



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:53 PM UTC

PDB ID : 4IL1 / pdb_00004il1
Title : Crystal Structure of the Rat Calcineurin
Authors : Ye, Q.; Faucher, F.; Jia, Z.
Deposited on : 2012-12-28
Resolution : 3.00 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)	:	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

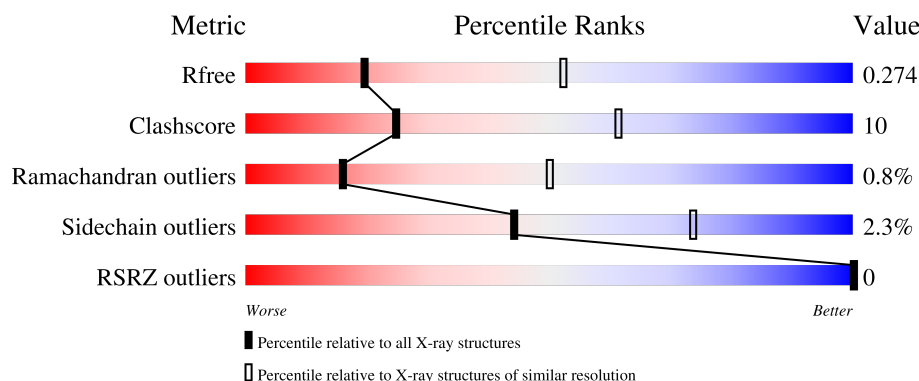
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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 $\leq 5\%$. 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	823	
1	B	823	
1	C	823	
1	D	823	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17255 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 Calmodulin, Calcineurin subunit B type 1, Serine/threonine-protein phosphatase 2B catalytic subunit alpha isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	529	Total	C	N	O	S	0	0	0
			4280	2737	718	796	29			
1	B	528	Total	C	N	O	S	0	0	0
			4277	2734	720	795	28			
1	C	529	Total	C	N	O	S	0	0	0
			4281	2739	718	796	28			
1	D	528	Total	C	N	O	S	0	0	0
			4277	2734	720	795	28			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	150	GLY	-	linker	UNP P62161
A	151	GLY	-	linker	UNP P62161
A	152	GLY	-	linker	UNP P62161
A	153	GLY	-	linker	UNP P62161
A	154	GLY	-	linker	UNP P62161
A	155	GLY	-	linker	UNP P62161
A	156	GLY	-	linker	UNP P62161
A	157	GLY	-	linker	UNP P62161
A	158	GLY	-	linker	UNP P62161
A	328	GLY	-	linker	UNP P63100
A	329	GLY	-	linker	UNP P63100
A	330	GLY	-	linker	UNP P63100
A	331	GLY	-	linker	UNP P63100
A	332	GLY	-	linker	UNP P63100
A	333	GLY	-	linker	UNP P63100
A	816	LEU	-	expression tag	UNP P63329
A	817	GLU	-	expression tag	UNP P63329
A	818	HIS	-	expression tag	UNP P63329
A	819	HIS	-	expression tag	UNP P63329
A	820	HIS	-	expression tag	UNP P63329

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Chain	Residue	Modelled	Actual	Comment	Reference
A	821	HIS	-	expression tag	UNP P63329
A	822	HIS	-	expression tag	UNP P63329
A	823	HIS	-	expression tag	UNP P63329
B	150	GLY	-	linker	UNP P62161
B	151	GLY	-	linker	UNP P62161
B	152	GLY	-	linker	UNP P62161
B	153	GLY	-	linker	UNP P62161
B	154	GLY	-	linker	UNP P62161
B	155	GLY	-	linker	UNP P62161
B	156	GLY	-	linker	UNP P62161
B	157	GLY	-	linker	UNP P62161
B	158	GLY	-	linker	UNP P62161
B	328	GLY	-	linker	UNP P63100
B	329	GLY	-	linker	UNP P63100
B	330	GLY	-	linker	UNP P63100
B	331	GLY	-	linker	UNP P63100
B	332	GLY	-	linker	UNP P63100
B	333	GLY	-	linker	UNP P63100
B	816	LEU	-	expression tag	UNP P63329
B	817	GLU	-	expression tag	UNP P63329
B	818	HIS	-	expression tag	UNP P63329
B	819	HIS	-	expression tag	UNP P63329
B	820	HIS	-	expression tag	UNP P63329
B	821	HIS	-	expression tag	UNP P63329
B	822	HIS	-	expression tag	UNP P63329
B	823	HIS	-	expression tag	UNP P63329
C	150	GLY	-	linker	UNP P62161
C	151	GLY	-	linker	UNP P62161
C	152	GLY	-	linker	UNP P62161
C	153	GLY	-	linker	UNP P62161
C	154	GLY	-	linker	UNP P62161
C	155	GLY	-	linker	UNP P62161
C	156	GLY	-	linker	UNP P62161
C	157	GLY	-	linker	UNP P62161
C	158	GLY	-	linker	UNP P62161
C	328	GLY	-	linker	UNP P63100
C	329	GLY	-	linker	UNP P63100
C	330	GLY	-	linker	UNP P63100
C	331	GLY	-	linker	UNP P63100
C	332	GLY	-	linker	UNP P63100
C	333	GLY	-	linker	UNP P63100
C	816	LEU	-	expression tag	UNP P63329

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Chain	Residue	Modelled	Actual	Comment	Reference
C	817	GLU	-	expression tag	UNP P63329
C	818	HIS	-	expression tag	UNP P63329
C	819	HIS	-	expression tag	UNP P63329
C	820	HIS	-	expression tag	UNP P63329
C	821	HIS	-	expression tag	UNP P63329
C	822	HIS	-	expression tag	UNP P63329
C	823	HIS	-	expression tag	UNP P63329
D	150	GLY	-	linker	UNP P62161
D	151	GLY	-	linker	UNP P62161
D	152	GLY	-	linker	UNP P62161
D	153	GLY	-	linker	UNP P62161
D	154	GLY	-	linker	UNP P62161
D	155	GLY	-	linker	UNP P62161
D	156	GLY	-	linker	UNP P62161
D	157	GLY	-	linker	UNP P62161
D	158	GLY	-	linker	UNP P62161
D	328	GLY	-	linker	UNP P63100
D	329	GLY	-	linker	UNP P63100
D	330	GLY	-	linker	UNP P63100
D	331	GLY	-	linker	UNP P63100
D	332	GLY	-	linker	UNP P63100
D	333	GLY	-	linker	UNP P63100
D	816	LEU	-	expression tag	UNP P63329
D	817	GLU	-	expression tag	UNP P63329
D	818	HIS	-	expression tag	UNP P63329
D	819	HIS	-	expression tag	UNP P63329
D	820	HIS	-	expression tag	UNP P63329
D	821	HIS	-	expression tag	UNP P63329
D	822	HIS	-	expression tag	UNP P63329
D	823	HIS	-	expression tag	UNP P63329

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	4	Total 4 Ca 4	0	0
2	B	4	Total 4 Ca 4	0	0
2	C	4	Total 4 Ca 4	0	0
2	D	4	Total 4 Ca 4	0	0

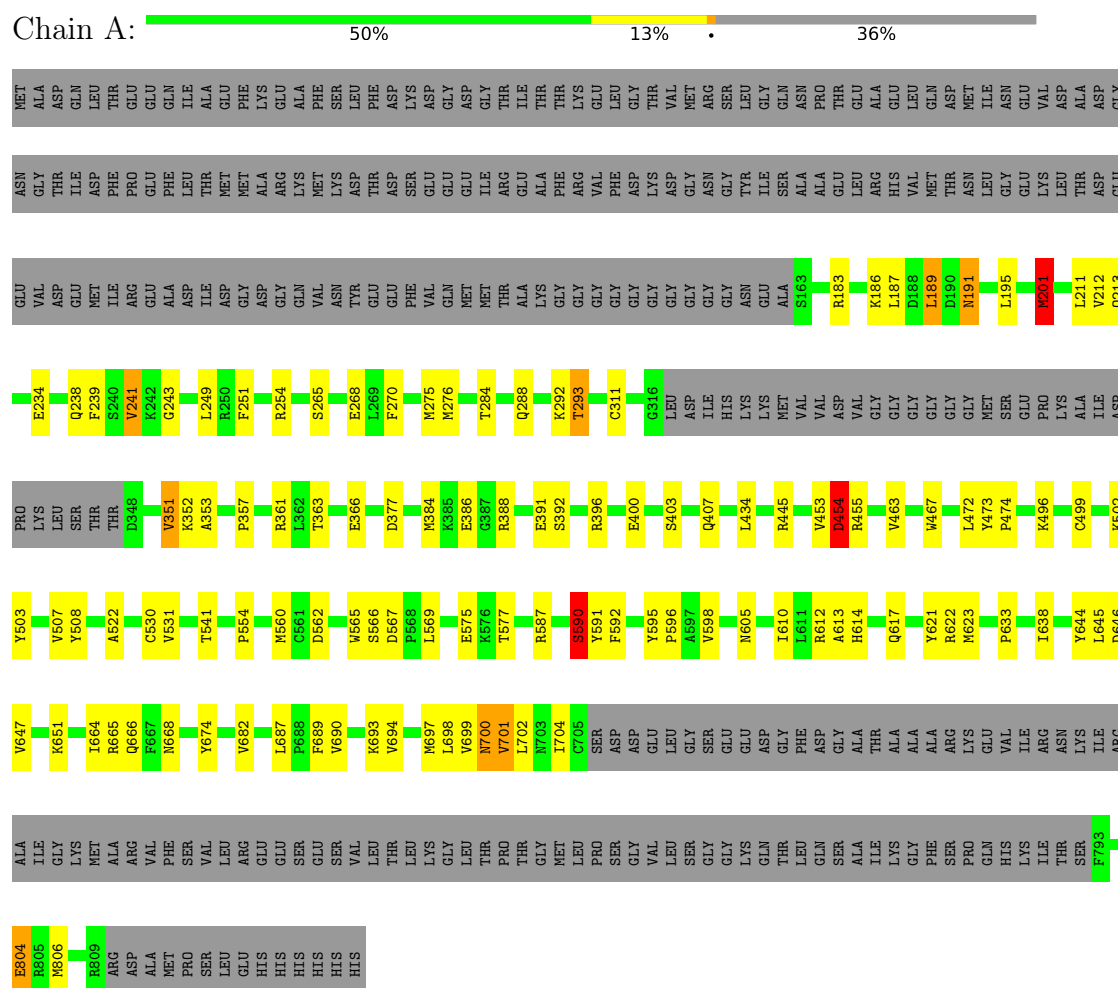
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	29	Total 29	O 29	0	0
3	B	26	Total 26	O 26	0	0
3	C	34	Total 34	O 34	0	0
3	D	35	Total 35	O 35	0	0

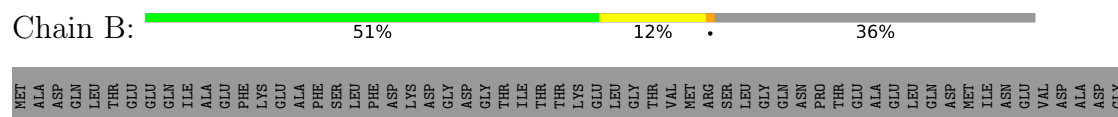
3 Residue-property plots

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 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: Calmodulin, Calcineurin subunit B type 1, Serine/threonine-protein phosphatase 2B catalytic subunit alpha isoform



- Molecule 1: Calmodulin, Calcineurin subunit B type 1, Serine/threonine-protein phosphatase 2B catalytic subunit alpha isoform





ARG	GLU	PRO	GLU	SER	GLN	GLU	SER	VAL	LEU	THR	LYS	GLY	LEU	THR	THR	GLY	MET	LEU	PRO	SER	GLY	VAL	LEU	SER	GLY	LYS	GLN	THR	LEU	GLN	SER	ALA	ILE	THR	SER	F793	G798	R801	E804	R805	M806	R809	ARG	ASP	ALA
MET	PRO	SER	LEU	GLU	HIS	HIS	HIS	HIS	HIS	HIS																																			

● Molecule 1: Calmodulin, Calcineurin subunit B type 1, Serine/threonine-protein phosphatase 2B catalytic subunit alpha isoform



MET	GLU	ASN	GLY	THR	ILE	GLN	LEU	ASP	THR	GLU	GLN	ILE	ALA	MET	PHE	LYS	GLY	ASP	PHE	ASP	LYS	GLY	ASP	GLY	THR	ILE	GLU	THR	THR	GLN	ASN	ALA	PRO	THR	GLU	ALA	GLU	VAL	GLN	ASP	MET	ILE	ASN	GLY	VAL	ASP	ALA	ASP	GLY	
ASN	GLY	THR	ILE	ASP	THR	GLN	LEU	ASP	THR	GLU	GLN	ILE	ALA	MET	PHE	LYS	GLY	ASP	PHE	ASP	LYS	GLY	ASP	GLY	THR	ILE	GLU	THR	THR	GLN	ASN	ALA	PRO	THR	GLU	ALA	GLU	VAL	GLN	ASP	MET	ILE	ASN	GLY	VAL	ASP	ALA	ASP	GLY	
GLU	VAL	ASP	GLU	MET	ILE	ARG	GLU	ALA	ASP	THR	ILE	ASP	ASP	THR	THR	ASP	GLY	GLN	VAL	PHE	GLU	GLY	THR	ALA	LYS	GLN	VAL	GLN	ASN	TYR	GLU	PHE	GLN	GLU	MET	MET	THR	ALA	LYS	GLY	THR	ALA	LYS	GLN	ASP	GLY	VAL	ASP	GLY	
L206	Q207	L211	T221	E231	Q238	F239	S240	G243	E246	L249	R250	M258	D259	G265	N266	L273	K274	M275	M276	T284	Q287	Q288	D291	K292	T293	C311	V314	G315	G316	LEU	ASP	ILE	HIS	LYS	LYS	MET	VAL	VAL	ASP	VAL	VAL	GLY	GLY	GLY	GLY					
GLY	GLY	MET	PRO	LYS	ALA	ILE	ASP	LYS	THR	D348	R349	V350	V351	K352	A353	V354	R361	L362	T363	E366	R388	R396	E400	I424	L431	L434	G438	A442	N443	L449	V453	D454	R455	L466	L472	Y473	P474	L479												
M483	F493	C499	K500	I501	K502	Y503	V507	D516	A522	C530	V531	T541	K552	A556	W565	S566	L569	Q573	N574	E575	E579	N584	R587	S590	Y591	F592	T593	S594	Y595	P596	A597	V598	N605	I610	L611	R612	A613	H614	Q617											
Y621	R622	I638	N643	Y644	L645	D646	V647	K656	M662	N663	I664	W675	D681	V682	L687	P688	F689	V690	K693	M697	L698	L702	N703	ILE	CYS	SER	ASP	ASP	GLY	LEU	SER	GLY	GLU	LYS	GLN	THR	ALA	ILE	GLY	ALA	ALA	ARG	LYS	GLN	VAL					
ILE	ARG	ASN	ILE	ARG	ALA	ILE	GLY	LYS	MET	ALA	ARG	VAL	PHE	SER	VAL	LEU	ARG	GLU	GLU	SER	VAL	LEU	THR	PRO	THR	GLY	MET	LEU	PRO	GLY	VAL	LEU	SER	GLY	GLY	LYS	GLN	THR	LEU	GLN	SER	ALA	ILE	LYS	GLY	PHE	SER	PRO	GLN	HIS
LYS	ILE	SER	F793	E794	E795	A796	K797	G798	R801	I802	R805	M806	R809	R810	ASP	ALA	MET	PRO	SER	SER	LEU	GLU	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS		

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	99.30Å 193.85Å 107.82Å 90.00° 90.09° 90.00°	Depositor
Resolution (Å)	10.00 – 3.00 10.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.4 (10.00-3.00) 99.5 (10.00-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.08 (at 2.98Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.241 , 0.273 0.243 , 0.274	Depositor DCC
R_{free} test set	2034 reflections (2.51%)	wwPDB-VP
Wilson B-factor (Å ²)	61.5	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 16.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.447 for h,-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	17255	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 37.56 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.2090e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.81	1/4379 (0.0%)	1.00	6/5914 (0.1%)
1	B	0.83	1/4376 (0.0%)	0.98	5/5909 (0.1%)
1	C	0.82	1/4380 (0.0%)	0.99	6/5916 (0.1%)
1	D	0.83	0/4376	1.00	8/5909 (0.1%)
All	All	0.82	3/17511 (0.0%)	0.99	25/23648 (0.1%)

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	C	0	1
1	D	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	351	VAL	CA-C	5.39	1.59	1.52
1	A	351	VAL	CA-C	5.18	1.58	1.53
1	C	589	CYS	CA-C	5.09	1.58	1.53

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	701	VAL	N-CA-C	-9.86	101.26	110.53
1	D	442	ALA	N-CA-C	-8.69	95.95	109.25
1	B	352	LYS	N-CA-C	7.43	120.53	108.34
1	C	588	GLY	N-CA-C	-7.34	100.35	112.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	454	ASP	N-CA-C	6.04	123.67	110.80
1	A	351	VAL	N-CA-C	5.96	115.92	106.32
1	D	353	ALA	N-CA-C	-5.87	105.77	113.17
1	D	454	ASP	N-CA-C	5.75	123.05	110.80
1	B	203	LEU	CB-CA-C	5.75	116.67	108.68
1	A	357	PRO	CA-C-N	5.71	125.64	119.76
1	A	357	PRO	C-N-CA	5.71	125.64	119.76
1	B	456	GLY	N-CA-C	-5.48	102.45	111.38
1	B	701	VAL	N-CA-C	-5.40	98.11	109.34
1	D	240	SER	N-CA-C	-5.38	103.52	111.81
1	C	357	PRO	CA-C-N	5.32	125.33	119.90
1	C	357	PRO	C-N-CA	5.32	125.33	119.90
1	D	454	ASP	CA-C-N	-5.22	113.93	122.54
1	D	454	ASP	C-N-CA	-5.22	113.93	122.54
1	D	795	GLU	N-CA-C	-5.21	106.88	113.18
1	C	351	VAL	CB-CA-C	5.18	118.08	110.98
1	C	418	VAL	CB-CA-C	-5.10	102.00	111.18
1	B	684	THR	N-CA-CB	5.10	117.71	110.06
1	C	456	GLY	N-CA-C	-5.02	103.20	111.38
1	D	501	ILE	CB-CA-C	-5.02	104.13	112.26
1	A	241	VAL	N-CA-C	-5.01	105.96	110.82

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	452	TYR	Peptide
1	D	449	LEU	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	4280	0	4186	96	0
1	B	4277	0	4183	65	0
1	C	4281	0	4187	79	0
1	D	4277	0	4182	95	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	4	0	0	0	0
2	B	4	0	0	0	0
2	C	4	0	0	0	0
2	D	4	0	0	0	0
3	A	29	0	0	2	0
3	B	26	0	0	1	0
3	C	34	0	0	1	0
3	D	35	0	0	1	0
All	All	17255	0	16738	333	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 10.

All (333) 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:C:453:VAL:O	1:C:459:SER:OG	1.62	1.15
1:A:187:LEU:HD23	1:A:195:LEU:HD21	1.26	1.08
1:A:455:ARG:HD3	1:A:644:TYR:OH	1.61	1.00
1:C:517:CYS:O	1:C:550:ARG:NH1	1.96	0.98
1:D:579:GLU:O	1:D:594:SER:OG	1.81	0.98
1:C:623:MET:HE3	1:C:633:PRO:HG2	1.47	0.96
1:C:352:LYS:HB3	1:C:353:ALA:HA	1.48	0.96
1:A:623:MET:HE3	1:A:633:PRO:HG2	1.49	0.94
1:C:239:PHE:CZ	1:C:694:VAL:HG21	2.02	0.94
1:A:187:LEU:CD2	1:A:195:LEU:HD21	1.99	0.93
1:D:273:LEU:HD11	1:D:682:VAL:HG11	1.50	0.93
1:C:239:PHE:HZ	1:C:694:VAL:HG21	1.34	0.91
1:C:555:PRO:HD2	1:C:560:MET:HG2	1.56	0.88
1:A:352:LYS:CG	1:A:353:ALA:HA	2.02	0.87
1:D:442:ALA:O	1:D:443:ASN:HB3	1.73	0.86
1:A:239:PHE:CZ	1:A:251:PHE:CZ	2.63	0.86
1:B:203:LEU:HD11	1:B:206:LEU:HB2	1.58	0.85
1:B:623:MET:HE1	1:D:167:GLU:OE2	1.77	0.84
1:C:352:LYS:HB3	1:C:353:ALA:CA	2.07	0.83
1:A:201:MET:HA	1:A:201:MET:HE2	1.61	0.82
1:C:203:LEU:HD12	1:C:204:PRO:HD2	1.63	0.81
1:A:352:LYS:HG3	1:A:353:ALA:HA	1.63	0.81
1:D:249:LEU:HD23	1:D:311:CYS:SG	2.23	0.79
1:A:249:LEU:HD23	1:A:311:CYS:SG	2.24	0.78
1:A:403:SER:O	1:A:407:GLN:NE2	2.16	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:249:LEU:HD23	1:C:311:CYS:SG	2.24	0.77
1:C:408:GLU:O	1:C:550:ARG:NH2	2.18	0.77
1:B:249:LEU:HD23	1:B:311:CYS:SG	2.24	0.77
1:B:437:VAL:HG13	1:B:665:ARG:HE	1.51	0.75
1:B:203:LEU:CD1	1:B:206:LEU:HB2	2.17	0.74
1:D:794:GLU:OE1	1:D:794:GLU:N	2.20	0.74
1:D:424:ILE:HD13	1:D:431:LEU:HD13	1.70	0.74
1:D:809:ARG:HG2	1:D:810:ARG:H	1.52	0.74
1:C:258:MET:HE3	1:C:275:MET:HE1	1.70	0.74
1:A:665:ARG:NH1	1:A:666:GLN:O	2.21	0.73
1:C:437:VAL:HG13	1:C:665:ARG:HE	1.52	0.73
1:A:698:LEU:O	1:A:701:VAL:HB	1.88	0.73
1:A:187:LEU:HD23	1:A:195:LEU:CD2	2.15	0.72
1:C:239:PHE:CZ	1:C:694:VAL:CG2	2.72	0.72
1:B:350:VAL:HG11	1:B:352:LYS:HD2	1.71	0.72
1:A:239:PHE:HZ	1:A:251:PHE:CZ	2.05	0.72
1:C:453:VAL:O	1:C:459:SER:CB	2.38	0.72
1:D:584:ASN:HB3	1:D:590:SER:O	1.90	0.71
1:A:187:LEU:CD2	1:A:195:LEU:CD2	2.69	0.71
1:D:350:VAL:HG11	1:D:352:LYS:NZ	2.06	0.70
1:C:499:CYS:O	1:C:502:LYS:O	2.11	0.69
1:A:499:CYS:O	1:A:502:LYS:O	2.11	0.69
1:D:499:CYS:O	1:D:502:LYS:O	2.11	0.68
1:B:499:CYS:O	1:B:502:LYS:O	2.11	0.68
1:A:623:MET:CE	1:A:633:PRO:HG2	2.24	0.68
1:B:437:VAL:HG13	1:B:665:ARG:NE	2.09	0.68
1:C:352:LYS:CB	1:C:353:ALA:HA	2.22	0.68
1:C:453:VAL:HG23	1:C:485:GLU:OE2	1.94	0.68
1:C:239:PHE:HE1	1:C:251:PHE:CE1	2.11	0.68
1:B:171:HIS:CG	1:B:241:VAL:CG1	2.77	0.67
1:C:798:GLY:O	1:C:801:ARG:NH1	2.27	0.67
1:D:258:MET:HE3	1:D:275:MET:HE1	1.75	0.67
1:C:623:MET:CE	1:C:633:PRO:HG2	2.22	0.67
1:D:798:GLY:O	1:D:801:ARG:NE	2.24	0.66
1:C:437:VAL:HG13	1:C:665:ARG:NE	2.09	0.66
1:A:212:VAL:HA	1:A:697:MET:HE1	1.77	0.66
1:C:584:ASN:HB3	1:C:590:SER:O	1.96	0.66
1:A:352:LYS:HG2	1:A:353:ALA:HA	1.78	0.65
1:A:352:LYS:HG2	1:A:353:ALA:CA	2.25	0.65
1:C:265:SER:HB3	1:C:349:ARG:HH11	1.61	0.65
1:B:171:HIS:CG	1:B:241:VAL:HG11	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:565:TRP:CZ2	1:D:806:MET:HE3	2.33	0.64
1:D:442:ALA:O	1:D:443:ASN:CB	2.43	0.64
1:D:575:GLU:HG3	1:D:594:SER:HB2	1.78	0.64
1:A:241:VAL:C	1:A:243:GLY:H	2.06	0.63
1:A:455:ARG:CD	1:A:644:TYR:OH	2.41	0.63
1:D:556:ALA:HB2	1:D:809:ARG:HH11	1.62	0.63
1:A:292:LYS:HE2	1:A:386:GLU:OE2	1.99	0.62
1:B:565:TRP:CZ2	1:B:806:MET:HE3	2.34	0.62
1:A:565:TRP:CZ2	1:A:806:MET:HE3	2.35	0.62
1:D:702:LEU:O	1:D:703:ASN:O	2.17	0.62
1:B:266:ASN:HB3	1:B:350:VAL:HG22	1.82	0.62
1:D:211:LEU:HD12	1:D:693:LYS:HB2	1.82	0.62
1:A:698:LEU:O	1:A:701:VAL:N	2.32	0.61
1:B:246:GLU:O	1:B:250:ARG:HG2	1.99	0.61
1:A:183:ARG:HG2	1:A:704:ILE:HG12	1.81	0.61
1:A:211:LEU:HD12	1:A:693:LYS:HB2	1.83	0.60
1:B:665:ARG:NH1	1:D:171:HIS:O	2.34	0.60
1:C:211:LEU:HD12	1:C:693:LYS:HB2	1.84	0.60
1:D:350:VAL:HG11	1:D:352:LYS:HZ2	1.66	0.60
1:C:552:LYS:NZ	3:C:1004:HOH:O	2.30	0.60
1:B:211:LEU:HD12	1:B:693:LYS:HB2	1.83	0.60
1:A:212:VAL:HA	1:A:697:MET:CE	2.32	0.59
1:A:700:ASN:OD1	1:A:700:ASN:C	2.45	0.59
1:A:455:ARG:HD3	1:A:644:TYR:HH	1.65	0.58
1:B:702:LEU:O	1:B:703:ASN:OD1	2.21	0.58
1:B:531:VAL:O	1:B:612:ARG:HA	2.04	0.58
1:D:352:LYS:HD2	1:D:354:VAL:O	2.03	0.58
1:C:293:THR:HG21	1:C:682:VAL:HG22	1.86	0.58
1:A:212:VAL:HG22	1:A:697:MET:HE2	1.86	0.58
1:D:584:ASN:CB	1:D:590:SER:O	2.51	0.58
1:A:211:LEU:HD11	1:A:690:VAL:HA	1.86	0.57
1:A:453:VAL:O	1:A:454:ASP:HB2	2.03	0.57
1:C:276:MET:HB2	1:C:689:PHE:CE2	2.39	0.57
1:A:702:LEU:HD11	3:A:1006:HOH:O	2.04	0.57
1:D:573:GLY:H	1:D:575:GLU:CD	2.13	0.57
1:A:455:ARG:HG2	1:A:455:ARG:HH11	1.69	0.56
1:B:361:ARG:NH2	1:B:388:ARG:NH2	2.53	0.56
1:A:293:THR:HG21	1:A:682:VAL:HG22	1.85	0.56
1:B:293:THR:HG21	1:B:682:VAL:HG22	1.86	0.56
1:D:352:LYS:CD	1:D:354:VAL:O	2.54	0.56
1:D:809:ARG:HG2	1:D:810:ARG:N	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:531:VAL:O	1:A:612:ARG:HA	2.05	0.56
1:A:623:MET:HE3	1:A:633:PRO:CG	2.31	0.56
1:B:171:HIS:ND1	1:B:237:SER:OG	2.39	0.56
1:C:531:VAL:O	1:C:612:ARG:HA	2.06	0.56
1:B:211:LEU:HD11	1:B:690:VAL:HA	1.88	0.56
1:D:587:ARG:HH21	1:D:614:HIS:CD2	2.24	0.56
1:A:183:ARG:HG2	1:A:704:ILE:CG1	2.36	0.56
1:B:453:VAL:O	1:B:454:ASP:HB2	2.05	0.56
1:D:556:ALA:HB2	1:D:809:ARG:NH1	2.20	0.56
1:D:238:GLN:O	1:D:239:PHE:CB	2.54	0.55
1:D:284:THR:O	1:D:288:GLN:HG3	2.06	0.55
1:A:213:GLN:HG2	1:A:275:MET:CE	2.36	0.55
1:C:238:GLN:OE1	1:C:247:GLN:NE2	2.40	0.55
1:D:453:VAL:O	1:D:454:ASP:HB2	2.05	0.55
1:B:543:ASP:HA	1:B:546:ARG:HG3	1.88	0.55
1:C:555:PRO:CD	1:C:560:MET:HG2	2.34	0.55
1:D:266:ASN:HB3	1:D:350:VAL:HG22	1.89	0.55
1:A:292:LYS:NZ	1:A:674:TYR:O	2.39	0.55
1:A:699:VAL:C	1:A:701:VAL:H	2.14	0.54
1:C:584:ASN:CB	1:C:590:SER:O	2.55	0.54
1:D:273:LEU:HD11	1:D:682:VAL:CG1	2.32	0.54
1:D:531:VAL:O	1:D:612:ARG:HA	2.07	0.54
1:B:284:THR:O	1:B:288:GLN:HG3	2.07	0.54
1:C:565:TRP:O	1:C:566:SER:C	2.49	0.54
1:C:587:ARG:NH1	1:C:804:GLU:HG3	2.23	0.54
1:D:794:GLU:O	1:D:797:LYS:HB3	2.08	0.54
1:A:690:VAL:O	1:A:694:VAL:HG23	2.07	0.54
1:D:238:GLN:O	1:D:239:PHE:HB2	2.08	0.54
1:A:239:PHE:CZ	1:A:251:PHE:CE1	2.95	0.54
1:C:565:TRP:CZ2	1:C:806:MET:HE3	2.43	0.54
1:D:221:THR:OG1	1:D:231:GLU:HG2	2.08	0.54
1:C:284:THR:O	1:C:288:GLN:HG3	2.08	0.53
1:C:234:GLU:O	1:C:238:GLN:HG3	2.08	0.53
1:C:265:SER:HB3	1:C:349:ARG:NH1	2.23	0.53
1:D:211:LEU:HD11	1:D:690:VAL:HA	1.91	0.53
1:A:213:GLN:CG	1:A:275:MET:HE1	2.39	0.53
1:C:702:LEU:O	1:C:703:ASN:HB3	2.09	0.53
1:D:291:ASP:OD2	1:D:352:LYS:HE2	2.09	0.53
1:A:352:LYS:HG2	1:A:353:ALA:HB2	1.91	0.52
1:C:258:MET:CE	1:C:275:MET:HE1	2.38	0.52
1:D:287:GLN:NE2	1:D:291:ASP:OD1	2.37	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:391:GLU:O	1:B:395:LEU:HD13	2.09	0.52
1:B:292:LYS:HE3	1:B:386:GLU:OE2	2.10	0.52
1:C:211:LEU:HD11	1:C:690:VAL:HA	1.92	0.52
1:C:437:VAL:HG13	1:C:665:ARG:CD	2.40	0.51
1:B:206:LEU:HD11	1:B:697:MET:HG3	1.93	0.51
1:D:258:MET:CE	1:D:275:MET:HE1	2.40	0.51
1:A:361:ARG:HH12	1:A:388:ARG:CZ	2.23	0.51
1:A:284:THR:O	1:A:288:GLN:HG3	2.09	0.51
1:D:556:ALA:N	1:D:809:ARG:HH12	2.08	0.51
1:C:541:THR:HA	1:C:605:ASN:OD1	2.11	0.51
1:C:270:PHE:CD1	1:C:351:VAL:HG11	2.46	0.51
1:C:703:ASN:O	1:C:704:ILE:HB	2.10	0.51
1:C:239:PHE:CE1	1:C:251:PHE:CE1	2.96	0.50
1:B:437:VAL:HG13	1:B:665:ARG:CD	2.41	0.50
1:C:472:LEU:C	1:C:474:PRO:HD3	2.36	0.50
1:C:623:MET:HE3	1:C:633:PRO:CG	2.29	0.50
1:A:702:LEU:CD1	3:A:1006:HOH:O	2.58	0.50
1:D:396:ARG:O	1:D:400:GLU:HB2	2.11	0.50
1:A:276:MET:HB2	1:A:689:PHE:CE2	2.46	0.50
1:B:522:ALA:HB3	1:B:530:CYS:HB2	1.93	0.50
1:A:352:LYS:HG2	1:A:353:ALA:CB	2.40	0.50
1:D:293:THR:HG23	1:D:681:ASP:OD1	2.12	0.50
1:A:239:PHE:CZ	1:A:694:VAL:HG11	2.47	0.50
1:D:201:MET:HE1	1:D:207:GLN:HA	1.94	0.49
1:D:265:SER:HB2	1:D:349:ARG:HG3	1.94	0.49
1:D:363:THR:HG23	1:D:366:GLU:OE1	2.12	0.49
1:B:396:ARG:O	1:B:400:GLU:HB2	2.12	0.49
1:B:565:TRP:O	1:B:566:SER:C	2.56	0.49
1:C:363:THR:HG23	1:C:366:GLU:OE1	2.13	0.49
1:C:567:ASP:OD2	1:C:587:ARG:NE	2.39	0.49
1:D:438:GLY:HA2	1:D:656:LYS:HE3	1.95	0.49
1:A:567:ASP:OD2	1:A:587:ARG:NE	2.42	0.49
1:C:396:ARG:O	1:C:400:GLU:HB2	2.13	0.49
1:A:396:ARG:O	1:A:400:GLU:HB2	2.13	0.49
1:D:556:ALA:N	1:D:809:ARG:NH1	2.60	0.49
1:D:702:LEU:O	1:D:703:ASN:C	2.56	0.49
1:C:555:PRO:HD2	1:C:560:MET:CG	2.37	0.49
1:B:201:MET:HE1	1:B:207:GLN:HA	1.95	0.48
1:D:311:CYS:HA	1:D:314:VAL:HG22	1.95	0.48
1:A:587:ARG:NH1	1:A:804:GLU:HG3	2.29	0.48
1:A:234:GLU:O	1:A:238:GLN:HG3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:699:VAL:C	1:A:701:VAL:N	2.72	0.48
1:A:352:LYS:CG	1:A:353:ALA:CA	2.79	0.48
1:D:203:LEU:HD12	1:D:206:LEU:HD12	1.96	0.48
1:D:516:ASP:OD2	1:D:552:LYS:C	2.56	0.48
1:C:473:TYR:N	1:C:474:PRO:HD3	2.29	0.48
1:C:522:ALA:HB3	1:C:530:CYS:HB2	1.95	0.48
1:D:472:LEU:C	1:D:474:PRO:HD3	2.38	0.48
1:A:201:MET:HE2	1:A:201:MET:CA	2.41	0.47
1:A:565:TRP:O	1:A:566:SER:C	2.57	0.47
1:B:541:THR:HA	1:B:605:ASN:OD1	2.14	0.47
1:B:567:ASP:OD2	1:B:587:ARG:NE	2.40	0.47
1:A:363:THR:HG23	1:A:366:GLU:OE1	2.13	0.47
1:C:621:TYR:CD2	1:C:664:ILE:HD13	2.49	0.47
1:D:643:ASN:HB3	3:D:1027:HOH:O	2.14	0.47
1:A:186:LYS:HD2	1:A:704:ILE:CD1	2.45	0.47
1:A:541:THR:HA	1:A:605:ASN:OD1	2.14	0.47
1:B:472:LEU:C	1:B:474:PRO:HD3	2.39	0.47
1:B:586:VAL:O	1:B:805:ARG:HG2	2.15	0.47
1:D:239:PHE:CD2	1:D:698:LEU:HD11	2.50	0.47
1:D:434:LEU:C	1:D:434:LEU:HD23	2.40	0.47
1:D:794:GLU:N	1:D:794:GLU:CD	2.72	0.47
1:A:213:GLN:HG2	1:A:275:MET:HE1	1.94	0.47
1:A:472:LEU:C	1:A:474:PRO:HD3	2.40	0.47
1:B:363:THR:HG23	1:B:366:GLU:OE1	2.15	0.47
1:A:612:ARG:NH2	1:A:614:HIS:HB3	2.30	0.47
1:B:598:VAL:HG13	1:B:610:ILE:HD12	1.97	0.47
1:B:350:VAL:CG1	1:B:352:LYS:HD2	2.42	0.46
1:D:239:PHE:HD2	1:D:698:LEU:HD11	1.80	0.46
1:B:810:ARG:HA	1:B:810:ARG:NE	2.30	0.46
1:C:418:VAL:HG12	1:C:419:THR:N	2.30	0.46
1:B:569:LEU:HD23	1:B:592:PHE:HB3	1.98	0.46
1:D:598:VAL:HG13	1:D:610:ILE:HD12	1.97	0.46
1:A:522:ALA:HB3	1:A:530:CYS:HB2	1.96	0.46
1:C:483:ASN:ND2	1:C:614:HIS:HE1	2.13	0.46
1:C:559:PRO:O	1:C:563:ILE:HG13	2.15	0.46
1:D:473:TYR:N	1:D:474:PRO:HD3	2.30	0.46
1:A:455:ARG:HG2	1:A:455:ARG:NH1	2.31	0.46
1:D:239:PHE:CD2	1:D:698:LEU:CD1	2.98	0.46
1:A:562:ASP:OD1	1:A:590:SER:HB2	2.16	0.46
1:D:569:LEU:HD23	1:D:592:PHE:HB3	1.98	0.46
1:A:621:TYR:CD2	1:A:664:ILE:HD13	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:698:LEU:O	1:A:701:VAL:CB	2.61	0.46
1:A:434:LEU:C	1:A:434:LEU:HD23	2.41	0.46
1:B:473:TYR:N	1:B:474:PRO:HD3	2.31	0.46
1:B:503:TYR:HB3	1:B:507:VAL:HG21	1.98	0.45
1:B:621:TYR:CD2	1:B:664:ILE:HD13	2.51	0.45
1:D:204:PRO:HG2	1:D:205:GLU:OE2	2.16	0.45
1:A:700:ASN:OD1	1:A:701:VAL:N	2.49	0.45
1:B:651:LYS:HD3	1:B:668:ASN:OD1	2.15	0.45
1:D:503:TYR:HB3	1:D:507:VAL:HG21	1.98	0.45
1:D:239:PHE:CE2	1:D:698:LEU:HD12	2.52	0.45
1:B:587:ARG:CZ	1:B:614:HIS:CE1	2.99	0.45
1:D:455:ARG:HH21	1:D:645:LEU:HD11	1.82	0.45
1:A:251:PHE:HA	1:A:254:ARG:HD2	1.99	0.45
1:A:569:LEU:HD23	1:A:592:PHE:HB3	1.97	0.45
1:B:203:LEU:C	1:B:203:LEU:HD12	2.42	0.45
1:B:263:TYR:CD2	1:B:304:ARG:NH1	2.85	0.45
1:D:793:PHE:C	1:D:795:GLU:H	2.25	0.45
1:C:503:TYR:HB3	1:C:507:VAL:HG21	1.98	0.45
1:D:579:GLU:O	1:D:594:SER:CB	2.62	0.45
1:B:204:PRO:HG2	1:B:205:GLU:OE2	2.16	0.45
1:C:453:VAL:HG11	1:C:490:THR:HG22	1.97	0.45
1:D:565:TRP:HB2	1:D:590:SER:HB2	1.99	0.45
1:D:621:TYR:CD2	1:D:664:ILE:HD13	2.52	0.45
1:A:503:TYR:HB3	1:A:507:VAL:HG21	1.99	0.45
1:B:276:MET:HB2	1:B:689:PHE:CE2	2.52	0.44
1:D:522:ALA:HB3	1:D:530:CYS:HB2	1.98	0.44
1:C:655:LEU:HD13	1:C:662:MET:HE1	1.97	0.44
1:A:613:ALA:CB	1:A:638:ILE:O	2.66	0.44
1:D:348:ASP:HB3	1:D:349:ARG:H	1.66	0.44
1:C:613:ALA:CB	1:C:638:ILE:O	2.65	0.44
1:D:466:LEU:HB3	1:D:479:LEU:HD21	1.99	0.44
1:D:613:ALA:CB	1:D:638:ILE:O	2.66	0.44
1:C:569:LEU:HD23	1:C:592:PHE:HB3	1.99	0.44
1:B:270:PHE:CD1	1:B:270:PHE:C	2.95	0.44
1:A:241:VAL:C	1:A:243:GLY:N	2.76	0.44
1:C:348:ASP:O	1:C:348:ASP:OD1	2.36	0.44
1:D:350:VAL:HG11	1:D:352:LYS:CE	2.48	0.44
1:D:565:TRP:O	1:D:566:SER:C	2.60	0.44
1:B:171:HIS:CD2	1:B:241:VAL:HG11	2.53	0.43
1:C:265:SER:CB	1:C:349:ARG:HD3	2.47	0.43
1:D:541:THR:HA	1:D:605:ASN:OD1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:617:GLN:OE1	1:A:622:ARG:HB2	2.18	0.43
1:B:617:GLN:OE1	1:B:622:ARG:HB2	2.18	0.43
1:D:186:LYS:NZ	1:D:703:ASN:O	2.38	0.43
1:D:239:PHE:O	1:D:239:PHE:CG	2.70	0.43
1:A:270:PHE:CD1	1:A:270:PHE:C	2.96	0.43
1:B:187:LEU:O	1:B:189:LEU:HD22	2.18	0.43
1:C:589:CYS:SG	1:C:590:SER:N	2.91	0.43
1:B:496:LYS:HA	1:B:508:TYR:CD1	2.54	0.43
1:B:613:ALA:CB	1:B:638:ILE:O	2.67	0.43
1:C:617:GLN:OE1	1:C:622:ARG:HB2	2.19	0.43
1:C:598:VAL:HG13	1:C:610:ILE:HD12	1.99	0.43
1:D:565:TRP:CE2	1:D:806:MET:HE3	2.53	0.43
1:A:463:VAL:O	1:A:467:TRP:HB2	2.19	0.43
1:B:197:VAL:HG23	3:B:1006:HOH:O	2.19	0.43
1:D:276:MET:HB2	1:D:689:PHE:CE2	2.54	0.43
1:A:187:LEU:HD21	1:A:195:LEU:CD2	2.49	0.43
1:A:239:PHE:HZ	1:A:251:PHE:CE1	2.33	0.43
1:D:802:ILE:O	1:D:805:ARG:HB2	2.17	0.43
1:A:554:PRO:HA	1:A:560:MET:HE3	2.01	0.43
1:A:651:LYS:HE2	1:A:668:ASN:OD1	2.18	0.43
1:C:587:ARG:HB2	1:C:588:GLY:O	2.18	0.42
1:A:598:VAL:HG13	1:A:610:ILE:HD12	2.00	0.42
1:B:497:GLN:HG2	1:B:678:ASN:OD1	2.20	0.42
1:C:241:VAL:O	1:C:242:LYS:C	2.60	0.42
1:C:703:ASN:O	1:C:704:ILE:CB	2.67	0.42
1:A:265:SER:HB3	1:A:268:GLU:HB2	2.02	0.42
1:C:187:LEU:O	1:C:189:LEU:HD22	2.20	0.42
1:D:292:LYS:HD2	1:D:675:TRP:CZ2	2.55	0.42
1:D:617:GLN:OE1	1:D:622:ARG:HB2	2.19	0.42
1:C:457:TYR:OH	1:C:677:PRO:HA	2.20	0.42
1:C:645:LEU:O	1:C:646:ASP:HB2	2.20	0.42
1:D:595:TYR:HB3	1:D:596:PRO:HD3	2.02	0.42
1:A:239:PHE:C	1:A:241:VAL:N	2.77	0.42
1:A:239:PHE:CD2	1:A:698:LEU:HD11	2.55	0.42
1:D:187:LEU:O	1:D:189:LEU:HD22	2.20	0.42
1:B:307:PHE:CZ	1:B:311:CYS:SG	3.13	0.41
1:D:361:ARG:HH11	1:D:388:ARG:NE	2.18	0.41
1:C:270:PHE:CD1	1:C:270:PHE:C	2.97	0.41
1:D:273:LEU:CD1	1:D:682:VAL:HG11	2.36	0.41
1:B:695:THR:O	1:B:699:VAL:HG23	2.20	0.41
1:C:695:THR:O	1:C:699:VAL:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:373:LYS:HD3	1:B:472:LEU:HD12	2.02	0.41
1:C:463:VAL:O	1:C:467:TRP:HB2	2.21	0.41
1:D:206:LEU:HD21	1:D:697:MET:HA	2.02	0.41
1:A:595:TYR:HB3	1:A:596:PRO:HD3	2.02	0.41
1:C:190:ASP:N	1:C:190:ASP:OD1	2.54	0.41
1:A:473:TYR:N	1:A:474:PRO:HD3	2.35	0.41
1:D:246:GLU:O	1:D:250:ARG:HB2	2.21	0.41
1:D:455:ARG:NH1	1:D:493:PHE:CE1	2.87	0.41
1:A:187:LEU:O	1:A:189:LEU:HD22	2.20	0.41
1:A:496:LYS:HA	1:A:508:TYR:CD1	2.56	0.41
1:A:645:LEU:O	1:A:646:ASP:HB2	2.21	0.41
1:B:265:SER:HB2	1:B:349:ARG:HD2	2.03	0.40
1:A:590:SER:OG	1:A:591:TYR:N	2.50	0.40
1:B:203:LEU:HD11	1:B:206:LEU:CB	2.42	0.40
1:C:497:GLN:HG2	1:C:678:ASN:OD1	2.22	0.40
1:D:259:ASP:OD1	1:D:259:ASP:C	2.64	0.40
1:B:601:PHE:C	1:B:601:PHE:CD1	2.99	0.40
1:D:483:ASN:ND2	1:D:614:HIS:CE1	2.90	0.40
1:A:189:LEU:C	1:A:191:ASN:H	2.30	0.40
1:B:463:VAL:O	1:B:467:TRP:HB2	2.21	0.40
1:D:424:ILE:CD1	1:D:431:LEU:HD13	2.47	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	523/823 (64%)	494 (94%)	24 (5%)	5 (1%)	12 45
1	B	522/823 (63%)	499 (96%)	21 (4%)	2 (0%)	30 65
1	C	523/823 (64%)	496 (95%)	23 (4%)	4 (1%)	16 50
1	D	522/823 (63%)	492 (94%)	25 (5%)	5 (1%)	12 45

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2090/3292 (64%)	1981 (95%)	93 (4%)	16 (1%)	16 50

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	454	ASP
1	A	590	SER
1	C	703	ASN
1	D	239	PHE
1	D	454	ASP
1	C	191	ASN
1	A	191	ASN
1	A	700	ASN
1	B	191	ASN
1	D	191	ASN
1	A	201	MET
1	B	614	HIS
1	C	590	SER
1	D	443	ASN
1	C	246	GLU
1	D	243	GLY

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	472/708 (67%)	457 (97%)	15 (3%)	34 67
1	B	471/708 (66%)	459 (98%)	12 (2%)	42 72
1	C	471/708 (66%)	464 (98%)	7 (2%)	57 80
1	D	471/708 (66%)	461 (98%)	10 (2%)	47 75
All	All	1885/2832 (67%)	1841 (98%)	44 (2%)	44 74

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	189	LEU
1	A	201	MET
1	A	293	THR
1	A	351	VAL
1	A	377	ASP
1	A	384	MET
1	A	391	GLU
1	A	392	SER
1	A	445	ARG
1	A	575	GLU
1	A	577	THR
1	A	590	SER
1	A	647	VAL
1	A	687	LEU
1	A	804	GLU
1	B	183	ARG
1	B	189	LEU
1	B	244	ASP
1	B	293	THR
1	B	300	ASP
1	B	351	VAL
1	B	378	ILE
1	B	413	ASP
1	B	647	VAL
1	B	651	LYS
1	B	684	THR
1	B	702	LEU
1	C	189	LEU
1	C	240	SER
1	C	293	THR
1	C	647	VAL
1	C	687	LEU
1	C	804	GLU
1	C	809	ARG
1	D	189	LEU
1	D	221	THR
1	D	351	VAL
1	D	352	LYS
1	D	516	ASP
1	D	579	GLU
1	D	647	VAL
1	D	662	MET
1	D	687	LEU

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Mol	Chain	Res	Type
1	D	794	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	247	GLN
1	A	443	ASN
1	A	483	ASN
1	A	574	ASN
1	A	663	ASN
1	B	208	GLN
1	B	247	GLN
1	B	574	ASN
1	B	604	HIS
1	B	663	ASN
1	C	208	GLN
1	C	238	GLN
1	C	247	GLN
1	C	488	HIS
1	C	614	HIS
1	C	668	ASN
1	D	191	ASN
1	D	425	HIS
1	D	483	ASN
1	D	488	HIS
1	D	540	ASN
1	D	580	HIS
1	D	700	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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 16 ligands modelled in this entry, 16 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [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	529/823 (64%)	-1.79	0 100 100	32, 59, 96, 154	0
1	B	528/823 (64%)	-1.79	0 100 100	33, 61, 100, 149	0
1	C	529/823 (64%)	-1.80	0 100 100	34, 58, 99, 144	0
1	D	528/823 (64%)	-1.78	0 100 100	35, 61, 95, 134	0
All	All	2114/3292 (64%)	-1.79	0 100 100	32, 60, 98, 154	0

There are no RSRZ outliers to report.

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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	CA	A	901	1/1	1.00	0.01	109,109,109,109	0
2	CA	A	902	1/1	1.00	0.01	65,65,65,65	0
2	CA	A	903	1/1	1.00	0.01	59,59,59,59	0
2	CA	A	904	1/1	1.00	0.01	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CA	B	901	1/1	1.00	0.01	85,85,85,85	0
2	CA	B	902	1/1	1.00	0.01	66,66,66,66	0
2	CA	B	903	1/1	1.00	0.01	67,67,67,67	0
2	CA	B	904	1/1	1.00	0.03	80,80,80,80	0
2	CA	C	901	1/1	1.00	0.01	102,102,102,102	0
2	CA	C	902	1/1	1.00	0.01	70,70,70,70	0
2	CA	C	903	1/1	1.00	0.00	65,65,65,65	0
2	CA	C	904	1/1	1.00	0.01	70,70,70,70	0
2	CA	D	901	1/1	1.00	0.01	91,91,91,91	0
2	CA	D	902	1/1	1.00	0.02	69,69,69,69	0
2	CA	D	903	1/1	1.00	0.01	69,69,69,69	0
2	CA	D	904	1/1	1.00	0.01	76,76,76,76	0

6.5 Other polymers [i](#)

There are no such residues in this entry.