:ARG:HD3	2.00	0.61
1:A:39:LYS:NZ	1:A:39:LYS:CA	2.64	0.59
1:B:36:VAL:CB	1:B:39:LYS:HE2	2.32	0.59
1:A:36:VAL:HB	1:A:39:LYS:CD	2.30	0.59
2:E:89:SER:OXT	3:E:97:HOH:O	2.16	0.59
1:C:52:GLY:HA2	1:C:74:ALA:HA	1.85	0.58
1:A:19:LYS:HE3	3:A:130:HOH:O	2.03	0.58
1:C:3:VAL:HG11	3:C:127:HOH:O	2.04	0.57
1:C:36:VAL:CG1	1:C:39:LYS:CG	2.83	0.57
2:F:56:PHE:O	2:F:59:SER:CB	2.53	0.56
1:C:101:ASP:OD2	1:C:105:THR:CG2	2.52	0.56
1:C:25:ILE:HG12	1:C:25:ILE:O	2.07	0.55
2:F:57:GLU:HB3	3:F:108:HOH:O	2.06	0.55
2:D:78:LYS:HD3	3:D:158:HOH:O	2.05	0.54
2:F:9:GLN:HG3	3:F:123:HOH:O	2.07	0.54
2:F:78:LYS:CE	2:F:84:ILE:O	2.55	0.54
1:A:39:LYS:HZ2	1:A:39:LYS:CA	2.18	0.54
2:E:21:LYS:HA	2:E:26:LEU:HB2	1.91	0.53
1:C:11:ALA:O	1:C:15:GLN:HG2	2.10	0.52
2:E:55:GLN:O	2:E:56:PHE:C	2.52	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:20:LEU:O	1:C:21:PRO:C	2.52	0.52
2:E:11:ARG:HG3	2:E:15:ASP:OD2	2.09	0.52
1:C:32:ALA:C	1:C:34:GLY:N	2.69	0.51
2:D:56:PHE:HE2	2:D:60:LYS:HD2	1.75	0.51
1:C:105:THR:CG2	3:C:112:HOH:O	2.59	0.50
2:E:57:GLU:H	2:E:57:GLU:CD	2.20	0.50
2:F:41:LEU:HA	2:F:45:VAL:HG22	1.93	0.50
1:C:105:THR:HG23	3:C:112:HOH:O	2.13	0.49
2:D:6:ASN:ND2	2:D:54:ARG:HH11	2.09	0.49
2:D:11:ARG:HA	2:D:62:LEU:CD1	2.38	0.49
1:C:84:ASN:O	1:C:87:ARG:NH1	2.45	0.49
2:F:29:TYR:O	2:F:30:TYR:C	2.56	0.48
2:D:78:LYS:HE2	2:D:84:ILE:O	2.14	0.48
1:A:14:LEU:O	1:A:18:HIS:HD2	1.97	0.47
1:C:24:TYR:CD1	1:C:52:GLY:HA3	2.49	0.47
2:E:7:GLY:HA3	2:E:54:ARG:O	2.14	0.47
1:C:35:TRP:CD1	1:C:41:ASN:OD1	2.68	0.47
1:C:12:ASP:O	1:C:15:GLN:HB2	2.15	0.47
1:C:32:ALA:O	1:C:34:GLY:N	2.48	0.47
1:A:27:LYS:HE3	3:A:229:HOH:O	2.14	0.47
2:F:26:LEU:HB3	2:F:27:PRO:HD2	1.97	0.47
1:C:25:ILE:CD1	1:C:49:LYS:CB	2.94	0.46
1:A:36:VAL:O	1:A:39:LYS:HG3	2.15	0.46
2:F:62:LEU:HD23	2:F:62:LEU:HA	1.59	0.46
1:B:27:LYS:HE3	3:B:196:HOH:O	2.16	0.46
1:A:49:LYS:HA	1:A:49:LYS:HD3	1.81	0.46
1:B:108:LYS:NZ	1:B:110:ARG:OXT	2.43	0.45
2:E:78:LYS:HE2	2:E:84:ILE:O	2.17	0.45
1:C:36:VAL:O	1:C:39:LYS:HB2	2.16	0.45
2:D:56:PHE:CE2	2:D:60:LYS:HD2	2.52	0.45
2:D:62:LEU:HD22	2:D:62:LEU:HA	1.62	0.45
2:D:6:ASN:ND2	2:D:54:ARG:HD2	2.32	0.45
2:D:62:LEU:N	2:D:62:LEU:CD2	2.73	0.45
2:F:64:GLU:O	2:F:65:ASN:CB	2.66	0.44
1:B:36:VAL:CG2	1:B:39:LYS:HE2	2.46	0.44
1:B:84:ASN:HB2	3:B:213:HOH:O	2.18	0.44
2:E:83:ASP:OD1	2:E:83:ASP:C	2.58	0.44
2:F:40:ALA:O	2:F:44:TRP:HB3	2.17	0.44
1:C:84:ASN:O	1:C:87:ARG:NH2	2.51	0.44
1:C:20:LEU:C	1:C:21:PRO:O	2.56	0.44
1:A:52:GLY:HA2	1:A:74:ALA:HA	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:8:GLU:HB3	2:D:55:GLN:HG3	2.00	0.43
2:D:6:ASN:HD21	2:D:54:ARG:NH1	2.09	0.43
1:C:73:GLU:HB3	1:C:89:LEU:HD13	2.00	0.43
2:D:26:LEU:HB3	2:D:27:PRO:HD2	2.00	0.43
2:F:44:TRP:CD1	2:F:44:TRP:C	2.96	0.42
1:B:41:ASN:O	1:B:44:ASP:HB2	2.19	0.42
1:A:23:ASN:O	1:A:49:LYS:HA	2.20	0.42
1:A:36:VAL:CG1	1:A:39:LYS:HG2	2.49	0.42
2:F:8:GLU:OE1	2:F:55:GLN:HG3	2.20	0.42
1:C:30:ALA:C	1:C:35:TRP:HB3	2.45	0.42
2:F:47:TYR:HB3	2:F:48:PRO:CA	2.47	0.41
1:A:36:VAL:CB	1:A:39:LYS:HD2	2.50	0.41
1:A:82:PHE:HD1	3:A:134:HOH:O	2.03	0.41
2:D:86:ILE:HD13	2:D:86:ILE:HG21	1.88	0.41
1:C:5:ASN:C	1:C:5:ASN:OD1	2.59	0.41
1:A:21:PRO:HB2	1:A:23:ASN:OD1	2.21	0.41
1:A:36:VAL:CB	1:A:39:LYS:CD	2.97	0.41
1:C:7:PHE:CE1	1:C:98:LYS:HB2	2.56	0.41
1:C:31:GLN:O	1:C:34:GLY:N	2.54	0.41
2:D:18:GLN:HE22	2:D:32:GLU:CD	2.29	0.41
2:E:39:ASP:O	2:E:43:GLY:N	2.54	0.41
2:F:20:LEU:HA	2:F:20:LEU:HD23	1.79	0.41
2:F:47:TYR:CB	2:F:48:PRO:HA	2.45	0.40

All (1) 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)
3:A:208:HOH:O	3:B:166:HOH:O[2_555]	2.10	0.10

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	106/110 (96%)	104 (98%)	2 (2%)	0	100	100
1	B	108/110 (98%)	106 (98%)	2 (2%)	0	100	100
1	C	106/110 (96%)	92 (87%)	13 (12%)	1 (1%)	14	9
2	D	84/89 (94%)	80 (95%)	4 (5%)	0	100	100
2	E	82/89 (92%)	78 (95%)	4 (5%)	0	100	100
2	F	87/89 (98%)	81 (93%)	5 (6%)	1 (1%)	11	7
All	All	573/597 (96%)	541 (94%)	30 (5%)	2 (0%)	36	35

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	33	LEU
2	F	44	TRP

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	91/92 (99%)	90 (99%)	1 (1%)	65	73
1	B	92/92 (100%)	89 (97%)	3 (3%)	33	34
1	C	83/92 (90%)	74 (89%)	9 (11%)	6	3
2	D	72/76 (95%)	68 (94%)	4 (6%)	19	16
2	E	66/76 (87%)	63 (96%)	3 (4%)	24	23
2	F	71/76 (93%)	69 (97%)	2 (3%)	38	41
All	All	475/504 (94%)	453 (95%)	22 (5%)	24	22

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	LYS
1	B	28	SER
1	B	66	LYS

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Mol	Chain	Res	Type
1	B	67	SER
1	C	3	VAL
1	C	23	ASN
1	C	25	ILE
1	C	28	SER
1	C	38	SER
1	C	66	LYS
1	C	70	THR
1	C	98	LYS
1	C	105	THR
2	D	28	GLU
2	D	46	GLU
2	D	62	LEU
2	D	89	SER
2	E	15	ASP
2	E	55	GLN
2	E	80	GLU
2	F	18	GLN
2	F	59	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	GLN
1	A	104	GLN
1	B	15	GLN
1	B	31	GLN
1	B	104	GLN
1	C	18	HIS
1	C	104	GLN
2	D	6	ASN
2	E	55	GLN
2	E	72	GLN
2	F	6	ASN
2	F	18	GLN
2	F	55	GLN
2	F	61	GLN
2	F	72	GLN

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

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.