



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:50 PM UTC

PDB ID : 5CTQ / pdb_00005ctq
Title : Crystal structure of human SART3/TIP110 half-a TPR (HAT) domain
Authors : Park, J.K.; Kim, E.E.
Deposited on : 2015-07-24
Resolution : 2.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

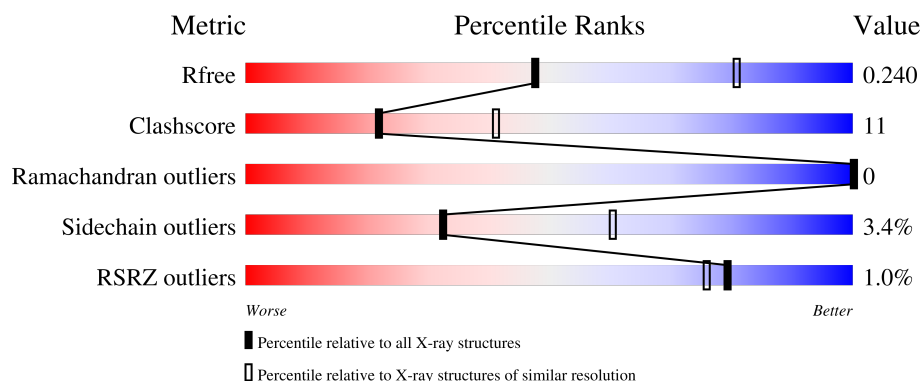
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	561	69% 20% 8%
1	B	561	64% 21% 13%
1	C	561	66% 20% 12%
1	D	561	63% 24% 11%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 16916 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 Squamous cell carcinoma antigen recognized by T-cells 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	518	Total	C	N	O	S	0	0	0
			4298	2717	753	806	22			
1	B	490	Total	C	N	O	S	0	0	0
			4071	2581	708	760	22			
1	C	495	Total	C	N	O	S	0	0	0
			4108	2603	714	769	22			
1	D	502	Total	C	N	O	S	0	0	0
			4158	2633	723	780	22			

There are 172 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	51	MET	-	initiating methionine	UNP Q15020
A	52	GLY	-	expression tag	UNP Q15020
A	53	SER	-	expression tag	UNP Q15020
A	54	SER	-	expression tag	UNP Q15020
A	55	HIS	-	expression tag	UNP Q15020
A	56	HIS	-	expression tag	UNP Q15020
A	57	HIS	-	expression tag	UNP Q15020
A	58	HIS	-	expression tag	UNP Q15020
A	59	HIS	-	expression tag	UNP Q15020
A	60	HIS	-	expression tag	UNP Q15020
A	61	SER	-	expression tag	UNP Q15020
A	62	SER	-	expression tag	UNP Q15020
A	63	GLY	-	expression tag	UNP Q15020
A	64	LEU	-	expression tag	UNP Q15020
A	65	VAL	-	expression tag	UNP Q15020
A	66	PRO	-	expression tag	UNP Q15020
A	67	ARG	-	expression tag	UNP Q15020
A	68	GLY	-	expression tag	UNP Q15020
A	69	SER	-	expression tag	UNP Q15020
A	70	HIS	-	expression tag	UNP Q15020
A	71	MET	-	expression tag	UNP Q15020

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Chain	Residue	Modelled	Actual	Comment	Reference
A	72	ALA	-	expression tag	UNP Q15020
A	73	SER	-	expression tag	UNP Q15020
A	74	MET	-	expression tag	UNP Q15020
A	75	THR	-	expression tag	UNP Q15020
A	76	GLY	-	expression tag	UNP Q15020
A	77	GLY	-	expression tag	UNP Q15020
A	78	GLN	-	expression tag	UNP Q15020
A	79	GLN	-	expression tag	UNP Q15020
A	80	MET	-	expression tag	UNP Q15020
A	81	GLY	-	expression tag	UNP Q15020
A	82	ARG	-	expression tag	UNP Q15020
A	83	GLY	-	expression tag	UNP Q15020
A	84	SER	-	expression tag	UNP Q15020
A	85	GLU	-	expression tag	UNP Q15020
A	86	PHE	-	expression tag	UNP Q15020
A	87	GLU	-	expression tag	UNP Q15020
A	88	ASN	-	expression tag	UNP Q15020
A	89	LEU	-	expression tag	UNP Q15020
A	90	TYR	-	expression tag	UNP Q15020
A	91	PHE	-	expression tag	UNP Q15020
A	92	GLN	-	expression tag	UNP Q15020
A	93	GLY	-	expression tag	UNP Q15020
B	51	MET	-	initiating methionine	UNP Q15020
B	52	GLY	-	expression tag	UNP Q15020
B	53	SER	-	expression tag	UNP Q15020
B	54	SER	-	expression tag	UNP Q15020
B	55	HIS	-	expression tag	UNP Q15020
B	56	HIS	-	expression tag	UNP Q15020
B	57	HIS	-	expression tag	UNP Q15020
B	58	HIS	-	expression tag	UNP Q15020
B	59	HIS	-	expression tag	UNP Q15020
B	60	HIS	-	expression tag	UNP Q15020
B	61	SER	-	expression tag	UNP Q15020
B	62	SER	-	expression tag	UNP Q15020
B	63	GLY	-	expression tag	UNP Q15020
B	64	LEU	-	expression tag	UNP Q15020
B	65	VAL	-	expression tag	UNP Q15020
B	66	PRO	-	expression tag	UNP Q15020
B	67	ARG	-	expression tag	UNP Q15020
B	68	GLY	-	expression tag	UNP Q15020
B	69	SER	-	expression tag	UNP Q15020
B	70	HIS	-	expression tag	UNP Q15020

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Chain	Residue	Modelled	Actual	Comment	Reference
B	71	MET	-	expression tag	UNP Q15020
B	72	ALA	-	expression tag	UNP Q15020
B	73	SER	-	expression tag	UNP Q15020
B	74	MET	-	expression tag	UNP Q15020
B	75	THR	-	expression tag	UNP Q15020
B	76	GLY	-	expression tag	UNP Q15020
B	77	GLY	-	expression tag	UNP Q15020
B	78	GLN	-	expression tag	UNP Q15020
B	79	GLN	-	expression tag	UNP Q15020
B	80	MET	-	expression tag	UNP Q15020
B	81	GLY	-	expression tag	UNP Q15020
B	82	ARG	-	expression tag	UNP Q15020
B	83	GLY	-	expression tag	UNP Q15020
B	84	SER	-	expression tag	UNP Q15020
B	85	GLU	-	expression tag	UNP Q15020
B	86	PHE	-	expression tag	UNP Q15020
B	87	GLU	-	expression tag	UNP Q15020
B	88	ASN	-	expression tag	UNP Q15020
B	89	LEU	-	expression tag	UNP Q15020
B	90	TYR	-	expression tag	UNP Q15020
B	91	PHE	-	expression tag	UNP Q15020
B	92	GLN	-	expression tag	UNP Q15020
B	93	GLY	-	expression tag	UNP Q15020
C	51	MET	-	initiating methionine	UNP Q15020
C	52	GLY	-	expression tag	UNP Q15020
C	53	SER	-	expression tag	UNP Q15020
C	54	SER	-	expression tag	UNP Q15020
C	55	HIS	-	expression tag	UNP Q15020
C	56	HIS	-	expression tag	UNP Q15020
C	57	HIS	-	expression tag	UNP Q15020
C	58	HIS	-	expression tag	UNP Q15020
C	59	HIS	-	expression tag	UNP Q15020
C	60	HIS	-	expression tag	UNP Q15020
C	61	SER	-	expression tag	UNP Q15020
C	62	SER	-	expression tag	UNP Q15020
C	63	GLY	-	expression tag	UNP Q15020
C	64	LEU	-	expression tag	UNP Q15020
C	65	VAL	-	expression tag	UNP Q15020
C	66	PRO	-	expression tag	UNP Q15020
C	67	ARG	-	expression tag	UNP Q15020
C	68	GLY	-	expression tag	UNP Q15020
C	69	SER	-	expression tag	UNP Q15020

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Chain	Residue	Modelled	Actual	Comment	Reference
C	70	HIS	-	expression tag	UNP Q15020
C	71	MET	-	expression tag	UNP Q15020
C	72	ALA	-	expression tag	UNP Q15020
C	73	SER	-	expression tag	UNP Q15020
C	74	MET	-	expression tag	UNP Q15020
C	75	THR	-	expression tag	UNP Q15020
C	76	GLY	-	expression tag	UNP Q15020
C	77	GLY	-	expression tag	UNP Q15020
C	78	GLN	-	expression tag	UNP Q15020
C	79	GLN	-	expression tag	UNP Q15020
C	80	MET	-	expression tag	UNP Q15020
C	81	GLY	-	expression tag	UNP Q15020
C	82	ARG	-	expression tag	UNP Q15020
C	83	GLY	-	expression tag	UNP Q15020
C	84	SER	-	expression tag	UNP Q15020
C	85	GLU	-	expression tag	UNP Q15020
C	86	PHE	-	expression tag	UNP Q15020
C	87	GLU	-	expression tag	UNP Q15020
C	88	ASN	-	expression tag	UNP Q15020
C	89	LEU	-	expression tag	UNP Q15020
C	90	TYR	-	expression tag	UNP Q15020
C	91	PHE	-	expression tag	UNP Q15020
C	92	GLN	-	expression tag	UNP Q15020
C	93	GLY	-	expression tag	UNP Q15020
D	51	MET	-	initiating methionine	UNP Q15020
D	52	GLY	-	expression tag	UNP Q15020
D	53	SER	-	expression tag	UNP Q15020
D	54	SER	-	expression tag	UNP Q15020
D	55	HIS	-	expression tag	UNP Q15020
D	56	HIS	-	expression tag	UNP Q15020
D	57	HIS	-	expression tag	UNP Q15020
D	58	HIS	-	expression tag	UNP Q15020
D	59	HIS	-	expression tag	UNP Q15020
D	60	HIS	-	expression tag	UNP Q15020
D	61	SER	-	expression tag	UNP Q15020
D	62	SER	-	expression tag	UNP Q15020
D	63	GLY	-	expression tag	UNP Q15020
D	64	LEU	-	expression tag	UNP Q15020
D	65	VAL	-	expression tag	UNP Q15020
D	66	PRO	-	expression tag	UNP Q15020
D	67	ARG	-	expression tag	UNP Q15020
D	68	GLY	-	expression tag	UNP Q15020

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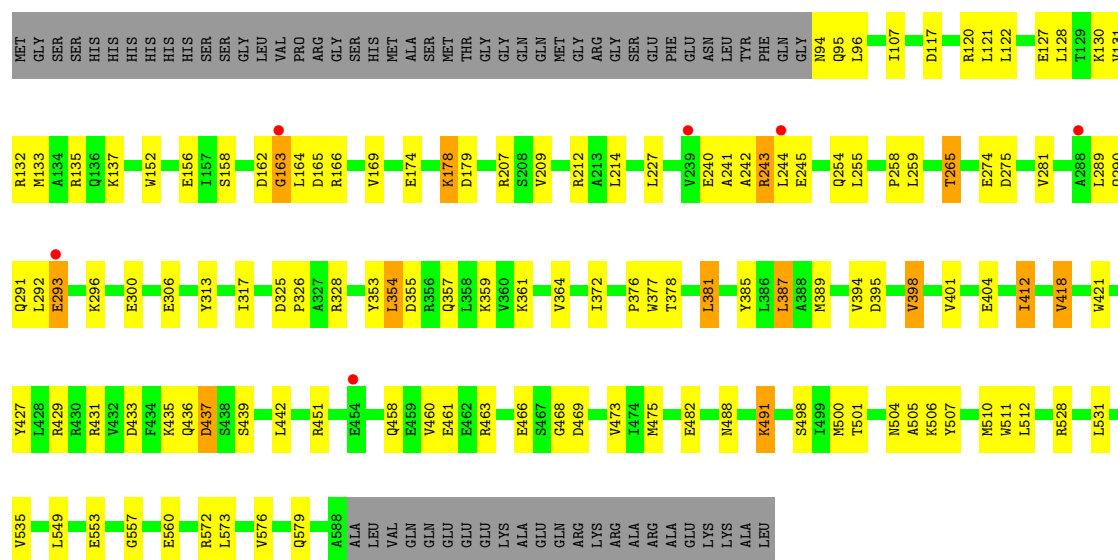
Chain	Residue	Modelled	Actual	Comment	Reference
D	69	SER	-	expression tag	UNP Q15020
D	70	HIS	-	expression tag	UNP Q15020
D	71	MET	-	expression tag	UNP Q15020
D	72	ALA	-	expression tag	UNP Q15020
D	73	SER	-	expression tag	UNP Q15020
D	74	MET	-	expression tag	UNP Q15020
D	75	THR	-	expression tag	UNP Q15020
D	76	GLY	-	expression tag	UNP Q15020
D	77	GLY	-	expression tag	UNP Q15020
D	78	GLN	-	expression tag	UNP Q15020
D	79	GLN	-	expression tag	UNP Q15020
D	80	MET	-	expression tag	UNP Q15020
D	81	GLY	-	expression tag	UNP Q15020
D	82	ARG	-	expression tag	UNP Q15020
D	83	GLY	-	expression tag	UNP Q15020
D	84	SER	-	expression tag	UNP Q15020
D	85	GLU	-	expression tag	UNP Q15020
D	86	PHE	-	expression tag	UNP Q15020
D	87	GLU	-	expression tag	UNP Q15020
D	88	ASN	-	expression tag	UNP Q15020
D	89	LEU	-	expression tag	UNP Q15020
D	90	TYR	-	expression tag	UNP Q15020
D	91	PHE	-	expression tag	UNP Q15020
D	92	GLN	-	expression tag	UNP Q15020
D	93	GLY	-	expression tag	UNP Q15020

- Molecule 2 is water.

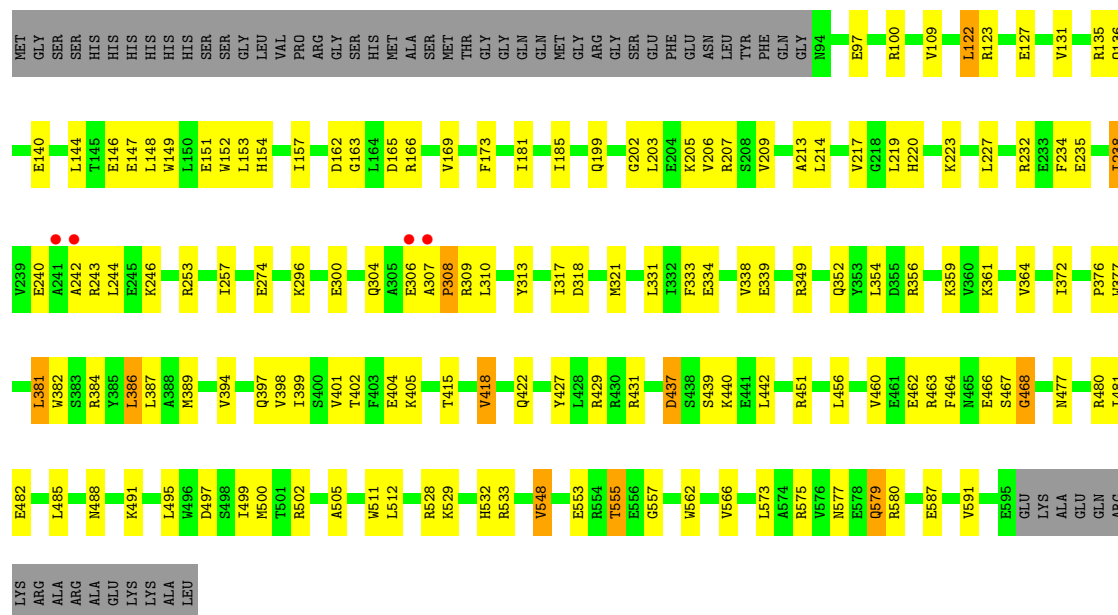
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	69	Total O 69 69	0	0
2	B	57	Total O 57 57	0	0
2	C	86	Total O 86 86	0	0
2	D	69	Total O 69 69	0	0



• Molecule 1: Squamous cell carcinoma antigen recognized by T-cells 3



• Molecule 1: Squamous cell carcinoma antigen recognized by T-cells 3



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	120.91Å 80.53Å 146.64Å 90.00° 99.36° 90.00°	Depositor
Resolution (Å)	38.15 – 2.60 38.15 – 2.60	Depositor EDS
% Data completeness (in resolution range)	95.8 (38.15-2.60) 95.6 (38.15-2.60)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 2.58Å)	Xtriage
Refinement program	PHENIX 1.7.3 _928	Depositor
R, R_{free}	0.235 , 0.281 0.238 , 0.240	Depositor DCC
R_{free} test set	4155 reflections (4.76%)	wwPDB-VP
Wilson B-factor (Å ²)	44.0	Xtriage
Anisotropy	0.222	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 17.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	16916	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.84% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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	0.54	0/4385	1.00	24/5921 (0.4%)
1	B	0.49	0/4158	1.00	14/5623 (0.2%)
1	C	0.57	1/4195 (0.0%)	1.08	21/5672 (0.4%)
1	D	0.49	0/4245	0.95	12/5740 (0.2%)
All	All	0.53	1/16983 (0.0%)	1.01	71/22956 (0.3%)

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	1
1	B	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	293	GLU	CA-C	5.05	1.59	1.52

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	163	GLY	N-CA-C	-15.25	95.95	113.79
1	C	243	ARG	N-CA-C	11.98	127.67	113.18
1	C	95	GLN	N-CA-C	10.15	123.59	111.82
1	C	241	ALA	N-CA-C	-9.86	101.01	113.43
1	D	238	ILE	N-CA-C	-9.72	94.45	108.36
1	A	241	ALA	N-CA-C	8.71	124.84	114.04
1	B	238	ILE	N-CA-C	8.34	124.11	112.35
1	A	437	ASP	N-CA-C	-8.04	96.12	109.46
1	A	307	ALA	CA-C-N	7.68	145.43	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	307	ALA	C-N-CA	7.68	145.43	127.00
1	A	307	ALA	C-N-CD	-7.67	103.71	120.60
1	C	240	GLU	N-CA-C	7.61	121.90	107.75
1	B	160	ALA	N-CA-C	-7.53	98.52	109.59
1	B	243	ARG	N-CA-C	-7.39	104.25	113.20
1	C	354	LEU	N-CA-C	7.34	118.92	111.07
1	A	243	ARG	N-CA-C	-7.16	104.54	113.20
1	D	238	ILE	N-CA-CB	7.08	119.48	110.99
1	B	242	ALA	N-CA-C	6.97	122.89	113.97
1	C	244	LEU	N-CA-C	6.86	118.75	111.28
1	A	459	GLU	N-CA-C	6.76	118.30	111.07
1	A	107	ILE	N-CA-C	-6.65	104.37	110.82
1	B	163	GLY	N-CA-C	6.53	122.12	113.37
1	A	200	LYS	N-CA-C	6.44	119.12	111.33
1	C	460	VAL	N-CA-C	6.23	117.01	110.72
1	A	504	ASN	N-CA-C	-6.20	104.99	113.30
1	B	179	ASP	N-CA-C	6.15	117.68	110.97
1	A	242	ALA	N-CA-C	6.13	121.82	113.97
1	C	361	LYS	N-CA-C	6.00	118.35	111.02
1	A	533	ARG	CB-CG-CD	-6.00	97.50	111.30
1	C	281	VAL	N-CA-C	5.96	116.74	110.72
1	C	412	ILE	CG1-CB-CG2	-5.94	92.88	110.70
1	D	310	LEU	N-CA-C	5.94	117.43	111.07
1	A	262	MET	N-CA-C	-5.77	105.50	112.54
1	C	274	GLU	N-CA-C	-5.76	104.60	111.69
1	C	463	ARG	N-CA-C	5.76	117.64	111.36
1	C	293	GLU	N-CA-C	-5.73	105.17	111.82
1	D	242	ALA	N-CA-C	-5.72	106.65	113.97
1	D	361	LYS	N-CA-C	5.70	117.97	111.02
1	B	241	ALA	N-CA-C	5.69	121.09	114.04
1	A	466	GLU	N-CA-C	-5.66	100.46	109.23
1	A	239	VAL	N-CA-C	5.52	117.86	108.86
1	B	164	LEU	CA-C-N	5.50	132.06	121.18
1	B	164	LEU	C-N-CA	5.50	132.06	121.18
1	A	440	LYS	N-CA-C	-5.48	105.31	111.28
1	D	440	LYS	N-CA-C	-5.45	105.42	111.36
1	D	468	GLY	N-CA-C	-5.45	108.13	115.21
1	B	349	ARG	CG-CD-NE	5.39	123.85	112.00
1	D	437	ASP	CA-C-N	-5.36	115.21	122.77
1	D	437	ASP	C-N-CA	-5.36	115.21	122.77
1	C	163	GLY	CA-C-O	5.35	124.22	119.56
1	C	178	LYS	N-CA-C	5.32	117.16	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	178	LYS	N-CA-C	5.31	117.15	111.36
1	A	307	ALA	N-CA-C	-5.31	96.14	111.00
1	A	437	ASP	CA-C-N	5.28	131.21	121.70
1	A	437	ASP	C-N-CA	5.28	131.21	121.70
1	D	555	THR	N-CA-C	5.21	119.69	113.23
1	A	240	GLU	N-CA-C	5.21	119.61	112.68
1	B	244	LEU	N-CA-C	-5.19	105.11	111.75
1	A	500	MET	N-CA-C	5.18	117.83	111.82
1	A	436	GLN	N-CA-C	5.17	117.02	108.13
1	C	436	GLN	N-CA-C	-5.13	100.53	108.90
1	A	578	GLU	CA-CB-CG	5.13	124.35	114.10
1	D	274	GLU	N-CA-C	-5.13	105.38	111.69
1	B	468	GLY	N-CA-C	-5.12	108.55	115.21
1	C	292	LEU	N-CA-C	5.10	116.92	111.36
1	C	275	ASP	N-CA-C	5.07	117.07	110.08
1	C	179	ASP	N-CA-C	5.05	116.48	110.97
1	C	128	LEU	N-CA-C	5.05	116.87	111.36
1	B	463	ARG	N-CA-C	5.04	116.86	111.36
1	D	308	PRO	N-CA-C	-5.03	106.54	113.53
1	A	128	LEU	N-CA-C	5.00	116.82	111.36

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	306	GLU	Peptide
1	B	438	SER	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	4298	0	4220	86	0
1	B	4071	0	3984	84	0
1	C	4108	0	4019	81	0
1	D	4158	0	4061	111	0
2	A	69	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	57	0	0	2	0
2	C	86	0	0	1	0
2	D	69	0	0	5	0
All	All	16916	0	16284	352	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 11.

All (352) 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:D:306:GLU:HG2	1:D:308:PRO:HD2	1.09	1.08
1:A:502:ARG:HB2	1:A:502:ARG:CZ	1.93	0.98
1:B:239:VAL:HG11	1:B:243:ARG:H	1.29	0.98
1:A:502:ARG:NH1	1:A:502:ARG:CB	2.30	0.94
1:D:306:GLU:HG2	1:D:308:PRO:CD	1.97	0.93
1:A:605:ARG:NH1	2:A:702:HOH:O	2.00	0.93
1:A:502:ARG:NH1	1:A:502:ARG:HB3	1.84	0.91
1:D:306:GLU:CG	1:D:308:PRO:HD2	1.99	0.91
1:B:122:LEU:HB3	1:B:131:VAL:HG22	1.53	0.90
1:B:519:ARG:NH2	1:B:556:GLU:OE1	2.04	0.89
1:D:306:GLU:O	1:D:309:ARG:HB3	1.74	0.88
1:B:358:LEU:HD12	1:C:107:ILE:HD11	1.58	0.85
1:A:419:GLU:OE1	2:A:701:HOH:O	1.95	0.83
1:D:97:GLU:OE2	1:D:100:ARG:NH2	2.12	0.82
1:B:438:SER:HB2	1:B:439:SER:HA	1.60	0.81
1:D:404:GLU:OE2	1:D:451:ARG:NH2	2.14	0.81
1:A:404:GLU:OE2	1:A:451:ARG:NH2	2.14	0.80
1:A:502:ARG:HB3	1:A:502:ARG:HH11	1.47	0.79
1:B:498:SER:HB3	1:B:502:ARG:HH12	1.49	0.78
1:A:502:ARG:CZ	1:A:502:ARG:CB	2.59	0.77
1:D:402:THR:HA	1:D:405:LYS:HE2	1.67	0.76
1:D:235:GLU:HA	1:D:243:ARG:NH1	2.00	0.76
1:B:215:SER:HA	1:C:96:LEU:HD13	1.66	0.75
1:B:354:LEU:HB3	1:B:364:VAL:HG12	1.71	0.72
1:C:404:GLU:OE2	1:C:451:ARG:NH2	2.23	0.72
1:A:451:ARG:NH1	2:A:703:HOH:O	2.23	0.72
1:B:404:GLU:OE2	1:B:451:ARG:NH2	2.23	0.72
1:A:122:LEU:HB3	1:A:131:VAL:HG22	1.73	0.71
1:B:437:ASP:OD1	1:B:437:ASP:N	2.19	0.71
1:A:379:VAL:HG21	1:A:416:ASP:HB3	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:456:LEU:HA	1:D:460:VAL:HG12	1.73	0.71
1:D:122:LEU:HB3	1:D:131:VAL:HG22	1.73	0.70
1:D:203:LEU:HD11	1:D:243:ARG:NH2	2.06	0.70
1:D:307:ALA:O	1:D:339:GLU:OE2	2.09	0.70
1:C:207:ARG:HH22	1:C:243:ARG:NE	1.89	0.70
1:A:397:GLN:OE1	1:A:397:GLN:N	2.25	0.69
1:B:500:MET:HE1	1:B:510:MET:HB3	1.75	0.69
1:D:422:GLN:OE1	1:D:477:ASN:ND2	2.24	0.69
1:A:533:ARG:NH1	1:A:536:GLN:OE1	2.24	0.69
1:D:500:MET:HE3	1:D:505:ALA:HA	1.76	0.68
1:C:258:PRO:HG3	1:C:291:GLN:HB3	1.76	0.67
1:D:384:ARG:NH1	2:D:703:HOH:O	2.27	0.67
1:A:502:ARG:CB	1:A:502:ARG:HH11	2.04	0.67
1:C:500:MET:HE3	1:C:505:ALA:HA	1.76	0.67
1:D:439:SER:HB3	1:D:442:LEU:HB2	1.77	0.66
1:A:502:ARG:HB2	1:A:502:ARG:NH1	2.06	0.65
1:A:502:ARG:CG	1:A:502:ARG:O	2.44	0.65
1:D:497:ASP:OD1	2:D:701:HOH:O	2.13	0.65
1:B:163:GLY:N	1:B:164:LEU:HA	2.10	0.65
1:A:456:LEU:HD13	1:A:460:VAL:HG11	1.79	0.65
1:C:500:MET:HE2	1:C:511:TRP:CE2	2.31	0.65
1:D:235:GLU:OE1	1:D:243:ARG:NE	2.30	0.65
1:D:307:ALA:HA	1:D:309:ARG:CZ	2.28	0.64
1:D:500:MET:CE	1:D:505:ALA:HA	2.27	0.64
1:B:572:ARG:HH11	1:B:575:ARG:HH21	1.44	0.64
1:C:127:GLU:O	1:C:131:VAL:HG23	1.97	0.64
1:D:296:LYS:O	1:D:300:GLU:HG2	1.99	0.63
1:A:174:GLU:OE2	1:A:212:ARG:NH2	2.31	0.63
1:B:334:GLU:OE2	1:B:370:ARG:NH2	2.31	0.63
1:D:235:GLU:O	1:D:243:ARG:HD3	1.98	0.62
1:D:427:TYR:CZ	1:D:431:ARG:HD2	2.35	0.62
1:C:354:LEU:HB3	1:C:364:VAL:HG22	1.82	0.62
1:A:239:VAL:HG11	1:A:243:ARG:HB2	1.82	0.61
1:D:467:SER:CB	1:D:502:ARG:HH22	2.14	0.61
1:A:482:GLU:HG2	1:A:491:LYS:HB3	1.82	0.61
1:C:576:VAL:O	1:C:579:GLN:HG2	2.00	0.61
1:D:382:TRP:O	1:D:386:LEU:HD13	2.00	0.61
1:C:132:ARG:NH2	1:C:156:GLU:OE1	2.34	0.61
1:A:306:GLU:HG2	1:A:309:ARG:HH21	1.66	0.61
1:C:439:SER:HB2	1:C:442:LEU:HB2	1.82	0.60
1:D:154:HIS:O	1:D:157:ILE:HG13	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:239:VAL:HG11	1:B:243:ARG:N	2.10	0.60
1:C:122:LEU:HD21	1:C:130:LYS:HE3	1.83	0.60
1:B:528:ARG:NH1	1:B:553:GLU:OE1	2.35	0.60
1:D:502:ARG:O	1:D:502:ARG:HG2	2.01	0.60
1:C:163:GLY:O	1:C:166:ARG:HB3	2.02	0.59
1:D:199:GLN:N	1:D:199:GLN:OE1	2.35	0.59
1:D:356:ARG:O	1:D:359:LYS:NZ	2.35	0.59
1:B:482:GLU:HG2	1:B:491:LYS:HB3	1.85	0.58
1:C:122:LEU:HB3	1:C:131:VAL:HG22	1.85	0.58
1:A:536:GLN:OE1	1:C:458:GLN:NE2	2.37	0.58
1:D:127:GLU:O	1:D:131:VAL:HG23	2.03	0.58
1:D:577:ASN:O	1:D:580:ARG:HG3	2.03	0.58
1:B:207:ARG:HH22	1:B:243:ARG:NH1	2.01	0.58
1:D:165:ASP:O	1:D:169:VAL:HG23	2.04	0.57
1:D:235:GLU:HA	1:D:243:ARG:HH11	1.69	0.57
1:B:439:SER:O	1:B:443:GLU:HG2	2.04	0.57
1:B:221:MET:HE2	1:B:328:ARG:NH2	2.20	0.57
1:C:500:MET:CE	1:C:505:ALA:HA	2.35	0.57
1:B:127:GLU:O	1:B:131:VAL:HG23	2.04	0.57
1:A:238:ILE:HD12	1:A:239:VAL:HB	1.87	0.56
1:C:398:VAL:HA	1:C:401:VAL:HG12	1.88	0.56
1:D:123:ARG:NH1	1:D:135:ARG:HH22	2.02	0.56
1:D:439:SER:HB3	1:D:442:LEU:CB	2.34	0.56
1:D:162:ASP:HB3	1:D:165:ASP:OD1	2.05	0.56
1:D:207:ARG:HH21	1:D:243:ARG:HE	1.52	0.56
1:C:254:GLN:NE2	1:C:265:THR:HG21	2.21	0.56
1:D:238:ILE:HG22	1:D:243:ARG:NH1	2.21	0.55
1:A:127:GLU:O	1:A:131:VAL:HG23	2.06	0.55
1:B:334:GLU:CD	1:B:370:ARG:HH22	2.13	0.55
1:C:535:VAL:O	1:C:572:ARG:NH1	2.40	0.55
1:A:162:ASP:OD1	1:A:163:GLY:N	2.38	0.55
1:D:500:MET:HE2	1:D:511:TRP:CE2	2.42	0.55
1:A:502:ARG:O	1:A:502:ARG:HG2	2.06	0.55
1:A:418:VAL:HG12	1:A:456:LEU:HD11	1.89	0.55
1:D:352:GLN:HG3	1:D:356:ARG:NH1	2.22	0.55
1:C:133:MET:HE3	1:C:137:LYS:HE3	1.89	0.55
1:B:572:ARG:HH11	1:B:575:ARG:NH2	2.04	0.54
1:C:433:ASP:OD1	1:C:435:LYS:HB2	2.07	0.54
1:A:398:VAL:HA	1:A:401:VAL:HG12	1.87	0.54
1:B:577:ASN:ND2	2:B:701:HOH:O	2.23	0.54
1:C:528:ARG:NH1	1:C:553:GLU:OE1	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:306:GLU:O	1:D:309:ARG:CB	2.53	0.54
1:A:147:GLU:HG2	1:A:148:LEU:HD12	1.89	0.53
1:C:469:ASP:OD1	1:C:473:VAL:HG22	2.07	0.53
1:B:174:GLU:OE2	1:B:212:ARG:NH2	2.42	0.53
1:D:202:GLY:O	1:D:206:VAL:HG23	2.09	0.53
1:A:456:LEU:HA	1:A:460:VAL:HG12	1.90	0.52
1:B:270:GLU:OE1	1:B:277:ILE:HG13	2.09	0.52
1:C:506:LYS:HE3	1:C:507:TYR:CZ	2.45	0.52
1:B:510:MET:HA	1:B:510:MET:HE2	1.91	0.52
1:A:354:LEU:HB3	1:A:364:VAL:HG12	1.91	0.52
1:B:506:LYS:HE3	1:B:507:TYR:CZ	2.45	0.52
1:D:482:GLU:HG2	1:D:491:LYS:HB3	1.91	0.51
1:C:376:PRO:HD2	1:C:377:TRP:CE3	2.45	0.51
1:A:525:GLN:HE22	1:A:528:ARG:HH12	1.57	0.51
1:C:174:GLU:OE2	1:C:212:ARG:NH2	2.43	0.51
1:D:147:GLU:O	1:D:151:GLU:HG2	2.11	0.51
1:A:155:ASP:O	1:A:159:MET:HE2	2.10	0.51
1:A:325:ASP:OD2	1:A:328:ARG:HG3	2.11	0.51
1:B:531:LEU:HD13	1:B:549:LEU:HA	1.93	0.51
1:A:528:ARG:HD3	1:A:553:GLU:OE2	2.10	0.51
1:B:293:GLU:OE1	1:B:296:LYS:NZ	2.28	0.51
1:D:481:ILE:HG23	1:D:485:LEU:HD12	1.92	0.51
1:C:482:GLU:HG2	1:C:491:LYS:HB3	1.92	0.50
1:D:144:LEU:HB2	1:D:149:TRP:NE1	2.26	0.50
1:D:495:LEU:O	1:D:499:ILE:HG13	2.11	0.50
1:C:385:TYR:CZ	1:C:389:MET:HE3	2.47	0.50
1:B:491:LYS:NZ	2:B:705:HOH:O	2.45	0.50
1:D:240:GLU:O	1:D:244:LEU:HB2	2.11	0.50
1:A:165:ASP:O	1:A:169:VAL:HG23	2.12	0.50
1:B:389:MET:HE3	1:B:394:VAL:HG11	1.94	0.50
1:B:482:GLU:HG3	1:B:488:ASN:HB3	1.94	0.50
1:C:313:TYR:O	1:C:317:ILE:HG13	2.12	0.50
1:D:181:ILE:HG22	1:D:338:VAL:HG21	1.94	0.50
1:A:437:ASP:OD1	1:A:438:SER:HA	2.12	0.50
1:D:467:SER:HB3	1:D:502:ARG:HH22	1.76	0.49
1:A:495:LEU:O	1:A:499:ILE:HG13	2.12	0.49
1:A:376:PRO:HD2	1:A:377:TRP:CE3	2.47	0.49
1:C:394:VAL:HG12	1:C:398:VAL:HG13	1.95	0.49
1:A:482:GLU:HG3	1:A:488:ASN:HB3	1.95	0.49
1:C:439:SER:HB2	1:C:442:LEU:CB	2.43	0.49
1:D:467:SER:HB2	1:D:502:ARG:HH22	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:587:GLU:O	1:A:591:VAL:HG23	2.12	0.49
1:B:214:LEU:O	1:C:96:LEU:HD22	2.13	0.49
1:B:498:SER:HB3	1:B:502:ARG:NH1	2.21	0.49
1:B:559:LEU:O	1:B:559:LEU:HD12	2.12	0.49
1:A:127:GLU:HG3	1:A:130:LYS:HE2	1.95	0.49
1:A:533:ARG:HD2	1:A:533:ARG:HA	1.60	0.48
1:A:469:ASP:OD1	1:A:473:VAL:HG22	2.12	0.48
1:B:161:GLN:O	1:B:165:ASP:OD1	2.31	0.48
1:B:308:PRO:HB2	1:B:340:ASN:OD1	2.13	0.48
1:A:300:GLU:O	1:A:304:GLN:HG2	2.13	0.48
1:B:376:PRO:HD2	1:B:377:TRP:CE3	2.48	0.48
1:B:490:GLN:NE2	1:B:494:GLU:OE2	2.46	0.48
1:A:305:ALA:O	1:A:306:GLU:HG3	2.13	0.48
1:D:307:ALA:HA	1:D:309:ARG:NH2	2.28	0.48
1:A:94:ASN:HD21	1:A:124:LEU:HD23	1.78	0.48
1:C:162:ASP:C	1:C:164:LEU:H	2.20	0.48
1:D:307:ALA:HB3	1:D:308:PRO:HD3	1.96	0.48
1:D:389:MET:HE3	1:D:394:VAL:HG11	1.95	0.48
1:B:179:ASP:O	1:B:370:ARG:HD2	2.14	0.48
1:B:398:VAL:HA	1:B:401:VAL:HG12	1.96	0.48
1:B:461:GLU:OE1	1:B:466:GLU:N	2.46	0.48
1:C:466:GLU:HG2	1:C:468:GLY:H	1.77	0.48
1:D:136:GLN:O	1:D:140:GLU:HG3	2.13	0.48
1:C:429:ARG:HD2	1:D:555:THR:O	2.14	0.47
1:D:313:TYR:O	1:D:317:ILE:HG13	2.13	0.47
1:D:532:HIS:HE1	2:D:713:HOH:O	1.97	0.47
1:D:562:TRP:O	1:D:566:VAL:HG23	2.14	0.47
1:B:469:ASP:OD1	1:B:473:VAL:HG22	2.13	0.47
1:D:220:HIS:CE1	1:D:223:LYS:HE3	2.49	0.47
1:B:490:GLN:O	1:B:494:GLU:HG3	2.14	0.47
1:B:153:LEU:HD23	1:B:172:LEU:HD23	1.96	0.47
1:B:563:ASP:O	1:B:567:GLN:HG2	2.13	0.47
1:C:306:GLU:HA	1:C:306:GLU:OE1	2.14	0.47
1:A:379:VAL:HG22	1:A:411:PHE:CE2	2.49	0.47
1:B:439:SER:HB3	1:B:442:LEU:HB3	1.96	0.47
1:B:184:ASN:O	1:B:188:GLU:HB2	2.15	0.47
1:B:493:ARG:NH2	1:B:518:GLU:OE2	2.47	0.47
1:B:563:ASP:O	1:B:566:VAL:HG22	2.15	0.47
1:D:512:LEU:HD21	1:D:548:VAL:HG11	1.97	0.47
1:B:279:GLU:O	1:B:282:ILE:HG22	2.15	0.47
1:B:505:ALA:O	1:B:511:TRP:NE1	2.41	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:500:MET:HE2	1:C:511:TRP:CZ2	2.50	0.47
1:D:153:LEU:HD13	1:D:173:PHE:CE2	2.50	0.47
1:A:306:GLU:HG2	1:A:309:ARG:NH2	2.29	0.46
1:C:395:ASP:HB2	1:C:398:VAL:HG12	1.97	0.46
1:D:376:PRO:HD2	1:D:377:TRP:CE3	2.51	0.46
1:C:504:ASN:ND2	1:C:510:MET:HE2	2.31	0.46
1:B:424:TYR:CE2	1:B:428:LEU:HD11	2.51	0.46
1:C:174:GLU:O	1:C:178:LYS:HD2	2.16	0.46
1:C:353:TYR:CE1	1:C:357:GLN:HG3	2.51	0.46
1:C:557:GLY:O	1:D:429:ARG:NH2	2.43	0.46
1:B:427:TYR:CZ	1:B:431:ARG:HD2	2.50	0.46
1:C:560:GLU:H	1:C:560:GLU:CD	2.24	0.46
1:D:356:ARG:NH2	2:D:708:HOH:O	2.48	0.46
1:B:491:LYS:O	1:B:491:LYS:HD3	2.16	0.46
1:B:506:LYS:HB2	1:B:539:SER:OG	2.16	0.46
1:A:352:GLN:HG3	1:A:356:ARG:NH1	2.31	0.45
1:A:582:LYS:O	1:A:585:GLU:HB2	2.16	0.45
1:A:181:ILE:HD11	1:A:335:ARG:HA	1.99	0.45
1:A:507:TYR:HB2	1:A:510:MET:HB2	1.98	0.45
1:D:533:ARG:NH2	2:D:702:HOH:O	2.25	0.45
1:A:422:GLN:HE21	1:B:554:ARG:CZ	2.29	0.45
1:D:397:GLN:O	1:D:401:VAL:HG23	2.16	0.45
1:C:429:ARG:NH2	1:D:557:GLY:O	2.47	0.45
1:D:488:ASN:OD1	1:D:491:LYS:HB2	2.16	0.45
1:D:500:MET:HE2	1:D:511:TRP:CZ2	2.52	0.45
1:D:123:ARG:NH1	1:D:135:ARG:NH2	2.64	0.45
1:D:219:LEU:HB2	1:D:331:LEU:HD22	1.97	0.45
1:D:300:GLU:O	1:D:304:GLN:HG2	2.16	0.45
1:D:415:THR:O	1:D:418:VAL:HG22	2.15	0.45
1:D:203:LEU:HD11	1:D:243:ARG:HH22	1.80	0.45
1:A:308:PRO:C	1:A:309:ARG:HG2	2.41	0.45
1:A:382:TRP:CE3	1:A:406:ALA:HB2	2.52	0.45
1:B:437:ASP:O	1:B:438:SER:C	2.60	0.45
1:C:207:ARG:HH22	1:C:243:ARG:HE	1.63	0.45
1:D:402:THR:HA	1:D:405:LYS:CE	2.42	0.45
1:D:529:LYS:O	1:D:533:ARG:HG3	2.17	0.45
1:A:422:GLN:NE2	1:B:554:ARG:CZ	2.80	0.44
1:C:255:LEU:HD21	1:C:265:THR:CG2	2.46	0.44
1:C:290:GLN:HA	1:C:293:GLU:OE1	2.18	0.44
1:D:243:ARG:O	1:D:246:LYS:HB3	2.17	0.44
1:D:466:GLU:HG2	1:D:468:GLY:H	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:456:LEU:HA	1:D:460:VAL:CG1	2.44	0.44
1:A:121:LEU:HD23	1:A:121:LEU:HA	1.70	0.44
1:A:412:ILE:O	1:A:464:PHE:HE2	2.00	0.44
1:D:333:PHE:HZ	1:D:349:ARG:HG2	1.82	0.44
1:B:131:VAL:HG12	1:B:135:ARG:HD2	1.99	0.44
1:C:325:ASP:OD2	1:C:328:ARG:HG3	2.17	0.44
1:C:531:LEU:HD13	1:C:549:LEU:HA	1.99	0.44
1:D:307:ALA:O	1:D:309:ARG:HG2	2.17	0.44
1:A:334:GLU:O	1:A:338:VAL:HG23	2.17	0.44
1:B:253:ARG:NH1	1:C:94:ASN:HA	2.33	0.44
1:B:260:TYR:CE2	1:B:292:LEU:HD11	2.53	0.44
1:B:436:GLN:O	1:B:439:SER:HB2	2.17	0.44
1:A:553:GLU:HG3	1:A:565:ALA:HB2	1.99	0.44
1:A:378:THR:OG1	1:A:381:LEU:HD22	2.18	0.44
1:B:395:ASP:HB2	1:B:398:VAL:HG12	2.00	0.44
1:C:491:LYS:O	1:C:491:LYS:HD3	2.17	0.44
1:D:334:GLU:O	1:D:338:VAL:HG23	2.18	0.44
1:C:353:TYR:CD1	1:C:357:GLN:HG3	2.53	0.44
1:A:254:GLN:NE2	1:A:265:THR:HG21	2.33	0.43
1:B:333:PHE:HZ	1:B:349:ARG:HG2	1.83	0.43
1:C:117:ASP:HA	1:C:120:ARG:HG2	2.01	0.43
1:D:528:ARG:NH1	1:D:553:GLU:OE1	2.51	0.43
1:D:235:GLU:C	1:D:243:ARG:HD3	2.44	0.43
1:D:306:GLU:HG2	1:D:307:ALA:N	2.33	0.43
1:B:213:ALA:HB1	1:B:227:LEU:CD2	2.49	0.43
1:B:554:ARG:CZ	1:B:554:ARG:HB3	2.48	0.43
1:D:317:ILE:O	1:D:321:MET:HG3	2.19	0.43
1:B:98:ILE:HD13	1:B:122:LEU:HD12	2.01	0.43
1:D:146:GLU:HG3	1:D:185:ILE:HG13	2.00	0.43
1:D:207:ARG:NH2	1:D:243:ARG:HE	2.16	0.43
1:A:395:ASP:HB2	1:A:398:VAL:HG12	2.01	0.43
1:B:543:GLU:OE1	1:B:543:GLU:N	2.45	0.43
1:A:219:LEU:HB2	1:A:331:LEU:HD22	2.01	0.43
1:A:577:ASN:O	1:A:581:MET:HB2	2.18	0.43
1:D:163:GLY:O	1:D:166:ARG:HB3	2.19	0.43
1:D:227:LEU:HA	1:D:227:LEU:HD23	1.80	0.43
1:A:405:LYS:HD2	1:A:405:LYS:HA	1.67	0.42
1:B:135:ARG:HD3	1:B:152:TRP:CG	2.54	0.42
1:B:262:MET:HE3	1:B:289:LEU:HD23	2.00	0.42
1:C:255:LEU:HD23	1:C:255:LEU:HA	1.84	0.42
1:A:379:VAL:HG21	1:A:416:ASP:CB	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:GLU:O	1:B:107:ILE:HG12	2.19	0.42
1:B:500:MET:HE2	1:B:500:MET:HA	2.02	0.42
1:C:135:ARG:HD3	1:C:152:TRP:CG	2.54	0.42
1:A:427:TYR:CZ	1:A:431:ARG:HD2	2.54	0.42
1:A:372:ILE:HD13	1:A:372:ILE:HA	1.81	0.42
1:B:352:GLN:HG3	1:B:356:ARG:NH1	2.34	0.42
1:C:255:LEU:HD21	1:C:265:THR:HG22	2.01	0.42
1:C:296:LYS:O	1:C:300:GLU:HG3	2.20	0.42
1:C:498:SER:O	1:C:501:THR:HB	2.19	0.42
1:D:307:ALA:N	1:D:308:PRO:CD	2.81	0.42
1:D:372:ILE:HD13	1:D:381:LEU:HB3	2.02	0.42
1:D:148:LEU:HD23	1:D:148:LEU:HA	1.88	0.42
1:A:153:LEU:HD13	1:A:173:PHE:CE2	2.54	0.42
1:C:227:LEU:HD23	1:C:227:LEU:HA	1.89	0.42
1:B:174:GLU:CD	1:B:212:ARG:HH22	2.28	0.42
1:C:387:LEU:HD13	1:C:387:LEU:HA	1.92	0.42
1:D:318:ASP:OD1	1:D:349:ARG:NH2	2.52	0.42
1:D:575:ARG:O	1:D:579:GLN:HG3	2.20	0.42
1:A:296:LYS:N	1:A:297:PRO:HD2	2.35	0.42
1:B:170:TYR:CD1	1:B:189:TYR:HE1	2.38	0.42
1:B:342:LEU:O	1:B:344:PRO:HD3	2.20	0.42
1:D:463:ARG:HG3	1:D:464:PHE:CD2	2.55	0.42
1:A:174:GLU:CD	1:A:212:ARG:HH22	2.26	0.41
1:A:488:ASN:ND2	1:A:491:LYS:HB2	2.35	0.41
1:C:355:ASP:O	1:C:359:LYS:HG2	2.20	0.41
1:C:512:LEU:HD23	1:C:512:LEU:HA	1.91	0.41
1:B:270:GLU:OE1	1:B:270:GLU:HA	2.20	0.41
1:C:482:GLU:HG3	1:C:488:ASN:HB3	2.02	0.41
1:A:306:GLU:CG	1:A:309:ARG:HH21	2.33	0.41
1:A:394:VAL:HG12	1:A:398:VAL:HG13	2.01	0.41
1:C:207:ARG:HH22	1:C:243:ARG:CD	2.33	0.41
1:C:372:ILE:HA	1:C:372:ILE:HD13	1.76	0.41
1:D:372:ILE:HD13	1:D:372:ILE:HA	1.82	0.41
1:D:587:GLU:O	1:D:591:VAL:HG23	2.20	0.41
1:C:475:MET:HG3	2:C:721:HOH:O	2.20	0.41
1:A:389:MET:HE3	1:A:394:VAL:HG11	2.03	0.41
1:A:576:VAL:O	1:A:579:GLN:HG2	2.20	0.41
1:C:461:GLU:HA	1:C:466:GLU:O	2.20	0.41
1:D:122:LEU:HB3	1:D:131:VAL:CG2	2.47	0.41
1:D:235:GLU:OE1	1:D:243:ARG:CZ	2.69	0.41
1:D:389:MET:HE2	1:D:399:ILE:HG12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:GLU:O	1:A:178:LYS:HD3	2.21	0.41
1:A:544:HIS:O	1:A:548:VAL:HG23	2.20	0.41
1:A:563:ASP:O	1:A:566:VAL:HG22	2.20	0.41
1:C:120:ARG:HG3	1:C:121:LEU:N	2.36	0.41
1:D:253:ARG:O	1:D:257:ILE:HD13	2.20	0.41
1:B:251:PHE:O	1:B:255:LEU:HG	2.21	0.41
1:B:292:LEU:HD12	1:B:292:LEU:O	2.20	0.41
1:B:506:LYS:HE3	1:B:507:TYR:CE1	2.56	0.41
1:D:477:ASN:OD1	1:D:480:ARG:NH2	2.50	0.41
1:D:205:LYS:HD3	1:D:205:LYS:HA	1.62	0.41
1:A:525:GLN:NE2	1:A:528:ARG:HH12	2.18	0.41
1:B:337:LEU:HD22	1:B:347:TRP:CE2	2.56	0.41
1:C:242:ALA:O	1:C:245:GLU:OE1	2.39	0.41
1:C:293:GLU:OE1	1:C:293:GLU:N	2.54	0.41
1:A:308:PRO:HB2	1:A:340:ASN:OD1	2.20	0.41
1:C:437:ASP:OD1	1:C:437:ASP:N	2.52	0.41
1:D:217:VAL:HG23	1:D:227:LEU:HD12	2.01	0.41
1:A:107:ILE:HG13	1:A:108:ASN:N	2.36	0.40
1:A:239:VAL:HG21	1:A:243:ARG:H	1.85	0.40
1:A:529:LYS:HB2	1:A:529:LYS:HE2	1.76	0.40
1:C:531:LEU:O	1:C:535:VAL:HG23	2.21	0.40
1:D:135:ARG:HD3	1:D:152:TRP:CG	2.56	0.40
1:D:234:PHE:O	1:D:243:ARG:NH1	2.54	0.40
1:C:165:ASP:O	1:C:169:VAL:HG23	2.21	0.40
1:C:378:THR:HB	1:C:381:LEU:HD22	2.02	0.40
1:C:418:VAL:HG11	1:C:469:ASP:HB2	2.03	0.40
1:C:427:TYR:CZ	1:C:431:ARG:HD2	2.56	0.40
1:C:372:ILE:HD13	1:C:381:LEU:HB3	2.02	0.40
1:D:213:ALA:HB1	1:D:227:LEU:HD13	2.03	0.40
1:D:235:GLU:CA	1:D:243:ARG:HD3	2.51	0.40
1:B:133:MET:SD	1:B:137:LYS:HE3	2.61	0.40
1:C:421:TRP:CH2	1:C:451:ARG:HG2	2.57	0.40
1:D:354:LEU:HB3	1:D:364:VAL:HG22	2.02	0.40
1:C:289:LEU:HA	1:C:289:LEU:HD23	1.69	0.40
1:C:325:ASP:HA	1:C:326:PRO:HD2	1.96	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	516/561 (92%)	509 (99%)	7 (1%)	0	100	100
1	B	488/561 (87%)	477 (98%)	11 (2%)	0	100	100
1	C	493/561 (88%)	482 (98%)	11 (2%)	0	100	100
1	D	500/561 (89%)	490 (98%)	10 (2%)	0	100	100
All	All	1997/2244 (89%)	1958 (98%)	39 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	453/487 (93%)	438 (97%)	15 (3%)	33	61
1	B	432/487 (89%)	416 (96%)	16 (4%)	30	57
1	C	435/487 (89%)	422 (97%)	13 (3%)	36	64
1	D	439/487 (90%)	424 (97%)	15 (3%)	32	60
All	All	1759/1948 (90%)	1700 (97%)	59 (3%)	32	60

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	98	ILE
1	A	122	LEU

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Mol	Chain	Res	Type
1	A	127	GLU
1	A	209	VAL
1	A	214	LEU
1	A	310	LEU
1	A	381	LEU
1	A	387	LEU
1	A	398	VAL
1	A	418	VAL
1	A	491	LYS
1	A	502	ARG
1	A	573	LEU
1	A	605	ARG
1	A	611	LEU
1	B	109	VAL
1	B	122	LEU
1	B	124	LEU
1	B	209	VAL
1	B	214	LEU
1	B	239	VAL
1	B	259	LEU
1	B	381	LEU
1	B	387	LEU
1	B	398	VAL
1	B	412	ILE
1	B	418	VAL
1	B	437	ASP
1	B	491	LYS
1	B	559	LEU
1	B	573	LEU
1	C	158	SER
1	C	209	VAL
1	C	214	LEU
1	C	259	LEU
1	C	265	THR
1	C	381	LEU
1	C	387	LEU
1	C	398	VAL
1	C	412	ILE
1	C	418	VAL
1	C	437	ASP
1	C	491	LYS
1	C	573	LEU

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Mol	Chain	Res	Type
1	D	109	VAL
1	D	122	LEU
1	D	209	VAL
1	D	214	LEU
1	D	232	ARG
1	D	381	LEU
1	D	386	LEU
1	D	387	LEU
1	D	398	VAL
1	D	418	VAL
1	D	437	ASP
1	D	462	GLU
1	D	548	VAL
1	D	573	LEU
1	D	579	GLN

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	94	ASN
1	A	422	GLN
1	A	525	GLN
1	B	397	GLN
1	B	490	GLN
1	B	521	HIS
1	B	525	GLN
1	C	304	GLN
1	C	458	GLN
1	C	504	ASN
1	C	532	HIS
1	D	291	GLN
1	D	369	ASN
1	D	521	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	518/561 (92%)	-0.09	5 (0%) 79 76	40, 62, 99, 140	0
1	B	490/561 (87%)	-0.13	5 (1%) 79 76	43, 63, 98, 145	0
1	C	495/561 (88%)	-0.09	6 (1%) 76 73	41, 60, 96, 144	0
1	D	502/561 (89%)	-0.11	4 (0%) 82 80	40, 64, 98, 135	0
All	All	2005/2244 (89%)	-0.10	20 (0%) 79 76	40, 62, 98, 145	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	307	ALA	4.7
1	A	502	ARG	4.2
1	C	293	GLU	3.7
1	B	583	ALA	3.5
1	D	241	ALA	2.8
1	B	162	ASP	2.6
1	A	240	GLU	2.4
1	A	241	ALA	2.4
1	C	163	GLY	2.4
1	A	242	ALA	2.2
1	C	239	VAL	2.2
1	A	239	VAL	2.2
1	C	288	ALA	2.2
1	D	242	ALA	2.2
1	B	242	ALA	2.1
1	B	164	LEU	2.1
1	C	244	LEU	2.1
1	D	306	GLU	2.0
1	C	454	GLU	2.0
1	B	161	GLN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.