



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:47 PM GMT

PDB ID : 1CID
Title : CRYSTAL STRUCTURE OF DOMAINS 3 & 4 OF RAT CD4 AND THEIR
RELATIONSHIP TO THE NH2-TERMINAL DOMAINS
Authors : Brady, R.L.; Dodson, E.J.; Lange, G.
Deposited on : 1993-01-28
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

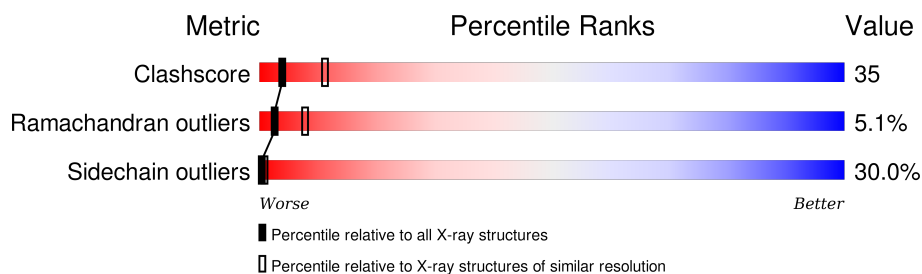
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	177	<div> <div></div> <div>19%</div> <div>37%</div> <div>33%</div> <div>11%</div> </div>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 1396 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 T CELL SURFACE GLYCOPROTEIN CD4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	177	Total	C	N	O	S	9	0	0
			1381	867	232	276	6			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	S	0	0
			1	1		

- Molecule 3 is water.

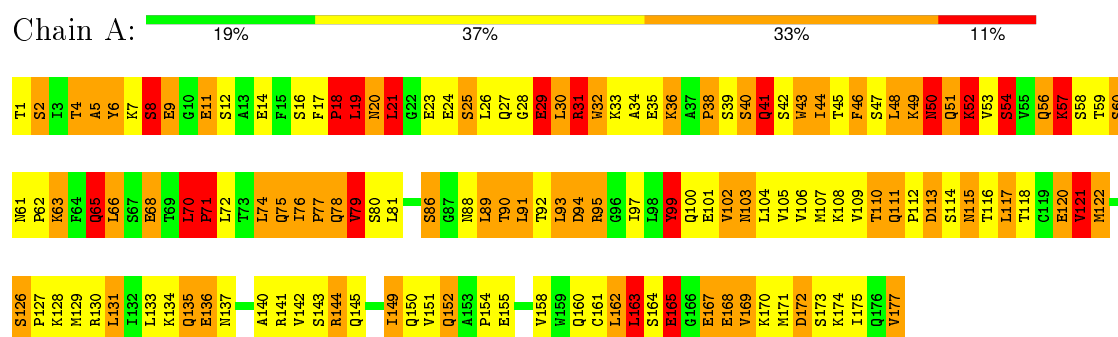
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	14	Total	O	0	0
			14	14		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

• Molecule 1: T CELL SURFACE GLYCOPROTEIN CD4



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	77.80 Å 77.80 Å 82.50 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.233 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1396	wwPDB-VP
Average B, all atoms (Å ²)	44.0	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: SO4

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	1.25	2/1402 (0.1%)	3.11	184/1895 (9.7%)

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	A	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	143	SER	CA-CB	-6.21	1.43	1.52
1	A	177	VAL	C-OXT	5.21	1.33	1.23

All (184) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	130	ARG	NE-CZ-NH2	17.89	129.24	120.30
1	A	79	VAL	CA-CB-CG2	-13.31	90.93	110.90
1	A	120	GLU	OE1-CD-OE2	12.63	138.46	123.30
1	A	93	LEU	CA-C-O	12.63	146.62	120.10
1	A	177	VAL	CA-C-O	-12.56	93.73	120.10
1	A	79	VAL	CA-CB-CG1	11.78	128.57	110.90
1	A	78	GLN	CA-CB-CG	11.60	138.93	113.40
1	A	71	PRO	N-CA-C	10.77	140.10	112.10
1	A	163	LEU	CA-CB-CG	10.71	139.94	115.30
1	A	14	GLU	OE1-CD-OE2	10.67	136.11	123.30
1	A	130	ARG	NE-CZ-NH1	-10.58	115.01	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	75	GLN	N-CA-CB	-10.18	92.27	110.60
1	A	40	SER	N-CA-CB	10.05	125.57	110.50
1	A	93	LEU	CA-C-N	-9.89	95.43	117.20
1	A	99	TYR	CB-CG-CD1	9.82	126.89	121.00
1	A	104	LEU	O-C-N	9.79	138.37	122.70
1	A	168	GLU	OE1-CD-OE2	9.77	135.02	123.30
1	A	162	LEU	CA-CB-CG	9.74	137.70	115.30
1	A	5	ALA	O-C-N	9.59	138.04	122.70
1	A	144	ARG	CD-NE-CZ	9.56	136.99	123.60
1	A	75	GLN	CA-CB-CG	9.52	134.35	113.40
1	A	6	TYR	CB-CG-CD1	-9.36	115.39	121.00
1	A	169	VAL	O-C-N	9.27	137.53	122.70
1	A	43	TRP	CB-CG-CD1	9.24	139.01	127.00
1	A	173	SER	N-CA-CB	-9.24	96.64	110.50
1	A	24	GLU	C-N-CA	9.22	144.76	121.70
1	A	70	LEU	O-C-N	8.98	138.17	121.10
1	A	8	SER	N-CA-CB	8.97	123.95	110.50
1	A	155	GLU	CG-CD-OE1	-8.96	100.39	118.30
1	A	103	ASN	O-C-N	8.90	136.94	122.70
1	A	78	GLN	CB-CG-CD	8.87	134.66	111.60
1	A	91	LEU	CA-CB-CG	8.82	135.60	115.30
1	A	70	LEU	CB-CA-C	8.75	126.83	110.20
1	A	66	LEU	CA-CB-CG	8.73	135.38	115.30
1	A	130	ARG	CD-NE-CZ	8.68	135.75	123.60
1	A	167	GLU	CA-CB-CG	8.60	132.31	113.40
1	A	11	GLU	CG-CD-OE2	8.54	135.38	118.30
1	A	120	GLU	N-CA-CB	8.50	125.90	110.60
1	A	101	GLU	N-CA-CB	8.48	125.86	110.60
1	A	40	SER	CA-C-N	-8.48	98.55	117.20
1	A	94	ASP	N-CA-C	-8.45	88.18	111.00
1	A	6	TYR	CD1-CE1-CZ	-8.44	112.20	119.80
1	A	92	THR	C-N-CA	8.33	142.53	121.70
1	A	111	GLN	CG-CD-OE1	8.26	138.13	121.60
1	A	5	ALA	N-CA-CB	8.18	121.55	110.10
1	A	143	SER	CA-CB-OG	8.14	133.17	111.20
1	A	144	ARG	NE-CZ-NH2	8.10	124.35	120.30
1	A	134	LYS	CB-CG-CD	-7.96	90.90	111.60
1	A	61	ASN	O-C-N	7.96	136.22	121.10
1	A	77	PRO	N-CA-C	7.91	132.66	112.10
1	A	141	ARG	NE-CZ-NH2	-7.87	116.36	120.30
1	A	11	GLU	O-C-N	-7.74	110.32	122.70
1	A	75	GLN	CB-CA-C	7.70	125.79	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	78	GLN	CB-CA-C	7.68	125.75	110.40
1	A	59	THR	N-CA-CB	7.68	124.89	110.30
1	A	59	THR	O-C-N	7.55	134.79	122.70
1	A	117	LEU	N-CA-CB	7.54	125.49	110.40
1	A	42	SER	N-CA-CB	7.52	121.78	110.50
1	A	11	GLU	N-CA-CB	-7.45	97.18	110.60
1	A	65	GLN	CB-CA-C	-7.43	95.53	110.40
1	A	29	GLU	N-CA-CB	-7.43	97.22	110.60
1	A	70	LEU	CA-C-O	-7.42	104.53	120.10
1	A	174	LYS	CB-CA-C	-7.39	95.62	110.40
1	A	107	MET	CG-SD-CE	7.34	111.94	100.20
1	A	95	ARG	CD-NE-CZ	7.33	133.86	123.60
1	A	134	LYS	CB-CA-C	-7.28	95.84	110.40
1	A	24	GLU	CA-C-O	7.23	135.28	120.10
1	A	171	MET	O-C-N	7.21	134.23	122.70
1	A	168	GLU	CA-C-N	-7.13	101.51	117.20
1	A	172	ASP	CB-CG-OD1	6.98	124.58	118.30
1	A	18	PRO	N-CA-CB	-6.93	94.98	102.60
1	A	61	ASN	CA-C-O	-6.88	105.65	120.10
1	A	70	LEU	CB-CG-CD1	-6.88	99.31	111.00
1	A	29	GLU	CA-CB-CG	6.87	128.52	113.40
1	A	168	GLU	CA-C-O	6.85	134.48	120.10
1	A	75	GLN	CA-C-O	-6.83	105.76	120.10
1	A	57	LYS	CA-C-O	6.80	134.38	120.10
1	A	27	GLN	N-CA-C	-6.79	92.66	111.00
1	A	43	TRP	CB-CG-CD2	-6.77	117.80	126.60
1	A	68	GLU	CA-CB-CG	6.74	128.24	113.40
1	A	21	LEU	CA-CB-CG	6.74	130.80	115.30
1	A	172	ASP	CB-CG-OD2	-6.72	112.25	118.30
1	A	160	GLN	CB-CA-C	6.57	123.53	110.40
1	A	92	THR	CA-C-O	6.55	133.85	120.10
1	A	52	LYS	N-CA-CB	6.54	122.38	110.60
1	A	56	GLN	CB-CA-C	6.54	123.47	110.40
1	A	14	GLU	N-CA-CB	6.53	122.36	110.60
1	A	95	ARG	CA-CB-CG	6.42	127.53	113.40
1	A	60	SER	CA-CB-OG	6.39	128.44	111.20
1	A	9	GLU	N-CA-CB	-6.36	99.15	110.60
1	A	171	MET	CG-SD-CE	-6.31	90.11	100.20
1	A	46	PHE	O-C-N	6.30	132.78	122.70
1	A	8	SER	CA-C-N	-6.30	103.34	117.20
1	A	19	LEU	C-N-CA	6.29	137.42	121.70
1	A	4	THR	N-CA-CB	6.29	122.24	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	52	LYS	CB-CG-CD	6.27	127.91	111.60
1	A	76	ILE	CB-CA-C	6.27	124.14	111.60
1	A	78	GLN	N-CA-C	-6.25	94.11	111.00
1	A	115	ASN	O-C-N	6.25	132.70	122.70
1	A	4	THR	O-C-N	6.21	132.63	122.70
1	A	155	GLU	OE1-CD-OE2	6.21	130.75	123.30
1	A	29	GLU	CG-CD-OE2	6.19	130.68	118.30
1	A	65	GLN	O-C-N	6.19	132.60	122.70
1	A	145	GLN	N-CA-CB	-6.13	99.56	110.60
1	A	70	LEU	CB-CG-CD2	6.11	121.39	111.00
1	A	155	GLU	CA-CB-CG	-6.07	100.04	113.40
1	A	143	SER	N-CA-CB	6.05	119.58	110.50
1	A	34	ALA	CB-CA-C	6.04	119.17	110.10
1	A	133	LEU	C-N-CA	6.04	136.80	121.70
1	A	65	GLN	N-CA-CB	6.01	121.42	110.60
1	A	68	GLU	CA-C-N	6.01	130.42	117.20
1	A	140	ALA	N-CA-CB	-6.01	101.69	110.10
1	A	151	VAL	CA-CB-CG1	5.93	119.80	110.90
1	A	141	ARG	CD-NE-CZ	-5.89	115.35	123.60
1	A	149	ILE	CA-CB-CG2	-5.88	99.14	110.90
1	A	109	VAL	O-C-N	5.84	132.04	122.70
1	A	121	VAL	CG1-CB-CG2	-5.83	101.56	110.90
1	A	68	GLU	OE1-CD-OE2	-5.78	116.36	123.30
1	A	40	SER	CA-C-O	5.77	132.21	120.10
1	A	165	GLU	N-CA-CB	5.76	120.97	110.60
1	A	11	GLU	CA-CB-CG	5.74	126.02	113.40
1	A	92	THR	CA-C-N	-5.74	104.58	117.20
1	A	35	GLU	CB-CG-CD	5.73	129.67	114.20
1	A	120	GLU	CB-CA-C	-5.67	99.06	110.40
1	A	36	LYS	O-C-N	5.66	131.76	122.70
1	A	56	GLN	N-CA-C	-5.66	95.72	111.00
1	A	5	ALA	CA-C-N	-5.61	104.87	117.20
1	A	14	GLU	CG-CD-OE2	-5.59	107.11	118.30
1	A	11	GLU	OE1-CD-OE2	-5.57	116.62	123.30
1	A	152	GLN	CA-C-N	-5.55	104.99	117.20
1	A	86	SER	CA-CB-OG	-5.54	96.24	111.20
1	A	26	LEU	C-N-CA	5.52	135.51	121.70
1	A	35	GLU	C-N-CA	-5.51	107.93	121.70
1	A	126	SER	CA-CB-OG	5.50	126.06	111.20
1	A	134	LYS	CD-CE-NZ	5.50	124.36	111.70
1	A	14	GLU	CB-CA-C	-5.48	99.43	110.40
1	A	130	ARG	O-C-N	5.46	131.43	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	43	TRP	CD1-NE1-CE2	-5.45	104.09	109.00
1	A	6	TYR	CB-CG-CD2	5.40	124.24	121.00
1	A	105	VAL	N-CA-CB	5.40	123.39	111.50
1	A	74	LEU	CB-CA-C	5.39	120.45	110.20
1	A	117	LEU	O-C-N	5.38	131.32	122.70
1	A	88	ASN	CA-CB-CG	5.36	125.20	113.40
1	A	131	LEU	CA-CB-CG	5.34	127.57	115.30
1	A	120	GLU	O-C-N	5.32	131.20	122.70
1	A	11	GLU	C-N-CA	5.31	134.98	121.70
1	A	99	TYR	CG-CD1-CE1	5.30	125.54	121.30
1	A	62	PRO	CA-N-CD	-5.29	104.10	111.50
1	A	137	ASN	C-N-CA	5.28	134.89	121.70
1	A	117	LEU	CA-C-O	-5.27	109.04	120.10
1	A	151	VAL	CA-C-N	-5.25	105.64	117.20
1	A	29	GLU	CB-CG-CD	-5.25	100.04	114.20
1	A	54	SER	N-CA-CB	5.25	118.37	110.50
1	A	154	PRO	N-CD-CG	-5.25	95.33	103.20
1	A	105	VAL	C-N-CA	5.23	134.78	121.70
1	A	57	LYS	CA-C-N	-5.22	105.71	117.20
1	A	155	GLU	CG-CD-OE2	5.22	128.75	118.30
1	A	75	GLN	CA-C-N	5.22	128.68	117.20
1	A	28	GLY	N-CA-C	-5.21	100.08	113.10
1	A	122	MET	CG-SD-CE	-5.21	91.87	100.20
1	A	32	TRP	CD2-CE3-CZ3	5.20	125.56	118.80
1	A	78	GLN	O-C-N	5.19	131.00	122.70
1	A	12	SER	CA-C-N	5.18	128.59	117.20
1	A	99	TYR	CB-CG-CD2	-5.17	117.90	121.00
1	A	11	GLU	CG-CD-OE1	-5.17	107.97	118.30
1	A	24	GLU	N-CA-C	5.14	124.88	111.00
1	A	50	ASN	O-C-N	-5.11	114.52	122.70
1	A	18	PRO	N-CA-C	5.11	125.39	112.10
1	A	169	VAL	CB-CA-C	5.11	121.11	111.40
1	A	160	GLN	N-CA-CB	-5.10	101.42	110.60
1	A	31	ARG	CA-CB-CG	5.09	124.60	113.40
1	A	57	LYS	N-CA-C	5.09	124.73	111.00
1	A	122	MET	CB-CG-SD	-5.08	97.15	112.40
1	A	110	THR	C-N-CA	5.08	134.39	121.70
1	A	16	SER	CB-CA-C	5.06	119.72	110.10
1	A	122	MET	CA-CB-CG	-5.06	104.70	113.30
1	A	165	GLU	CB-CG-CD	-5.04	100.58	114.20
1	A	113	ASP	CA-C-N	5.03	128.27	117.20
1	A	62	PRO	CA-C-N	5.02	128.25	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	136	GLU	N-CA-CB	5.02	119.63	110.60
1	A	80	SER	CB-CA-C	5.02	119.63	110.10
1	A	6	TYR	CG-CD1-CE1	5.01	125.31	121.30
1	A	113	ASP	CA-C-O	-5.00	109.60	120.10
1	A	114	SER	N-CA-CB	5.00	118.00	110.50

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	70	LEU	Mainchain,Peptide

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	1381	0	1401	96	0
2	A	1	0	0	0	0
3	A	14	0	0	2	1
All	All	1396	0	1401	96	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 35.

All (96) 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:57:LYS:O	3:A:222:HOH:O	1.61	1.14
1:A:32:TRP:HZ3	1:A:102:VAL:HG12	1.28	0.97
1:A:25:SER:HA	1:A:48:LEU:O	1.71	0.89
1:A:49:LYS:O	1:A:50:ASN:ND2	2.05	0.88
1:A:41:GLN:HG3	1:A:43:TRP:CH2	2.09	0.88
1:A:1:THR:O	1:A:100:GLN:OE1	1.93	0.86
1:A:32:TRP:CZ3	1:A:102:VAL:HG12	2.13	0.84
1:A:112:PRO:HG2	1:A:116:THR:CG2	2.13	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:MET:HG3	1:A:165:GLU:HB2	1.65	0.77
1:A:36:LYS:O	1:A:38:PRO:HD3	1.83	0.77
1:A:19:LEU:O	1:A:21:LEU:HD23	1.85	0.76
1:A:32:TRP:HZ3	1:A:102:VAL:CG1	1.99	0.72
1:A:33:LYS:HE2	1:A:40:SER:HB2	1.72	0.71
1:A:8:SER:O	1:A:11:GLU:HB2	1.91	0.70
1:A:30:LEU:O	1:A:43:TRP:HA	1.95	0.66
1:A:41:GLN:HG3	1:A:43:TRP:CZ3	2.31	0.66
1:A:131:LEU:HB3	1:A:149:ILE:HD13	1.79	0.65
1:A:115:ASN:HB3	1:A:152:GLN:HE22	1.61	0.65
1:A:6:TYR:C	1:A:7:LYS:HG2	2.16	0.64
1:A:111:GLN:CD	1:A:177:VAL:HG13	2.17	0.64
1:A:21:LEU:HD13	1:A:70:LEU:HD13	1.81	0.62
1:A:99:TYR:HD1	1:A:100:GLN:N	1.97	0.62
1:A:112:PRO:HG2	1:A:116:THR:HG21	1.81	0.62
1:A:57:LYS:NZ	1:A:58:SER:O	2.27	0.61
1:A:108:LYS:HE3	1:A:110:THR:HG21	1.83	0.60
1:A:142:VAL:HG13	1:A:144:ARG:HD3	1.85	0.59
1:A:46:PHE:HB2	1:A:54:SER:O	2.03	0.59
1:A:47:SER:HB3	1:A:56:GLN:OE1	2.04	0.58
1:A:120:GLU:HG2	3:A:226:HOH:O	2.04	0.58
1:A:33:LYS:NZ	1:A:40:SER:OG	2.18	0.58
1:A:111:GLN:NE2	1:A:177:VAL:HG13	2.19	0.58
1:A:99:TYR:CD1	1:A:100:GLN:N	2.73	0.57
1:A:136:GLU:HB2	1:A:158:VAL:HB	1.88	0.56
1:A:1:THR:C	1:A:100:GLN:OE1	2.44	0.56
1:A:44:ILE:HD12	1:A:58:SER:HB3	1.88	0.54
1:A:112:PRO:HG2	1:A:116:THR:HG22	1.90	0.54
1:A:50:ASN:C	1:A:51:GLN:HG2	2.28	0.54
1:A:50:ASN:O	1:A:51:GLN:HG2	2.08	0.53
1:A:29:GLU:CD	1:A:31:ARG:HE	2.12	0.53
1:A:44:ILE:HA	1:A:58:SER:HA	1.90	0.53
1:A:126:SER:O	1:A:129:MET:HB2	2.09	0.52
1:A:33:LYS:HZ1	1:A:40:SER:CB	2.19	0.52
1:A:112:PRO:HD2	1:A:116:THR:HB	1.90	0.52
1:A:108:LYS:HE3	1:A:110:THR:CG2	2.40	0.52
1:A:46:PHE:HA	1:A:54:SER:O	2.10	0.52
1:A:46:PHE:CA	1:A:54:SER:O	2.58	0.51
1:A:106:VAL:O	1:A:121:VAL:HA	2.11	0.50
1:A:81:LEU:HD23	1:A:106:VAL:HG12	1.93	0.50
1:A:46:PHE:CB	1:A:54:SER:O	2.59	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:THR:HG22	1:A:97:ILE:CG2	2.41	0.49
1:A:4:THR:HG22	1:A:5:ALA:N	2.28	0.49
1:A:111:GLN:OE1	1:A:177:VAL:HG13	2.12	0.49
1:A:86:SER:HB2	1:A:102:VAL:O	2.13	0.48
1:A:164:SER:HB3	1:A:169:VAL:HG22	1.94	0.48
1:A:112:PRO:HD2	1:A:116:THR:O	2.14	0.47
1:A:47:SER:CB	1:A:56:GLN:OE1	2.62	0.47
1:A:135:GLN:O	1:A:136:GLU:C	2.53	0.47
1:A:46:PHE:HZ	1:A:89:LEU:HD11	1.79	0.47
1:A:81:LEU:HD23	1:A:106:VAL:CG1	2.44	0.47
1:A:165:GLU:HB3	1:A:170:LYS:HE2	1.96	0.47
1:A:164:SER:HA	1:A:168:GLU:O	2.16	0.46
1:A:32:TRP:CZ3	1:A:102:VAL:CG1	2.86	0.46
1:A:86:SER:CB	1:A:102:VAL:O	2.65	0.45
1:A:45:THR:O	1:A:56:GLN:O	2.34	0.45
1:A:53:VAL:HG12	1:A:54:SER:N	2.30	0.45
1:A:1:THR:O	1:A:100:GLN:NE2	2.50	0.45
1:A:65:GLN:HE22	1:A:77:PRO:HG3	1.82	0.45
1:A:117:LEU:HD11	1:A:175:ILE:HG21	1.99	0.44
1:A:163:LEU:HD12	1:A:170:LYS:HB2	1.99	0.44
1:A:52:LYS:HE2	1:A:68:GLU:HB3	2.00	0.44
1:A:1:THR:O	1:A:100:GLN:CD	2.55	0.44
1:A:144:ARG:HB2	1:A:149:ILE:HG21	2.00	0.44
1:A:47:SER:N	1:A:54:SER:O	2.46	0.44
1:A:41:GLN:HG3	1:A:43:TRP:HH2	1.76	0.43
1:A:112:PRO:HD2	1:A:116:THR:C	2.38	0.43
1:A:31:ARG:HB3	1:A:31:ARG:NH1	2.33	0.43
1:A:17:PHE:HA	1:A:18:PRO:HD3	1.56	0.43
1:A:52:LYS:NZ	1:A:68:GLU:HB3	2.34	0.43
1:A:11:GLU:O	1:A:79:VAL:HB	2.19	0.43
1:A:41:GLN:CG	1:A:43:TRP:CZ3	3.02	0.42
1:A:90:THR:HG22	1:A:97:ILE:HG21	2.00	0.42
1:A:63:LYS:O	1:A:77:PRO:HD3	2.20	0.42
1:A:161:CYS:O	1:A:172:ASP:HA	2.19	0.42
1:A:113:ASP:OD1	1:A:116:THR:N	2.52	0.42
1:A:70:LEU:HA	1:A:71:PRO:HA	1.26	0.42
1:A:128:LYS:O	1:A:165:GLU:HA	2.20	0.41
1:A:19:LEU:H	1:A:19:LEU:HG	1.47	0.41
1:A:48:LEU:HD11	1:A:70:LEU:HD21	2.02	0.41
1:A:71:PRO:O	1:A:72:LEU:HB3	2.21	0.41
1:A:136:GLU:CD	1:A:158:VAL:HG11	2.42	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:LYS:HE2	1:A:40:SER:CB	2.45	0.40
1:A:19:LEU:C	1:A:21:LEU:HD23	2.42	0.40
1:A:163:LEU:CD1	1:A:170:LYS:HB2	2.52	0.40
1:A:144:ARG:HB2	1:A:149:ILE:CG2	2.51	0.40
1:A:41:GLN:HA	1:A:43:TRP:CZ3	2.57	0.40
1:A:8:SER:O	1:A:9:GLU:C	2.60	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:232:HOH:O	3:A:232:HOH:O[6_556]	0.47	1.73

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	175/177 (99%)	150 (86%)	16 (9%)	9 (5%)	2 8

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	20	ASN
1	A	21	LEU
1	A	41	GLN
1	A	39	SER
1	A	93	LEU
1	A	57	LYS
1	A	18	PRO
1	A	71	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	160/160 (100%)	112 (70%)	48 (30%)	0 1

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

Mol	Chain	Res	Type
1	A	2	SER
1	A	8	SER
1	A	19	LEU
1	A	20	ASN
1	A	21	LEU
1	A	23	GLU
1	A	25	SER
1	A	29	GLU
1	A	30	LEU
1	A	31	ARG
1	A	38	PRO
1	A	41	GLN
1	A	44	ILE
1	A	48	LEU
1	A	49	LYS
1	A	50	ASN
1	A	51	GLN
1	A	52	LYS
1	A	54	SER
1	A	57	LYS
1	A	60	SER
1	A	63	LYS
1	A	65	GLN
1	A	66	LEU
1	A	71	PRO
1	A	74	LEU
1	A	75	GLN
1	A	76	ILE
1	A	78	GLN
1	A	79	VAL

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Mol	Chain	Res	Type
1	A	89	LEU
1	A	90	THR
1	A	91	LEU
1	A	94	ASP
1	A	95	ARG
1	A	99	TYR
1	A	102	VAL
1	A	103	ASN
1	A	118	THR
1	A	121	VAL
1	A	122	MET
1	A	127	PRO
1	A	135	GLN
1	A	150	GLN
1	A	162	LEU
1	A	163	LEU
1	A	165	GLU
1	A	167	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	GLN
1	A	88	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry

Of 1 ligands modelled in this entry, 1 is modelled with single atom - 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 will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.