



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:18 AM UTC

PDB ID : 1EAI / pdb_00001eai
Title : COMPLEX OF ASCARIS CHYMOTRPSIN/ELASTASE INHIBITOR
WITH PORCINE ELASTASE
Authors : Huang, K.; Strynadka, N.C.J.; Bernard, V.D.; Peanasky, R.J.; James, M.N.G.
Deposited on : 1999-03-25
Resolution : 2.40 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

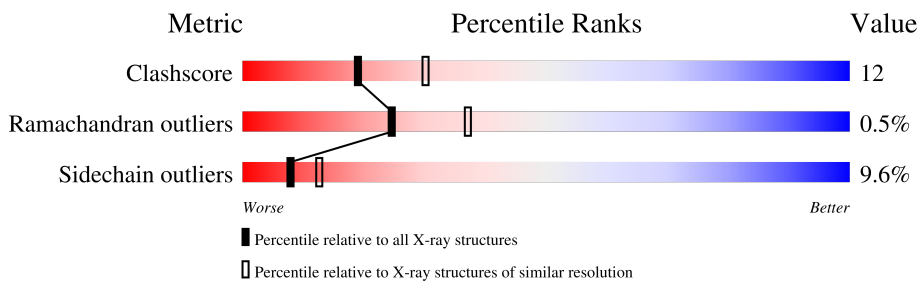
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)

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	240	63% 31% 6%
1	B	240	56% 32% 10% .
2	C	61	44% 41% 10% 5%
2	D	61	51% 34% 10% 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4686 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 PROTEIN (ELASTASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	240	Total	C	N	O	S	0	0	0
			1822	1135	329	348	10			
1	B	240	Total	C	N	O	S	0	0	0
			1822	1135	329	348	10			

- Molecule 2 is a protein called PROTEIN (CHYMOTRYPSIN/ELASTASE ISOINHIBITOR 1).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	61	Total	C	N	O	S	0	0	0
			448	260	84	91	13			
2	D	61	Total	C	N	O	S	0	0	0
			448	260	84	91	13			

- Molecule 3 is water.

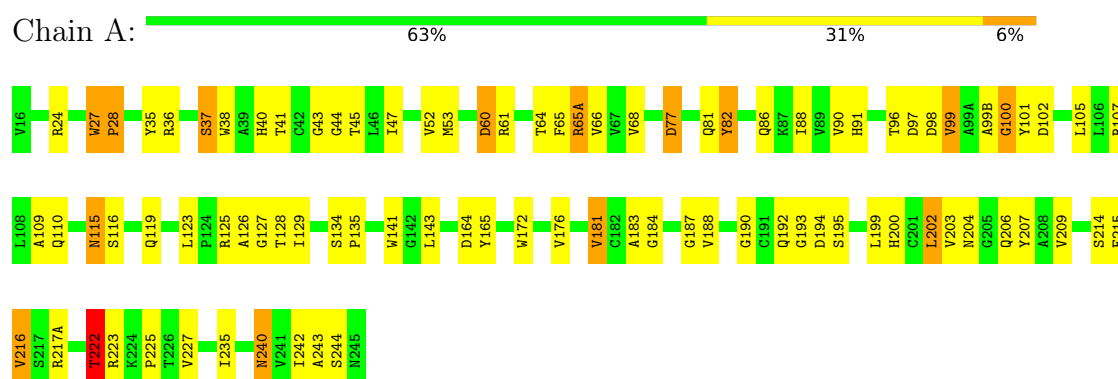
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	58	Total	O	0	0
			58	58		
3	B	61	Total	O	0	0
			61	61		
3	C	16	Total	O	0	0
			16	16		
3	D	11	Total	O	0	0
			11	11		

3 Residue-property plots

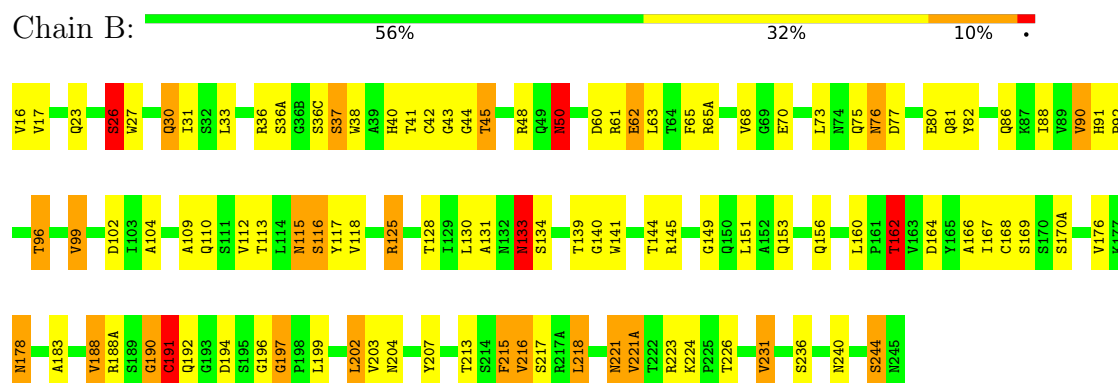
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

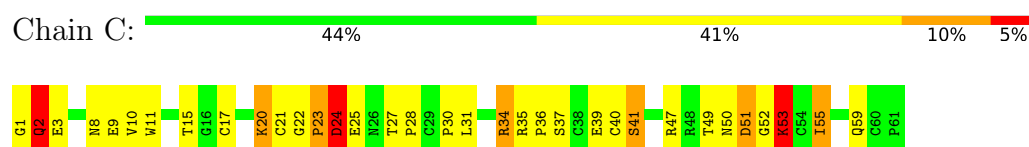
• Molecule 1: PROTEIN (ELASTASE)



• Molecule 1: PROTEIN (ELASTASE)

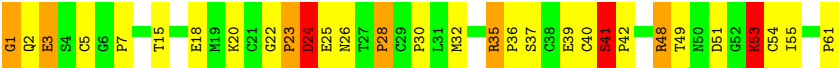


• Molecule 2: PROTEIN (CHYMOTRYPSIN/ELASTASE ISOINHIBITOR 1)



• Molecule 2: PROTEIN (CHYMOTRYPSIN/ELASTASE ISOINHIBITOR 1)





4 Data and refinement statistics

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

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	84.02Å 84.02Å 190.93Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.40	Depositor
% Data completeness (in resolution range)	92.0 (20.00-2.40)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.191 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4686	wwPDB-VP
Average B, all atoms (Å ²)	35.0	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	1.57	16/1862 (0.9%)	2.13	61/2543 (2.4%)
1	B	1.53	15/1862 (0.8%)	2.13	64/2543 (2.5%)
2	C	1.76	3/457 (0.7%)	2.67	44/615 (7.2%)
2	D	1.68	5/457 (1.1%)	2.34	34/615 (5.5%)
All	All	1.58	39/4638 (0.8%)	2.21	203/6316 (3.2%)

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	B	1	1
2	C	1	0
All	All	2	1

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	183	ALA	N-CA	8.97	1.57	1.45
1	B	40	HIS	CE1-NE2	8.37	1.41	1.32
1	A	40	HIS	CE1-NE2	7.73	1.40	1.32
1	B	197	GLY	N-CA	7.67	1.55	1.44
1	B	43	GLY	C-O	6.77	1.31	1.23
1	A	43	GLY	C-O	6.69	1.31	1.23
1	B	218	LEU	CA-C	-6.60	1.43	1.52
2	D	15	THR	C-N	6.42	1.40	1.32
1	B	197	GLY	C-O	6.18	1.32	1.24
1	B	226	THR	CA-C	6.08	1.60	1.52
2	D	54	CYS	C-N	6.02	1.39	1.33
1	A	181	VAL	C-N	5.99	1.41	1.33
2	C	53	LYS	CA-CB	-5.81	1.44	1.53
1	A	44	GLY	C-O	5.74	1.31	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	64	THR	CA-CB	5.68	1.61	1.53
1	B	42	CYS	C-N	5.66	1.39	1.33
1	B	191	CYS	N-CA	5.66	1.53	1.46
1	B	191	CYS	C-N	5.64	1.41	1.33
1	B	43	GLY	C-N	5.53	1.38	1.33
1	A	77	ASP	CG-OD1	5.51	1.35	1.25
1	A	193	GLY	C-O	5.49	1.31	1.24
2	D	54	CYS	CA-C	5.46	1.59	1.52
1	A	45	THR	N-CA	5.41	1.52	1.46
2	D	61	PRO	C-OXT	5.37	1.34	1.23
1	A	223	ARG	NE-CZ	5.36	1.39	1.33
1	A	127	GLY	CA-C	5.36	1.59	1.51
1	A	41	THR	CA-C	5.32	1.60	1.52
2	D	40	CYS	CA-C	5.31	1.59	1.52
2	C	34	ARG	NE-CZ	5.24	1.38	1.33
1	B	191	CYS	CA-C	5.24	1.59	1.52
1	A	141	TRP	NE1-CE2	5.21	1.43	1.37
1	B	141	TRP	CA-CB	5.21	1.61	1.53
1	B	40	HIS	CG-ND1	5.19	1.44	1.38
1	A	125	ARG	NE-CZ	5.19	1.38	1.33
1	A	53	MET	C-O	5.18	1.30	1.24
2	C	39	GLU	CA-C	5.09	1.59	1.52
1	B	139	THR	C-O	5.09	1.30	1.23
1	B	77	ASP	CG-OD1	5.01	1.34	1.25
1	A	214	SER	CA-C	5.01	1.59	1.52

All (203) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	51	ASP	N-CA-CB	-15.25	86.51	110.46
1	B	216	VAL	N-CA-CB	12.34	126.27	112.45
1	B	203	VAL	CB-CA-C	12.06	124.16	110.41
1	A	135	PRO	CB-CA-C	-11.56	98.96	111.56
1	A	24	ARG	CA-C-N	-10.22	104.94	123.34
1	A	24	ARG	C-N-CA	-10.22	104.94	123.34
1	B	190	GLY	O-C-N	-9.97	109.73	122.70
2	C	59	GLN	CA-CB-CG	-9.97	94.15	114.10
2	C	50	ASN	CA-C-N	9.56	139.84	122.06
2	C	50	ASN	C-N-CA	9.56	139.84	122.06
1	A	99	VAL	CB-CA-C	-9.54	99.54	112.04
1	B	102	ASP	CA-CB-CG	9.35	121.95	112.60
2	D	41	SER	N-CA-C	9.25	121.28	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	184	GLY	O-C-N	-9.03	114.10	122.86
1	A	37	SER	N-CA-C	8.98	124.03	109.94
1	A	240	ASN	CA-CB-CG	-8.85	103.75	112.60
2	D	55	ILE	N-CA-C	8.83	117.64	107.84
1	B	140	GLY	N-CA-C	8.62	123.64	110.18
1	B	178	ASN	CA-CB-CG	-8.59	104.01	112.60
1	A	216	VAL	N-CA-CB	8.37	125.04	111.23
2	C	53	LYS	CA-CB-CG	-8.08	97.93	114.10
2	D	23	PRO	CA-N-CD	-8.06	100.72	112.00
1	B	197	GLY	O-C-N	7.92	129.69	121.77
2	C	23	PRO	CA-N-CD	-7.89	100.95	112.00
1	A	134	SER	CA-C-N	7.89	129.93	120.23
1	A	134	SER	C-N-CA	7.89	129.93	120.23
1	B	191	CYS	N-CA-C	7.87	127.57	110.80
1	B	160	LEU	N-CA-CB	-7.79	100.63	111.77
1	B	26	SER	N-CA-CB	-7.74	98.38	110.30
1	B	188	VAL	N-CA-CB	-7.68	105.34	111.64
2	C	51	ASP	CA-CB-CG	7.56	120.16	112.60
2	C	8	ASN	CA-CB-CG	7.54	120.14	112.60
2	D	1	GLY	O-C-N	7.39	134.82	123.00
2	C	47	ARG	CG-CD-NE	-7.32	95.89	112.00
1	B	65(A)	ARG	NE-CZ-NH2	-7.26	112.66	119.20
2	C	15	THR	N-CA-CB	-7.25	99.27	110.29
1	A	82	TYR	CA-C-O	-7.24	112.61	120.36
2	C	23	PRO	CA-C-N	7.22	132.27	120.94
2	C	23	PRO	C-N-CA	7.22	132.27	120.94
1	B	197	GLY	N-CA-C	-7.21	97.64	112.34
2	D	41	SER	CA-C-N	7.19	126.81	119.19
2	D	41	SER	C-N-CA	7.19	126.81	119.19
1	B	162	THR	CA-CB-CG2	7.17	122.69	110.50
2	D	24	ASP	CA-CB-CG	-7.12	105.48	112.60
2	D	22	GLY	CA-C-N	-7.11	112.45	119.78
2	D	22	GLY	C-N-CA	-7.11	112.45	119.78
1	B	90	VAL	CA-CB-CG2	7.08	122.44	110.40
2	C	3	GLU	N-CA-CB	7.08	122.92	110.18
1	B	45	THR	CA-CB-OG1	6.97	120.05	109.60
2	C	20	LYS	CB-CA-C	-6.87	97.53	110.51
2	C	2	GLN	N-CA-CB	6.85	120.15	110.36
2	D	48	ARG	NE-CZ-NH1	6.78	128.28	121.50
2	C	25	GLU	CA-C-N	-6.78	112.49	122.86
2	C	25	GLU	C-N-CA	-6.78	112.49	122.86
1	B	197	GLY	CA-C-O	-6.75	111.87	121.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	44	GLY	CA-C-N	-6.68	111.90	122.73
1	A	44	GLY	C-N-CA	-6.68	111.90	122.73
2	C	23	PRO	N-CD-CG	6.65	113.17	103.20
2	C	28	PRO	CB-CA-C	-6.64	102.37	111.21
2	C	28	PRO	N-CA-C	6.64	121.61	111.19
2	D	1	GLY	CA-C-N	6.64	134.22	121.54
2	D	1	GLY	C-N-CA	6.64	134.22	121.54
1	A	235	ILE	N-CA-C	6.63	118.18	110.62
1	B	80	GLU	N-CA-C	6.63	119.50	110.55
2	D	48	ARG	N-CA-CB	6.62	120.95	110.23
1	A	181	VAL	CA-C-O	-6.50	113.39	120.67
1	A	65	PHE	CB-CA-C	-6.50	96.47	109.79
1	B	204	ASN	CB-CA-C	-6.49	101.33	111.39
1	A	102	ASP	CA-CB-CG	6.44	119.04	112.60
2	D	25	GLU	CA-C-N	-6.43	113.59	123.17
2	D	25	GLU	C-N-CA	-6.43	113.59	123.17
2	C	21	CYS	CA-C-N	-6.42	111.79	121.87
2	C	21	CYS	C-N-CA	-6.42	111.79	121.87
1	A	24	ARG	O-C-N	-6.36	114.14	122.59
1	A	188	VAL	N-CA-C	6.35	117.05	111.90
2	C	40	CYS	CA-C-O	-6.30	114.34	121.39
1	B	133	ASN	N-CA-C	6.27	120.27	112.24
1	A	215	PHE	N-CA-C	6.27	118.31	108.96
2	D	23	PRO	N-CD-CG	6.27	112.61	103.20
2	C	24	ASP	CA-CB-CG	-6.27	106.33	112.60
1	B	164	ASP	N-CA-C	6.25	118.62	110.43
2	C	2	GLN	CB-CA-C	6.25	122.50	109.68
1	B	37	SER	N-CA-C	6.25	120.21	108.65
1	B	221(A)	VAL	N-CA-CB	6.24	120.02	111.41
1	B	88	ILE	N-CA-C	6.23	116.99	107.77
1	A	165	TYR	CB-CA-C	6.21	120.63	110.88
1	B	166	ALA	N-CA-C	6.20	118.04	111.28
2	D	24	ASP	N-CA-CB	-6.18	101.52	110.36
2	C	27	THR	CA-C-N	6.14	125.90	119.76
2	C	27	THR	C-N-CA	6.14	125.90	119.76
2	D	3	GLU	N-CA-C	6.14	123.88	110.80
1	B	207	TYR	CB-CA-C	-6.13	99.09	109.83
1	B	236	SER	CA-CB-OG	-6.10	98.90	111.10
2	D	23	PRO	N-CA-CB	6.10	108.66	103.35
2	C	40	CYS	CB-CA-C	-6.10	101.50	111.68
2	D	7	PRO	CB-CA-C	-6.09	103.97	111.64
1	A	65(A)	ARG	NE-CZ-NH1	6.06	127.56	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	123	LEU	CA-C-N	6.05	126.24	120.31
1	A	123	LEU	C-N-CA	6.05	126.24	120.31
2	D	48	ARG	NE-CZ-NH2	-6.03	113.78	119.20
1	A	24	ARG	N-CA-C	5.97	123.52	110.80
1	B	30	GLN	OE1-CD-NE2	-5.92	116.68	122.60
2	D	30	PRO	N-CA-CB	5.91	108.82	103.33
1	A	192	GLN	CB-CG-CD	5.89	122.61	112.60
2	C	3	GLU	N-CA-C	5.88	119.98	112.34
1	A	100	GLY	CA-C-O	-5.85	116.53	122.56
1	A	98	ASP	N-CA-C	5.83	118.27	107.60
1	B	203	VAL	N-CA-CB	5.83	119.92	112.34
2	D	3	GLU	CA-C-N	-5.81	113.35	122.65
2	D	3	GLU	C-N-CA	-5.81	113.35	122.65
2	D	35	ARG	N-CA-C	5.80	117.01	109.64
1	B	231	VAL	N-CA-C	5.78	117.20	110.62
1	A	88	ILE	N-CA-C	5.76	116.24	108.17
1	B	73	LEU	N-CA-C	5.76	119.41	112.38
2	C	41	SER	N-CA-C	5.76	118.23	110.29
1	A	209	VAL	CA-C-O	-5.75	114.33	120.59
1	A	222	THR	CA-C-N	-5.74	114.93	125.02
1	A	222	THR	C-N-CA	-5.74	114.93	125.02
2	C	9	GLU	CA-C-N	-5.74	115.02	122.99
2	C	9	GLU	C-N-CA	-5.74	115.02	122.99
1	A	164	ASP	N-CA-C	5.72	117.93	110.43
1	B	88	ILE	N-CA-CB	-5.72	104.04	111.82
1	A	194	ASP	CA-CB-CG	5.71	118.31	112.60
1	A	107	ARG	NE-CZ-NH1	5.71	127.21	121.50
1	A	35	TYR	N-CA-CB	5.68	120.79	111.08
2	C	53	LYS	N-CA-CB	-5.66	101.84	110.49
1	B	42	CYS	CA-C-N	-5.65	116.46	122.67
1	B	42	CYS	C-N-CA	-5.65	116.46	122.67
1	B	202	LEU	CB-CA-C	-5.65	101.03	110.29
1	A	216	VAL	CG1-CB-CG2	-5.64	98.39	110.80
1	A	235	ILE	N-CA-CB	-5.64	103.42	110.47
2	C	52	GLY	N-CA-C	5.64	123.38	115.43
1	B	65	PHE	N-CA-C	5.63	119.24	110.17
2	C	10	VAL	CA-CB-CG2	5.62	119.96	110.40
1	B	221	ASN	CA-CB-CG	-5.62	106.98	112.60
1	B	48	ARG	CA-C-O	-5.60	115.46	121.45
1	B	215	PHE	N-CA-C	5.58	117.46	109.14
1	B	88	ILE	CB-CA-C	-5.57	102.89	110.42
2	C	2	GLN	OE1-CD-NE2	5.57	128.16	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	218	LEU	N-CA-CB	5.56	119.46	110.40
2	D	30	PRO	CA-C-O	-5.55	114.89	121.67
2	C	17	CYS	CA-C-N	5.53	131.77	122.87
2	C	17	CYS	C-N-CA	5.53	131.77	122.87
1	A	27	TRP	CA-C-N	5.53	126.75	119.84
1	A	27	TRP	C-N-CA	5.53	126.75	119.84
1	B	176	VAL	CA-CB-CG2	-5.50	101.05	110.40
2	D	53	LYS	CA-CB-CG	-5.50	103.10	114.10
2	C	55	ILE	CB-CA-C	-5.49	103.96	109.89
2	D	32	MET	CG-SD-CE	-5.48	88.84	100.90
1	B	183	ALA	CA-C-O	-5.48	113.97	120.43
2	C	39	GLU	N-CA-C	5.47	119.16	109.96
1	A	134	SER	O-C-N	5.47	128.58	121.64
1	A	47	ILE	N-CA-C	5.46	119.81	113.42
1	A	244	SER	N-CA-C	5.46	118.73	112.57
1	A	60	ASP	N-CA-C	5.45	119.03	112.38
2	D	39	GLU	N-CA-CB	-5.44	101.41	110.23
1	B	167	ILE	CB-CA-C	-5.44	104.95	112.24
2	C	22	GLY	CA-C-O	-5.44	113.74	121.52
1	A	126	ALA	N-CA-C	5.44	118.20	110.10
2	D	28	PRO	N-CA-C	5.43	119.83	111.57
1	B	70	GLU	N-CA-C	5.41	117.67	110.53
1	B	170(A)	SER	N-CA-C	5.40	117.86	111.33
1	B	110	GLN	N-CA-CB	-5.40	101.95	111.39
1	B	116	SER	CA-CB-OG	-5.38	100.35	111.10
1	A	134	SER	CA-C-O	-5.37	115.11	120.64
1	B	128	THR	N-CA-C	5.37	118.22	110.28
1	A	190	GLY	N-CA-C	-5.36	105.42	112.82
2	C	37	SER	N-CA-C	5.36	115.44	107.88
1	B	176	VAL	N-CA-C	5.35	116.48	109.58
1	A	47	ILE	CA-C-O	5.35	123.61	118.90
1	B	199	LEU	CB-CA-C	-5.32	102.17	110.74
1	A	115	ASN	CA-CB-CG	5.31	117.91	112.60
1	A	199	LEU	CA-C-O	-5.29	114.62	120.33
1	A	217(A)	ARG	N-CA-CB	5.29	119.17	110.39
1	B	118	VAL	N-CA-CB	-5.28	104.63	111.82
2	C	36	PRO	CA-C-O	-5.27	115.33	121.34
1	A	24	ARG	NE-CZ-NH1	-5.25	116.25	121.50
1	A	204	ASN	CB-CA-C	-5.25	104.43	111.89
1	B	50	ASN	CA-CB-CG	-5.25	107.35	112.60
2	D	35	ARG	CD-NE-CZ	5.25	131.75	124.40
1	A	41	THR	O-C-N	-5.25	116.53	122.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	48	ARG	CD-NE-CZ	5.23	131.73	124.40
2	D	26	ASN	CA-CB-CG	-5.23	107.37	112.60
1	B	168	CYS	N-CA-CB	5.21	117.78	110.12
1	B	169	SER	N-CA-C	5.19	118.74	112.93
2	D	55	ILE	O-C-N	-5.19	117.09	121.40
1	A	227	VAL	CB-CA-C	5.18	117.89	110.84
1	B	192	GLN	N-CA-CB	5.17	117.50	109.48
1	B	151	LEU	CA-C-O	-5.16	116.09	121.55
1	A	222	THR	N-CA-CB	5.15	117.61	109.83
1	B	65(A)	ARG	NE-CZ-NH1	5.13	126.64	121.50
1	B	236	SER	O-C-N	5.13	127.36	122.07
1	B	244	SER	CA-CB-OG	-5.12	100.87	111.10
1	A	99(B)	ALA	CA-C-N	-5.10	113.70	122.21
1	A	99(B)	ALA	C-N-CA	-5.10	113.70	122.21
1	B	104	ALA	N-CA-C	5.08	116.80	109.07
1	B	240	ASN	CA-CB-CG	5.07	117.67	112.60
1	B	27	TRP	CA-C-N	5.07	124.79	119.82
1	B	27	TRP	C-N-CA	5.07	124.79	119.82
2	C	2	GLN	N-CA-C	5.07	117.22	110.53
1	A	52	VAL	N-CA-C	5.02	115.94	108.46
1	A	243	ALA	N-CA-C	5.01	116.74	111.28
1	A	227	VAL	N-CA-C	5.00	115.52	108.36

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	203	VAL	CA
2	C	2	GLN	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	30	GLN	Sidechain

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	1822	0	1757	21	0
1	B	1822	0	1757	65	0
2	C	448	0	409	12	0
2	D	448	0	409	10	0
3	A	58	0	0	0	0
3	B	61	0	0	5	0
3	C	16	0	0	1	0
3	D	11	0	0	0	0
All	All	4686	0	4332	105	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 12.

All (105) 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:B:16:VAL:HG21	1:B:156:GLN:HB2	1.33	1.08
1:B:115:ASN:ND2	1:B:117:TYR:H	1.52	1.07
1:B:61:ARG:HB3	1:B:63:LEU:HD13	1.36	1.03
2:C:24:ASP:OD1	2:C:24:ASP:N	1.97	0.97
1:B:125:ARG:HH11	1:B:125:ARG:HG3	1.34	0.92
1:B:16:VAL:HG11	1:B:156:GLN:HB3	1.53	0.90
1:B:115:ASN:HD22	1:B:117:TYR:H	1.16	0.88
1:B:61:ARG:HB3	1:B:63:LEU:CD1	2.03	0.87
1:B:62:GLU:C	1:B:63:LEU:HD12	2.04	0.83
2:D:18:GLU:OE1	2:D:48:ARG:HD2	1.82	0.79
1:B:50:ASN:H	1:B:50:ASN:HD22	1.28	0.78
1:B:16:VAL:HG11	1:B:156:GLN:CB	2.13	0.77
1:B:23:GLN:O	1:B:26:SER:HB2	1.86	0.76
2:C:35:ARG:HG2	3:C:74:HOH:O	1.86	0.74
1:B:115:ASN:HD22	1:B:116:SER:N	1.85	0.74
1:A:36:ARG:NH1	2:D:51:ASP:O	2.23	0.72
2:D:20:LYS:O	2:D:23:PRO:HD2	1.89	0.72
1:B:125:ARG:HG3	1:B:125:ARG:NH1	2.02	0.71
1:B:16:VAL:CG2	1:B:156:GLN:HB2	2.17	0.70
2:C:2:GLN:HG3	2:C:11:TRP:CG	2.26	0.70
1:B:115:ASN:HD21	1:B:117:TYR:HD2	1.39	0.69
1:A:187:GLY:HA3	1:A:222:THR:HG22	1.76	0.67
1:B:33:LEU:O	1:B:41:THR:HG22	1.95	0.67
2:D:24:ASP:OD1	2:D:24:ASP:N	2.17	0.65
1:B:115:ASN:HD22	1:B:117:TYR:N	1.93	0.65
1:B:62:GLU:H	1:B:62:GLU:CD	2.06	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:20:LYS:O	2:C:23:PRO:HD2	1.98	0.63
1:B:16:VAL:HG12	3:B:271:HOH:O	1.98	0.62
1:B:197:GLY:HA2	1:B:213:THR:H	1.63	0.62
2:C:49:THR:OG1	2:C:51:ASP:HB3	1.99	0.61
1:B:60:ASP:OD2	1:B:96:THR:HG23	2.01	0.61
2:D:20:LYS:C	2:D:23:PRO:HD2	2.27	0.60
1:B:50:ASN:HD22	1:B:50:ASN:N	1.94	0.60
2:C:1:GLY:HA3	2:C:11:TRP:H	1.67	0.59
1:B:133:ASN:O	1:B:133:ASN:ND2	2.30	0.59
1:B:16:VAL:HB	3:B:272:HOH:O	2.01	0.59
1:B:75:GLN:O	3:B:246:HOH:O	2.17	0.59
1:A:216:VAL:HG13	2:C:31:LEU:HD11	1.85	0.58
1:B:62:GLU:OE1	1:B:62:GLU:N	2.35	0.58
1:A:38:TRP:CE3	1:A:65(A):ARG:HD2	2.39	0.58
1:B:218:LEU:H	1:B:218:LEU:HD12	1.68	0.57
1:B:133:ASN:HD22	1:B:133:ASN:C	2.11	0.56
1:B:91:HIS:CG	1:B:92:PRO:HD2	2.41	0.56
2:C:23:PRO:HA	2:C:24:ASP:OD1	2.06	0.55
1:B:134:SER:H	1:B:162:THR:HB	1.73	0.54
2:D:49:THR:OG1	2:D:53:LYS:HG3	2.07	0.54
1:B:215:PHE:CD2	2:D:28:PRO:HB3	2.43	0.54
1:B:197:GLY:CA	1:B:213:THR:H	2.22	0.53
1:B:115:ASN:HD22	1:B:115:ASN:C	2.17	0.53
1:B:221(A):VAL:HG22	1:B:224:LYS:HB2	1.91	0.53
1:B:62:GLU:O	1:B:63:LEU:HD12	2.09	0.53
1:B:244:SER:O	1:B:244:SER:OG	2.27	0.53
2:C:2:GLN:HG3	2:C:11:TRP:CB	2.39	0.52
1:B:115:ASN:ND2	1:B:117:TYR:N	2.37	0.52
2:C:55:ILE:HG13	2:C:55:ILE:O	2.09	0.52
1:B:81:GLN:HE22	1:B:113:THR:H	1.57	0.51
1:B:125:ARG:HH11	1:B:125:ARG:CG	2.17	0.51
1:B:131:ALA:O	1:B:162:THR:HG21	2.11	0.51
1:B:188:VAL:HG12	1:B:188(A):ARG:HG3	1.93	0.51
1:B:115:ASN:ND2	1:B:117:TYR:CD2	2.78	0.51
1:B:82:TYR:CD1	1:B:82:TYR:N	2.79	0.50
1:B:68:VAL:CG2	1:B:81:GLN:HB2	2.42	0.50
1:B:149:GLY:HA3	3:B:282:HOH:O	2.11	0.50
1:B:223:ARG:NH1	3:B:277:HOH:O	2.28	0.49
1:B:144:THR:O	1:B:145:ARG:HB3	2.12	0.49
1:A:109:ALA:C	1:A:110:GLN:HG3	2.35	0.48
1:B:37:SER:HB2	1:B:38:TRP:H	1.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:68:VAL:HG23	1:B:81:GLN:HB2	1.96	0.47
1:B:134:SER:N	1:B:162:THR:HB	2.30	0.47
1:B:81:GLN:NE2	1:B:112:VAL:HG13	2.29	0.47
2:D:1:GLY:N	2:D:5:CYS:HB2	2.30	0.47
1:B:31:ILE:HD12	1:B:31:ILE:C	2.40	0.46
2:D:36:PRO:O	2:D:37:SER:HB3	2.16	0.46
1:B:44:GLY:HA2	1:B:196:GLY:O	2.16	0.46
1:B:61:ARG:HE	1:B:63:LEU:HD11	1.80	0.46
1:B:217:SER:OG	1:B:218:LEU:HD12	2.15	0.46
1:B:221:ASN:OD1	1:B:221:ASN:N	2.40	0.46
1:B:50:ASN:N	1:B:50:ASN:ND2	2.61	0.46
1:A:68:VAL:HG22	1:A:81:GLN:HB2	1.98	0.45
1:A:90:VAL:HG12	1:A:91:HIS:N	2.28	0.45
1:B:16:VAL:HG12	1:B:16:VAL:O	2.15	0.45
2:D:41:SER:HA	2:D:42:PRO:HD3	1.62	0.45
1:B:190:GLY:O	1:B:194:ASP:OD2	2.34	0.45
1:A:172:TRP:CD1	1:A:225:PRO:HD2	2.52	0.44
1:A:68:VAL:CG2	1:A:81:GLN:HB2	2.46	0.44
1:A:90:VAL:CG1	1:A:91:HIS:N	2.78	0.44
1:A:128:THR:C	1:A:129:ILE:HG12	2.43	0.44
1:A:240:ASN:N	1:A:240:ASN:OD1	2.49	0.43
2:C:49:THR:OG1	2:C:53:LYS:HG3	2.19	0.43
1:A:115:ASN:OD1	1:A:116:SER:N	2.52	0.42
1:B:86:GLN:NE2	1:B:109:ALA:HA	2.34	0.42
1:A:82:TYR:N	1:A:82:TYR:CD1	2.86	0.42
1:B:76:ASN:ND2	1:B:76:ASN:C	2.78	0.42
1:A:37:SER:HB2	1:A:38:TRP:H	1.68	0.41
1:A:27:TRP:N	1:A:28:PRO:CD	2.82	0.41
1:B:17:VAL:HG23	1:B:191:CYS:HB2	2.01	0.41
1:B:216:VAL:HB	1:B:217:SER:H	1.74	0.41
2:C:30:PRO:HD2	2:C:34:ARG:NH2	2.36	0.41
1:A:202:LEU:HD22	1:A:207:TYR:CE1	2.55	0.41
1:A:28:PRO:HB2	1:A:119:GLN:HB2	2.02	0.41
1:A:172:TRP:NE1	1:A:225:PRO:HD2	2.36	0.41
1:A:100:GLY:O	1:A:101:TYR:HB2	2.22	0.40
1:A:90:VAL:HG12	1:A:91:HIS:O	2.21	0.40
1:B:99:VAL:H	1:B:99:VAL:HG23	1.48	0.40
1:B:62:GLU:O	1:B:62:GLU:HG2	2.21	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	238/240 (99%)	221 (93%)	16 (7%)	1 (0%)	30	43
1	B	238/240 (99%)	220 (92%)	18 (8%)	0	100	100
2	C	59/61 (97%)	56 (95%)	3 (5%)	0	100	100
2	D	59/61 (97%)	53 (90%)	4 (7%)	2 (3%)	3	2
All	All	594/602 (99%)	550 (93%)	41 (7%)	3 (0%)	24	37

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	2	GLN
2	D	3	GLU
1	A	28	PRO

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	198/198 (100%)	179 (90%)	19 (10%)	8	12
1	B	198/198 (100%)	177 (89%)	21 (11%)	6	10
2	C	53/53 (100%)	49 (92%)	4 (8%)	12	21
2	D	53/53 (100%)	49 (92%)	4 (8%)	12	21
All	All	502/502 (100%)	454 (90%)	48 (10%)	8	12

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	ASP
1	A	61	ARG
1	A	66	VAL
1	A	77	ASP
1	A	86	GLN
1	A	96	THR
1	A	97	ASP
1	A	99	VAL
1	A	105	LEU
1	A	143	LEU
1	A	176	VAL
1	A	181	VAL
1	A	195	SER
1	A	200	HIS
1	A	202	LEU
1	A	203	VAL
1	A	206	GLN
1	A	222	THR
1	A	242	ILE
1	B	26	SER
1	B	36	ARG
1	B	36(A)	SER
1	B	36(C)	SER
1	B	45	THR
1	B	50	ASN
1	B	62	GLU
1	B	76	ASN
1	B	90	VAL
1	B	96	THR
1	B	99	VAL
1	B	115	ASN
1	B	125	ARG
1	B	130	LEU
1	B	133	ASN
1	B	153	GLN
1	B	162	THR
1	B	178	ASN
1	B	191	CYS
1	B	202	LEU
1	B	231	VAL
2	C	2	GLN
2	C	24	ASP
2	C	41	SER

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Mol	Chain	Res	Type
2	C	53	LYS
2	D	24	ASP
2	D	35	ARG
2	D	41	SER
2	D	53	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	110	GLN
1	A	119	GLN
1	A	153	GLN
1	A	206	GLN
1	A	239	ASN
1	B	49	GLN
1	B	50	ASN
1	B	76	ASN
1	B	81	GLN
1	B	115	ASN
1	B	157	GLN
1	B	178	ASN
1	B	204	ASN
1	B	206	GLN

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 ⓘ

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.