



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:05 AM UTC

PDB ID : 5A23 / pdb_00005a23
Title : SdsA sulfatase triclinic form
Authors : De la Mora, E.; Flores-Hernandez, E.; Jakoncik, J.; Stojanoff, V.; Sanchez-Puig, N.; Moreno, A.
Deposited on : 2015-05-11
Resolution : 2.41 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

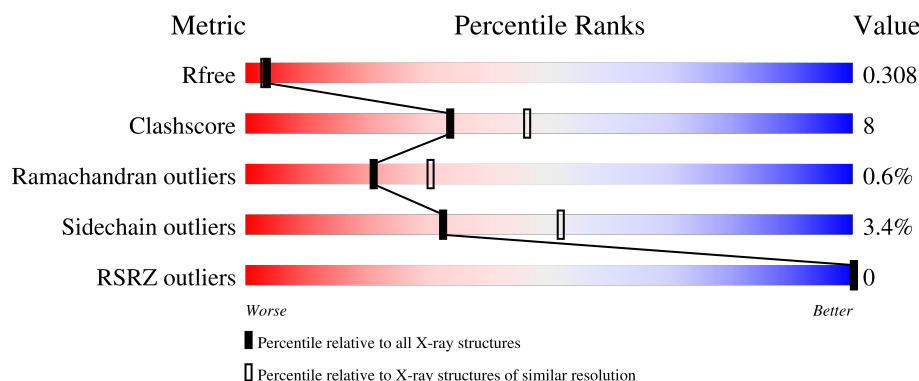
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

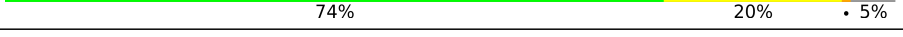
The reported resolution of this entry is 2.41 Å.

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	6062 (2.44-2.40)
Clashscore	190562	6562 (2.44-2.40)
Ramachandran outliers	187476	6481 (2.44-2.40)
Sidechain outliers	187428	6482 (2.44-2.40)
RSRZ outliers	180081	6066 (2.44-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	658	
1	B	658	
1	C	658	
1	D	658	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 19632 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 SDS HYDROLASE SDSA1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	628	Total	C	N	O	S	0	0	1
			4906	3096	887	913	10			
1	B	628	Total	C	N	O	S	0	0	1
			4906	3096	887	913	10			
1	C	628	Total	C	N	O	S	0	0	1
			4906	3096	887	913	10			
1	D	628	Total	C	N	O	S	0	0	1
			4906	3096	887	913	10			

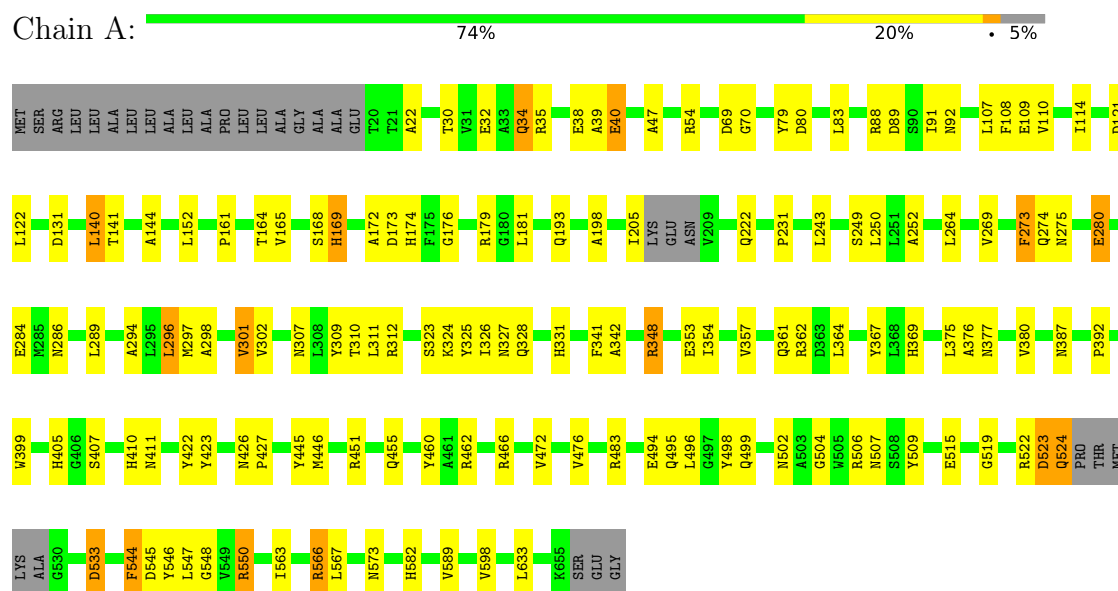
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

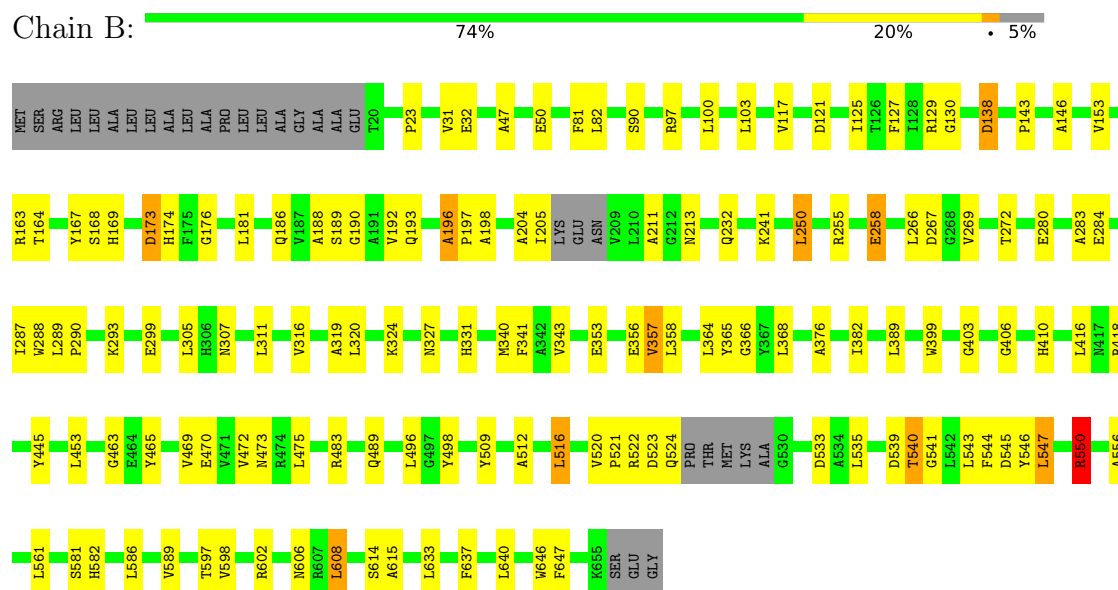
3 Residue-property plots

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.

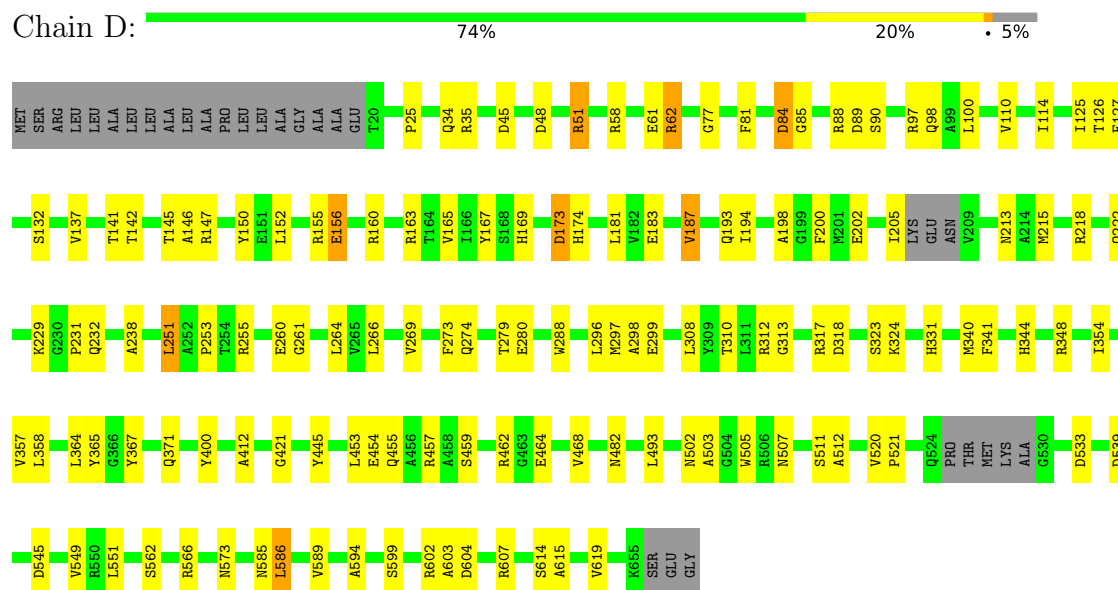
• Molecule 1: SDS HYDROLASE SDSA1



• Molecule 1: SDS HYDROLASE SDSA1



Chain C: 72% 21% • 5%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	86.90Å 86.80Å 129.03Å 107.59° 102.96° 95.59°	Depositor
Resolution (Å)	118.77 – 2.41 118.52 – 2.41	Depositor EDS
% Data completeness (in resolution range)	71.7 (118.77-2.41) 61.9 (118.52-2.41)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.27 (at 2.41Å)	Xtriage
Refinement program	REFMAC 5.8.0107	Depositor
R, R_{free}	0.253 , 0.307 0.258 , 0.308	Depositor DCC
R_{free} test set	4958 reflections (5.19%)	wwPDB-VP
Wilson B-factor (Å ²)	41.1	Xtriage
Anisotropy	0.154	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 29.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	19632	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.32% 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

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

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	1.33	22/5012 (0.4%)	1.29	37/6805 (0.5%)
1	B	1.12	11/5012 (0.2%)	1.19	11/6805 (0.2%)
1	C	1.18	7/5012 (0.1%)	1.22	18/6805 (0.3%)
1	D	1.24	10/5012 (0.2%)	1.23	17/6805 (0.2%)
All	All	1.22	50/20048 (0.2%)	1.23	83/27220 (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
1	C	0	1
All	All	0	3

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	294	ALA	CA-C	-8.12	1.42	1.52
1	B	196	ALA	CA-C	7.95	1.59	1.52
1	A	544	PHE	N-CA	7.06	1.54	1.46
1	A	161	PRO	C-O	6.85	1.31	1.23
1	A	302	VAL	N-CA	-6.79	1.37	1.46
1	A	280	GLU	CA-CB	6.50	1.63	1.53
1	D	586	LEU	N-CA	-6.45	1.38	1.46
1	D	412	ALA	N-CA	6.43	1.54	1.46
1	B	543	LEU	CA-C	-6.28	1.45	1.52
1	A	405	HIS	CA-C	6.25	1.60	1.53
1	A	181	LEU	C-O	-6.20	1.15	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	198	ALA	C-O	-6.04	1.16	1.23
1	B	121	ASP	N-CA	5.83	1.53	1.46
1	A	144	ALA	N-CA	5.83	1.53	1.46
1	D	318	ASP	CG-OD1	5.77	1.36	1.25
1	B	319	ALA	C-O	-5.65	1.16	1.24
1	C	197	PRO	CA-C	-5.64	1.45	1.52
1	C	307	ASN	CA-C	-5.62	1.45	1.52
1	A	108	PHE	C-O	-5.58	1.16	1.23
1	C	533	ASP	C-O	-5.55	1.17	1.24
1	D	114	ILE	CA-CB	5.53	1.61	1.54
1	D	288	TRP	CA-C	-5.52	1.46	1.52
1	B	167	TYR	CA-C	5.52	1.59	1.52
1	A	275	ASN	CA-C	-5.47	1.45	1.52
1	A	348	ARG	CA-CB	-5.47	1.44	1.53
1	B	368	LEU	C-O	-5.45	1.17	1.24
1	D	51	ARG	C-O	-5.41	1.17	1.24
1	A	354	ILE	C-O	-5.37	1.18	1.24
1	A	566	ARG	CA-C	5.37	1.59	1.52
1	A	331	HIS	CA-C	-5.35	1.45	1.52
1	C	587	ARG	C-O	-5.35	1.16	1.23
1	A	533	ASP	C-O	-5.32	1.17	1.24
1	D	142	THR	CA-C	5.30	1.57	1.52
1	C	126	THR	CA-C	-5.26	1.46	1.52
1	A	114	ILE	C-O	-5.24	1.18	1.24
1	A	301	VAL	CA-C	5.24	1.59	1.52
1	B	204	ALA	N-CA	5.21	1.52	1.46
1	A	179	ARG	N-CA	5.16	1.52	1.46
1	B	597	THR	CA-C	5.16	1.59	1.52
1	D	354	ILE	CA-C	-5.15	1.46	1.52
1	A	168	SER	C-O	5.14	1.30	1.24
1	B	547	LEU	N-CA	-5.13	1.40	1.46
1	A	399	TRP	C-O	-5.11	1.18	1.24
1	B	356	GLU	CA-C	5.09	1.59	1.52
1	D	274	GLN	CA-C	-5.08	1.46	1.53
1	C	172	ALA	N-CA	5.04	1.52	1.46
1	A	289	LEU	N-CA	-5.01	1.41	1.46
1	B	365	TYR	C-O	-5.00	1.18	1.24
1	D	503	ALA	N-CA	5.00	1.52	1.46
1	C	323	SER	C-O	-5.00	1.18	1.24

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	365	TYR	N-CA-C	-9.16	100.43	111.69
1	A	70	GLY	N-CA-C	8.82	125.58	115.08
1	D	187	VAL	N-CA-C	-8.33	102.22	110.30
1	B	550	ARG	CB-CA-C	-8.32	96.93	110.74
1	A	544	PHE	N-CA-C	8.27	120.29	111.28
1	D	141	THR	N-CA-C	8.23	120.33	111.36
1	A	252	ALA	CA-C-N	7.77	127.76	119.76
1	A	252	ALA	C-N-CA	7.77	127.76	119.76
1	A	289	LEU	CA-C-N	7.38	127.01	119.19
1	A	289	LEU	C-N-CA	7.38	127.01	119.19
1	B	324	LYS	N-CA-C	7.21	120.00	111.71
1	B	543	LEU	N-CA-C	-7.07	103.50	111.14
1	B	176	GLY	N-CA-C	6.96	122.58	114.16
1	C	168	SER	N-CA-C	-6.92	103.82	111.36
1	C	506	ARG	N-CA-C	-6.84	103.51	110.97
1	A	22	ALA	N-CA-C	6.84	119.52	110.36
1	A	168	SER	N-CA-C	-6.56	104.21	111.36
1	D	354	ILE	N-CA-C	-6.46	104.55	110.82
1	C	556	ALA	N-CA-C	6.32	120.85	113.20
1	D	25	PRO	N-CA-C	6.31	118.40	110.70
1	A	324	LYS	N-CA-C	6.27	117.78	111.07
1	A	548	GLY	N-CA-C	6.20	120.14	112.64
1	A	567	LEU	CA-C-N	6.20	126.09	119.28
1	A	567	LEU	C-N-CA	6.20	126.09	119.28
1	A	54	ARG	N-CA-C	6.19	119.20	110.23
1	A	47	ALA	CA-C-N	6.10	129.06	120.28
1	A	47	ALA	C-N-CA	6.10	129.06	120.28
1	D	323	SER	N-CA-C	-6.09	104.55	111.07
1	C	354	ILE	N-CA-C	-6.03	104.86	110.53
1	B	331	HIS	N-CA-C	5.78	118.52	111.82
1	C	178	VAL	N-CA-C	5.66	116.39	110.62
1	D	331	HIS	N-CA-C	5.64	119.42	112.54
1	C	372	THR	N-CA-C	-5.61	104.79	111.69
1	D	156	GLU	N-CA-C	5.55	118.52	111.69
1	D	545	ASP	N-CA-C	-5.51	105.17	111.07
1	B	357	VAL	CB-CA-C	-5.51	104.82	112.04
1	C	326	ILE	CA-C-N	5.50	127.58	120.44
1	C	326	ILE	C-N-CA	5.50	127.58	120.44
1	A	110	VAL	N-CA-C	-5.48	106.36	111.45
1	A	328	GLN	N-CA-C	-5.48	105.31	111.28
1	A	169	HIS	N-CA-C	5.47	115.77	108.38
1	C	471	VAL	N-CA-C	5.47	116.19	110.62
1	C	169	HIS	N-CA-C	5.45	115.73	108.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	110	VAL	CB-CA-C	-5.44	105.08	111.94
1	A	79	TYR	N-CA-C	5.43	119.61	112.92
1	D	308	LEU	N-CA-C	-5.41	106.53	113.23
1	A	284	GLU	N-CA-C	5.39	116.60	108.46
1	A	296	LEU	N-CA-C	-5.39	98.98	108.20
1	A	369	HIS	N-CA-C	5.38	117.00	111.03
1	A	273	PHE	N-CA-C	-5.36	100.96	109.59
1	A	109	GLU	N-CA-C	-5.34	100.02	108.73
1	D	551	LEU	N-CA-C	5.33	118.53	110.64
1	C	76	LEU	N-CA-C	5.32	119.93	113.38
1	B	289	LEU	CA-C-N	5.32	124.93	119.56
1	B	289	LEU	C-N-CA	5.32	124.93	119.56
1	A	422	TYR	N-CA-C	5.31	119.02	112.54
1	A	582	HIS	N-CA-C	5.31	117.02	108.32
1	A	302	VAL	N-CA-CB	-5.30	105.10	112.52
1	A	131	ASP	N-CA-C	5.28	117.03	111.28
1	A	375	LEU	N-CA-C	5.27	117.11	111.36
1	A	563	ILE	N-CA-C	5.25	115.60	107.78
1	A	307	ASN	N-CA-C	5.24	117.94	110.24
1	A	325	TYR	N-CA-C	5.23	117.06	111.36
1	B	307	ASN	N-CA-C	5.22	117.79	109.96
1	D	364	LEU	N-CA-C	5.21	116.76	111.14
1	C	69	ASP	N-CA-C	5.19	118.40	111.75
1	A	269	VAL	CA-C-N	5.19	124.95	119.76
1	A	269	VAL	C-N-CA	5.19	124.95	119.76
1	D	222	GLN	N-CA-C	5.19	117.34	111.11
1	D	165	VAL	N-CA-C	-5.18	101.02	108.89
1	A	165	VAL	N-CA-C	-5.17	100.87	108.11
1	A	280	GLU	N-CA-C	-5.16	105.66	111.28
1	C	141	THR	N-CA-C	5.14	119.27	112.89
1	D	533	ASP	CA-C-N	5.12	127.57	120.29
1	D	533	ASP	C-N-CA	5.12	127.57	120.29
1	C	260	GLU	N-CA-C	-5.11	107.00	113.18
1	C	541	GLY	N-CA-C	-5.10	106.61	112.73
1	B	320	LEU	N-CA-C	5.08	116.62	111.14
1	A	326	ILE	N-CA-C	5.04	115.65	110.36
1	C	184	PRO	N-CA-C	5.02	122.82	112.47
1	B	117	VAL	N-CA-C	-5.01	100.53	107.80
1	C	219	ALA	N-CA-C	5.01	117.63	111.82
1	C	108	PHE	N-CA-C	5.01	117.73	109.72

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	40	GLU	Peptide
1	B	523	ASP	Peptide
1	C	134	TRP	Peptide

5.2 Too-close contacts [i](#)

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	4906	0	4818	56	0
1	B	4906	0	4818	102	0
1	C	4906	0	4818	89	0
1	D	4906	0	4818	74	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	1	0
All	All	19632	0	19272	296	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 8.

All (296) 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:299:GLU:OE2	2:D:1001:ZN:ZN	1.17	0.91
1:C:35:ARG:C	1:C:38:GLU:HG2	2.00	0.86
1:C:35:ARG:NH2	1:C:89:ASP:OD1	2.12	0.81
1:C:35:ARG:O	1:C:38:GLU:HG2	1.82	0.77
1:B:146:ALA:HB1	1:B:181:LEU:HD21	1.65	0.77
1:D:562:SER:OG	1:D:594:ALA:HA	1.83	0.77
1:B:213:ASN:ND2	1:C:377:ASN:O	2.18	0.75
1:C:35:ARG:O	1:C:38:GLU:N	2.18	0.73
1:A:377:ASN:O	1:D:213:ASN:ND2	2.23	0.72
1:B:550:ARG:HE	1:B:640:LEU:HD22	1.55	0.72
1:B:169:HIS:CE1	1:B:299:GLU:HG3	2.26	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:547:LEU:CA	1:B:550:ARG:HD3	2.20	0.71
1:B:327:ASN:ND2	1:C:586:LEU:HD22	2.06	0.70
1:B:340:MET:SD	1:B:358:LEU:HD21	2.32	0.70
1:D:58:ARG:HH22	1:D:155:ARG:HB2	1.56	0.70
1:B:608:LEU:HD21	1:B:615:ALA:HB2	1.74	0.69
1:B:169:HIS:CD2	1:B:280:GLU:OE2	2.46	0.68
1:C:31:VAL:HG11	1:C:89:ASP:HB3	1.76	0.68
1:D:604:ASP:OD1	1:D:607:ARG:NH2	2.23	0.68
1:C:227:LEU:HD21	1:C:510:LEU:O	1.94	0.68
1:C:118:ARG:HG2	1:C:124:ASN:OD1	1.93	0.67
1:D:58:ARG:CZ	1:D:156:GLU:HG2	2.24	0.67
1:A:297:MET:O	1:A:298:ALA:C	2.37	0.66
1:D:84:ASP:OD2	1:D:88:ARG:NH1	2.28	0.66
1:A:545:ASP:OD1	1:D:324:LYS:NZ	2.24	0.66
1:B:299:GLU:HG2	1:B:343:VAL:CG2	2.25	0.66
1:C:35:ARG:O	1:C:38:GLU:CG	2.45	0.65
1:D:81:PHE:O	1:D:88:ARG:NH1	2.29	0.65
1:C:45:ASP:OD1	1:C:399:TRP:NE1	2.29	0.65
1:C:367:TYR:CZ	1:C:371:GLN:HG3	2.32	0.65
1:D:98:GLN:NE2	1:D:238:ALA:O	2.30	0.65
1:B:290:PRO:O	1:B:293:LYS:NZ	2.25	0.65
1:B:198:ALA:HB2	1:B:258:GLU:HG3	1.78	0.65
1:A:566:ARG:HG3	1:A:573:ASN:OD1	1.97	0.64
1:A:30:THR:OG1	1:A:495:GLN:OE1	2.14	0.64
1:C:538:MET:O	1:C:602:ARG:NH1	2.29	0.63
1:C:62:ARG:NH2	1:C:80:ASP:OD1	2.31	0.63
1:B:547:LEU:HB3	1:B:550:ARG:HD3	1.80	0.63
1:D:169:HIS:CD2	1:D:280:GLU:OE1	2.51	0.63
1:B:47:ALA:HA	1:B:50:GLU:OE2	1.99	0.62
1:C:63:LEU:O	1:C:75:GLN:HG3	1.99	0.62
1:B:547:LEU:C	1:B:550:ARG:HD3	2.25	0.62
1:B:547:LEU:CB	1:B:550:ARG:HD3	2.30	0.62
1:D:296:LEU:HA	1:D:341:PHE:O	2.00	0.62
1:C:31:VAL:CG1	1:C:89:ASP:HB3	2.30	0.61
1:B:382:ILE:HA	1:B:416:LEU:HD13	1.83	0.61
1:B:547:LEU:C	1:B:550:ARG:HH11	2.08	0.61
1:C:316:VAL:HG11	1:C:418:ARG:HB2	1.83	0.60
1:A:264:LEU:HD12	1:A:273:PHE:CE2	2.37	0.60
1:A:496:LEU:HD23	1:A:509:TYR:CE1	2.37	0.60
1:C:67:ASN:HB2	1:C:69:ASP:CG	2.27	0.60
1:B:190:GLY:HA3	1:D:255:ARG:HD2	1.82	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:TYR:CZ	1:A:392:PRO:HD3	2.36	0.59
1:C:535:LEU:O	1:C:602:ARG:NH2	2.36	0.58
1:D:90:SER:OG	1:D:231:PRO:O	2.21	0.58
1:C:80:ASP:HA	1:C:83:LEU:HD12	1.85	0.57
1:B:190:GLY:HA3	1:D:255:ARG:CD	2.34	0.57
1:C:118:ARG:CG	1:C:124:ASN:OD1	2.52	0.57
1:B:547:LEU:O	1:B:550:ARG:CD	2.53	0.57
1:C:437:ASP:O	1:C:441:ARG:NH2	2.31	0.57
1:D:566:ARG:HG2	1:D:573:ASN:OD1	2.04	0.57
1:B:586:LEU:HD22	1:C:327:ASN:ND2	2.19	0.57
1:A:122:LEU:HD22	1:A:243:LEU:HD13	1.86	0.57
1:B:539:ASP:OD2	1:B:541:GLY:N	2.37	0.57
1:A:39:ALA:O	1:A:40:GLU:HG2	2.05	0.56
1:B:547:LEU:O	1:B:550:ARG:HD3	2.05	0.56
1:B:550:ARG:HE	1:B:640:LEU:CD2	2.18	0.56
1:B:463:GLY:HA2	1:B:465:TYR:CE1	2.40	0.56
1:A:34:GLN:NE2	1:A:89:ASP:O	2.39	0.56
1:C:239:ILE:HD12	1:C:344:HIS:CE1	2.41	0.55
1:A:264:LEU:HD12	1:A:273:PHE:HE2	1.70	0.55
1:D:174:HIS:NE2	1:D:299:GLU:OE2	2.39	0.55
1:B:146:ALA:HB1	1:B:181:LEU:CD2	2.36	0.55
1:A:544:PHE:CD1	1:A:547:LEU:HD12	2.40	0.55
1:C:263:ASP:OD1	1:C:272:THR:HG23	2.06	0.54
1:A:222:GLN:OE1	1:A:312:ARG:N	2.41	0.54
1:A:274:GLN:OE1	1:A:286:ASN:ND2	2.41	0.54
1:B:197:PRO:HG2	1:B:283:ALA:HB1	1.90	0.54
1:B:547:LEU:O	1:B:550:ARG:CG	2.56	0.54
1:C:126:THR:HB	1:C:137:VAL:HB	1.89	0.53
1:A:327:ASN:ND2	1:D:586:LEU:HD22	2.24	0.53
1:B:602:ARG:NE	1:B:606:ASN:OD1	2.40	0.53
1:A:387:ASN:OD1	1:A:466:ARG:NH2	2.37	0.53
1:A:598:VAL:HG21	1:A:633:LEU:HD22	1.89	0.53
1:D:202:GLU:OE1	1:D:202:GLU:N	2.42	0.53
1:C:266:LEU:O	1:C:267:ASP:C	2.51	0.52
1:D:232:GLN:N	1:D:232:GLN:OE1	2.36	0.52
1:C:472:VAL:HB	1:C:489:GLN:OE1	2.09	0.52
1:D:150:TYR:OH	1:D:160:ARG:O	2.21	0.52
1:B:90:SER:HA	1:B:498:TYR:HB3	1.92	0.52
1:D:84:ASP:OD1	1:D:85:GLY:N	2.43	0.52
1:C:82:LEU:O	1:C:100:LEU:HD21	2.10	0.52
1:C:396:ASP:OD1	1:C:402:ARG:NH1	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:496:LEU:CD2	1:B:509:TYR:CZ	2.93	0.51
1:B:453:LEU:HD11	1:B:475:LEU:HD21	1.93	0.51
1:B:512:ALA:O	1:B:516:LEU:HD12	2.10	0.51
1:B:545:ASP:OD1	1:C:324:LYS:NZ	2.36	0.51
1:C:193:GLN:NE2	1:C:195:ILE:HD11	2.26	0.50
1:A:80:ASP:HA	1:A:83:LEU:HD12	1.93	0.50
1:B:521:PRO:HG2	1:B:646:TRP:CD2	2.46	0.50
1:D:279:THR:O	1:D:317:ARG:NE	2.32	0.50
1:B:496:LEU:HD22	1:B:509:TYR:CE1	2.47	0.50
1:B:138:ASP:OD2	1:B:174:HIS:ND1	2.44	0.50
1:C:179:ARG:HA	1:C:182:VAL:O	2.12	0.50
1:D:187:VAL:HG21	1:D:251:LEU:HD22	1.93	0.50
1:B:550:ARG:HD2	1:B:640:LEU:HD13	1.94	0.49
1:B:196:ALA:HB1	1:B:197:PRO:HD2	1.93	0.49
1:B:647:PHE:CD1	1:C:379:GLY:HA3	2.47	0.49
1:B:127:PHE:CZ	1:B:153:VAL:HG21	2.48	0.49
1:D:464:GLU:O	1:D:468:VAL:HG23	2.11	0.49
1:B:445:TYR:HH	1:C:459:SER:HG	1.61	0.49
1:D:367:TYR:CZ	1:D:371:GLN:HG3	2.48	0.49
1:D:146:ALA:HB1	1:D:181:LEU:HG	1.93	0.49
1:B:316:VAL:HG11	1:B:418:ARG:HB2	1.95	0.49
1:C:69:ASP:OD1	1:C:70:GLY:N	2.46	0.49
1:C:123:ALA:HB2	1:C:344:HIS:CE1	2.48	0.49
1:C:341:PHE:HB3	1:C:347:PRO:HB3	1.95	0.48
1:B:97:ARG:NH2	1:B:399:TRP:CD1	2.80	0.48
1:D:261:GLY:HA3	1:D:273:PHE:O	2.14	0.48
1:B:164:THR:HG23	1:B:193:GLN:CG	2.43	0.48
1:D:167:TYR:CD2	1:D:200:PHE:CZ	3.01	0.48
1:A:141:THR:O	1:A:176:GLY:HA3	2.14	0.48
1:C:298:ALA:O	1:C:343:VAL:HG22	2.14	0.48
1:C:308:LEU:HD12	1:C:411:ASN:HB3	1.95	0.48
1:D:340:MET:SD	1:D:358:LEU:HD21	2.53	0.48
1:B:522:ARG:O	1:B:524:GLN:NE2	2.46	0.48
1:B:546:TYR:O	1:B:547:LEU:C	2.56	0.48
1:A:423:TYR:O	1:D:218:ARG:NH2	2.32	0.47
1:C:69:ASP:OD1	1:C:71:SER:N	2.47	0.47
1:C:367:TYR:CE2	1:C:371:GLN:HG3	2.49	0.47
1:B:138:ASP:CG	1:B:174:HIS:HB3	2.40	0.47
1:C:193:GLN:HE22	1:C:266:LEU:CD2	2.28	0.47
1:C:198:ALA:HB2	1:C:258:GLU:CG	2.44	0.47
1:A:249:SER:HA	1:A:533:ASP:OD2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:189:SER:HB2	1:D:193:GLN:HE22	1.79	0.47
1:B:496:LEU:CD2	1:B:509:TYR:CE2	2.97	0.47
1:B:174:HIS:NE2	1:B:299:GLU:OE2	2.41	0.47
1:A:451:ARG:O	1:A:455:GLN:NE2	2.38	0.46
1:D:493:LEU:HD13	1:D:512:ALA:HB3	1.97	0.46
1:A:353:GLU:O	1:A:357:VAL:HG23	2.14	0.46
1:B:163:ARG:O	1:B:192:VAL:HA	2.15	0.46
1:C:95:LEU:HD11	1:C:236:ASP:HB3	1.96	0.46
1:C:99:ALA:HB2	1:C:236:ASP:HB2	1.96	0.46
1:B:173:ASP:HB3	1:B:174:HIS:CD2	2.50	0.46
1:D:299:GLU:OE2	1:D:344:HIS:NE2	2.49	0.46
1:C:307:ASN:ND2	1:C:405:HIS:CD2	2.83	0.46
1:C:435:PRO:O	1:C:439:ALA:HB2	2.16	0.46
1:D:357:VAL:HG22	1:D:400:TYR:CE2	2.51	0.46
1:B:23:PRO:HG2	1:B:232:GLN:HG3	1.98	0.46
1:D:169:HIS:CE1	1:D:299:GLU:HG3	2.51	0.46
1:B:305:LEU:HB3	1:B:403:GLY:HA2	1.98	0.46
1:D:45:ASP:O	1:D:97:ARG:NH2	2.46	0.46
1:A:121:ASP:OD2	1:A:140:LEU:HB3	2.16	0.46
1:B:547:LEU:HA	1:B:550:ARG:HD3	1.96	0.46
1:B:82:LEU:O	1:B:100:LEU:HD21	2.16	0.46
1:C:603:ALA:O	1:C:606:ASN:HB2	2.15	0.46
1:D:169:HIS:NE2	1:D:280:GLU:OE1	2.49	0.45
1:B:186:GLN:HB3	1:B:192:VAL:HG23	1.99	0.45
1:D:132:SER:OG	1:D:163:ARG:NE	2.47	0.45
1:B:445:TYR:HB3	1:C:446:MET:HG2	1.98	0.45
1:C:299:GLU:HG2	1:C:343:VAL:CG2	2.47	0.45
1:D:615:ALA:O	1:D:619:VAL:HG23	2.17	0.45
1:A:323:SER:OG	1:A:362:ARG:O	2.34	0.45
1:A:523:ASP:HA	1:A:524:GLN:HE21	1.81	0.45
1:B:193:GLN:HE22	1:B:266:LEU:HD22	1.81	0.45
1:C:124:ASN:HD22	1:C:344:HIS:HA	1.82	0.45
1:A:169:HIS:HE1	1:A:174:HIS:CE1	2.35	0.45
1:A:172:ALA:C	1:A:174:HIS:H	2.24	0.45
1:D:310:THR:HG21	1:D:312:ARG:CZ	2.46	0.45
1:D:549:VAL:HG12	1:D:549:VAL:O	2.16	0.45
1:A:494:GLU:HG2	1:A:498:TYR:CE2	2.52	0.45
1:C:520:VAL:O	1:C:521:PRO:C	2.57	0.45
1:D:194:ILE:HB	1:D:253:PRO:HA	1.98	0.45
1:D:215:MET:HG2	1:D:313:GLY:O	2.17	0.45
1:A:546:TYR:O	1:A:547:LEU:C	2.59	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:ALA:HA	1:A:380:VAL:O	2.17	0.44
1:B:272:THR:HB	1:B:288:TRP:HB3	1.99	0.44
1:D:34:GLN:HA	1:D:34:GLN:OE1	2.17	0.44
1:A:495:GLN:O	1:A:499:GLN:HG3	2.17	0.44
1:B:164:THR:HG23	1:B:193:GLN:HG3	1.99	0.44
1:D:81:PHE:O	1:D:84:ASP:OD2	2.35	0.44
1:A:91:ILE:HD11	1:A:231:PRO:HA	2.00	0.44
1:A:361:GLN:O	1:A:364:LEU:HB3	2.18	0.44
1:A:407:SER:HB3	1:A:410:HIS:ND1	2.32	0.44
1:A:506:ARG:O	1:A:507:ASN:C	2.59	0.44
1:D:297:MET:O	1:D:298:ALA:C	2.60	0.44
1:D:493:LEU:HD13	1:D:512:ALA:CB	2.47	0.44
1:A:169:HIS:CE1	1:A:174:HIS:NE2	2.86	0.44
1:D:202:GLU:N	1:D:202:GLU:CD	2.75	0.44
1:D:453:LEU:O	1:D:454:GLU:C	2.61	0.44
1:B:129:ARG:O	1:B:269:VAL:HG21	2.18	0.44
1:C:172:ALA:HA	1:C:175:PHE:CZ	2.52	0.44
1:D:566:ARG:NH1	1:D:573:ASN:HD21	2.14	0.44
1:B:90:SER:HB2	1:B:498:TYR:CD1	2.53	0.44
1:B:250:LEU:HB3	1:B:533:ASP:HB3	2.00	0.43
1:B:535:LEU:O	1:B:602:ARG:NH2	2.51	0.43
1:B:211:ALA:HB1	1:C:420:LEU:HD21	1.99	0.43
1:A:544:PHE:HA	1:A:547:LEU:HB2	1.99	0.43
1:B:353:GLU:O	1:B:357:VAL:HG23	2.18	0.43
1:B:127:PHE:CE1	1:B:153:VAL:HG21	2.54	0.43
1:B:598:VAL:HG21	1:B:633:LEU:HD22	2.00	0.43
1:D:45:ASP:OD1	1:D:45:ASP:C	2.62	0.43
1:D:602:ARG:O	1:D:603:ALA:C	2.62	0.43
1:B:496:LEU:HD22	1:B:509:TYR:CZ	2.54	0.43
1:C:163:ARG:O	1:C:192:VAL:HA	2.18	0.43
1:C:193:GLN:NE2	1:C:266:LEU:HD22	2.34	0.43
1:C:562:SER:OG	1:C:594:ALA:HA	2.19	0.43
1:C:169:HIS:CE1	1:C:299:GLU:HG3	2.53	0.43
1:C:198:ALA:HB2	1:C:258:GLU:HG3	2.00	0.43
1:A:91:ILE:HG22	1:A:92:ASN:O	2.18	0.43
1:B:250:LEU:CB	1:B:533:ASP:HB3	2.48	0.43
1:B:311:LEU:HD21	1:B:410:HIS:CD2	2.54	0.43
1:D:125:ILE:HG12	1:D:127:PHE:CE1	2.54	0.43
1:B:403:GLY:CA	1:B:406:GLY:O	2.66	0.43
1:B:470:GLU:HG2	1:C:442:TYR:OH	2.19	0.43
1:B:556:ALA:HB1	1:B:581:SER:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:147:ARG:HD3	1:D:147:ARG:HA	1.80	0.43
1:A:547:LEU:O	1:A:550:ARG:HB2	2.19	0.42
1:A:589:VAL:O	1:A:589:VAL:HG23	2.19	0.42
1:C:399:TRP:O	1:C:402:ARG:HG2	2.19	0.42
1:D:566:ARG:NH1	1:D:573:ASN:ND2	2.67	0.42
1:A:296:LEU:HD23	1:A:342:ALA:HA	2.01	0.42
1:C:117:VAL:CG1	1:C:120:PHE:CD1	3.03	0.42
1:D:367:TYR:CE1	1:D:371:GLN:HG3	2.54	0.42
1:A:426:ASN:HA	1:A:427:PRO:HD3	1.91	0.42
1:A:502:ASN:OD1	1:A:504:GLY:N	2.52	0.42
1:B:188:ALA:O	1:D:264:LEU:HD22	2.19	0.42
1:B:472:VAL:HB	1:B:489:GLN:OE1	2.20	0.42
1:C:169:HIS:CE1	1:C:174:HIS:CD2	3.07	0.42
1:C:579:LYS:O	1:C:580:ASN:C	2.62	0.42
1:B:483:ARG:HE	1:B:483:ARG:HB2	1.69	0.42
1:C:116:GLN:HG2	1:C:126:THR:OG1	2.19	0.42
1:C:296:LEU:HA	1:C:341:PHE:O	2.19	0.42
1:C:411:ASN:O	1:C:415:VAL:HG23	2.20	0.42
1:C:502:ASN:HB3	1:C:505:TRP:HB2	2.00	0.42
1:D:126:THR:HB	1:D:137:VAL:HB	2.01	0.42
1:A:107:LEU:HB2	1:A:152:LEU:CD2	2.49	0.42
1:B:544:PHE:HA	1:B:547:LEU:HB2	2.02	0.42
1:B:637:PHE:O	1:B:640:LEU:HG	2.19	0.42
1:A:446:MET:HG2	1:D:445:TYR:HB3	2.02	0.42
1:A:472:VAL:O	1:A:476:VAL:HG23	2.20	0.42
1:B:382:ILE:HB	1:B:416:LEU:HD22	2.01	0.42
1:C:582:HIS:CE1	1:C:584:ASN:OD1	2.73	0.42
1:B:189:SER:HB2	1:D:193:GLN:NE2	2.35	0.42
1:B:305:LEU:HD13	1:B:364:LEU:HD21	2.01	0.42
1:C:233:GLY:O	1:C:506:ARG:NE	2.49	0.42
1:B:366:GLY:HA3	1:C:582:HIS:CE1	2.55	0.42
1:C:26:PRO:HB2	1:C:31:VAL:CG1	2.50	0.42
1:B:130:GLY:HA3	1:B:267:ASP:HB3	2.02	0.41
1:C:30:THR:O	1:C:33:ALA:HB3	2.20	0.41
1:B:272:THR:O	1:B:287:ILE:HA	2.20	0.41
1:A:164:THR:HG23	1:A:193:GLN:HB2	2.02	0.41
1:B:173:ASP:CB	1:B:174:HIS:CD2	3.03	0.41
1:A:169:HIS:CE1	1:A:174:HIS:CD2	3.09	0.41
1:C:560:ALA:HA	1:C:578:LEU:O	2.20	0.41
1:D:48:ASP:HA	1:D:51:ARG:HB2	2.02	0.41
1:C:475:LEU:CD2	1:C:485:ALA:HB2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:576:LEU:C	1:C:577:GLU:HG3	2.46	0.41
1:C:402:ARG:HB2	1:C:404:TYR:CE2	2.56	0.41
1:D:502:ASN:HB3	1:D:505:TRP:HB2	2.02	0.41
1:B:31:VAL:O	1:B:32:GLU:C	2.64	0.41
1:B:103:LEU:HG	1:B:241:LYS:HD3	2.03	0.41
1:B:376:ALA:O	1:C:214:ALA:HB2	2.21	0.41
1:B:469:VAL:O	1:B:473:ASN:HB2	2.21	0.41
1:B:582:HIS:CE1	1:C:366:GLY:HA3	2.55	0.41
1:B:640:LEU:N	1:B:640:LEU:HD23	2.36	0.41
1:C:284:GLU:OE2	1:C:298:ALA:HB1	2.20	0.41
1:C:305:LEU:HB3	1:C:403:GLY:HA2	2.01	0.41
1:C:373:LEU:HD11	1:C:419:TYR:CE2	2.56	0.41
1:A:515:GLU:O	1:A:519:GLY:N	2.45	0.41
1:C:538:MET:O	1:C:602:ARG:NH2	2.50	0.41
1:D:266:LEU:O	1:D:269:VAL:N	2.48	0.41
1:A:35:ARG:NH2	1:A:38:GLU:OE2	2.43	0.41
1:B:280:GLU:OE2	1:B:284:GLU:OE1	2.39	0.41
1:B:550:ARG:CD	1:B:640:LEU:HD13	2.51	0.41
1:C:98:GLN:HE21	1:C:102:ASN:HD21	1.68	0.41
1:C:287:ILE:HD12	1:C:296:LEU:HD13	2.02	0.41
1:D:35:ARG:NH2	1:D:89:ASP:OD1	2.51	0.41
1:D:62:ARG:NH2	1:D:77:GLY:HA2	2.35	0.41
1:D:586:LEU:HD12	1:D:586:LEU:HA	1.95	0.41
1:C:373:LEU:HD21	1:C:419:TYR:CD2	2.56	0.41
1:D:507:ASN:O	1:D:511:SER:OG	2.27	0.41
1:A:309:TYR:CZ	1:D:421:GLY:HA3	2.57	0.40
1:B:168:SER:OG	1:B:169:HIS:N	2.54	0.40
1:B:389:LEU:HD23	1:B:389:LEU:C	2.46	0.40
1:A:407:SER:O	1:A:411:ASN:HB2	2.22	0.40
1:B:540:THR:HG22	1:B:544:PHE:CE2	2.56	0.40
1:D:58:ARG:NH2	1:D:152:LEU:O	2.55	0.40
1:D:459:SER:HA	1:D:462:ARG:HD2	2.03	0.40
1:A:410:HIS:CD2	1:A:410:HIS:C	2.99	0.40
1:B:280:GLU:HG3	1:B:284:GLU:OE1	2.22	0.40
1:C:538:MET:HE3	1:C:538:MET:HB2	1.95	0.40
1:D:173:ASP:CG	1:D:174:HIS:CD2	3.00	0.40
1:A:445:TYR:HA	1:D:455:GLN:OE1	2.21	0.40
1:B:366:GLY:HA3	1:C:582:HIS:NE2	2.36	0.40
1:D:145:THR:O	1:D:146:ALA:C	2.62	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	622/658 (94%)	581 (93%)	37 (6%)	4 (1%)	21	30
1	B	622/658 (94%)	586 (94%)	33 (5%)	3 (0%)	24	35
1	C	622/658 (94%)	571 (92%)	49 (8%)	2 (0%)	36	49
1	D	622/658 (94%)	575 (92%)	41 (7%)	6 (1%)	12	18
All	All	2488/2632 (94%)	2313 (93%)	160 (6%)	15 (1%)	21	30

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	140	LEU
1	B	81	PHE
1	B	138	ASP
1	B	173	ASP
1	C	38	GLU
1	A	173	ASP
1	A	460	TYR
1	D	173	ASP
1	D	539	ASP
1	D	84	ASP
1	D	198	ALA
1	D	482	ASN
1	A	301	VAL
1	D	521	PRO
1	C	385	VAL

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	499/521 (96%)	482 (97%)	17 (3%)	32	52
1	B	499/521 (96%)	484 (97%)	15 (3%)	36	56
1	C	499/521 (96%)	479 (96%)	20 (4%)	28	45
1	D	499/521 (96%)	484 (97%)	15 (3%)	36	56
All	All	1996/2084 (96%)	1929 (97%)	67 (3%)	32	52

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	GLU
1	A	34	GLN
1	A	69	ASP
1	A	88	ARG
1	A	205	ILE
1	A	250	LEU
1	A	280	GLU
1	A	310	THR
1	A	311	LEU
1	A	341	PHE
1	A	348	ARG
1	A	462	ARG
1	A	483	ARG
1	A	522	ARG
1	A	523	ASP
1	A	524	GLN
1	A	550	ARG
1	B	125	ILE
1	B	143	PRO
1	B	205	ILE
1	B	250	LEU
1	B	255	ARG
1	B	258	GLU
1	B	341	PHE
1	B	516	LEU
1	B	520	VAL
1	B	540	THR
1	B	550	ARG
1	B	561	LEU
1	B	589	VAL
1	B	608	LEU

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Mol	Chain	Res	Type
1	B	614	SER
1	C	38	GLU
1	C	50	GLU
1	C	59	ARG
1	C	62	ARG
1	C	71	SER
1	C	110	VAL
1	C	205	ILE
1	C	245	ARG
1	C	250	LEU
1	C	296	LEU
1	C	315	GLU
1	C	355	VAL
1	C	381	THR
1	C	416	LEU
1	C	450	GLU
1	C	520	VAL
1	C	559	LYS
1	C	567	LEU
1	C	592	GLU
1	C	644	ASP
1	D	61	GLU
1	D	62	ARG
1	D	100	LEU
1	D	183	GLU
1	D	205	ILE
1	D	229	LYS
1	D	251	LEU
1	D	260	GLU
1	D	348	ARG
1	D	457	ARG
1	D	520	VAL
1	D	585	ASN
1	D	589	VAL
1	D	599	SER
1	D	614	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	ASN
1	A	524	GLN

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Mol	Chain	Res	Type
1	B	124	ASN
1	B	193	GLN
1	B	371	GLN
1	B	384	GLN
1	C	67	ASN
1	C	98	GLN
1	C	185	GLN
1	C	193	GLN
1	C	307	ASN
1	C	405	HIS
1	C	473	ASN
1	D	307	ASN
1	D	331	HIS
1	D	426	ASN
1	D	582	HIS

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 8 ligands modelled in this entry, 8 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 [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	628/658 (95%)	-1.31	0 100 100	13, 38, 73, 104	0
1	B	628/658 (95%)	-1.23	0 100 100	23, 50, 84, 118	0
1	C	628/658 (95%)	-1.26	0 100 100	20, 45, 75, 123	0
1	D	628/658 (95%)	-1.30	0 100 100	18, 42, 73, 107	0
All	All	2512/2632 (95%)	-1.28	0 100 100	13, 44, 79, 123	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	ZN	A	1001	1/1	1.00	0.01	39,39,39,39	0
2	ZN	A	1002	1/1	1.00	0.01	44,44,44,44	0
2	ZN	B	1001	1/1	1.00	0.02	57,57,57,57	0
2	ZN	B	1002	1/1	1.00	0.02	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZN	C	1001	1/1	1.00	0.01	52,52,52,52	0
2	ZN	C	1002	1/1	1.00	0.01	50,50,50,50	0
2	ZN	D	1001	1/1	1.00	0.01	27,27,27,27	1
2	ZN	D	1002	1/1	1.00	0.02	48,48,48,48	1

6.5 Other polymers [i](#)

There are no such residues in this entry.