



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:31 AM UTC

PDB ID : 3BF0 / pdb_00003bf0
Title : Crystal structure of Escherichia coli Signal peptide peptidase (SppA), Native crystals
Authors : Paetzel, M.
Deposited on : 2007-11-20
Resolution : 2.55 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
Xtrriage (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

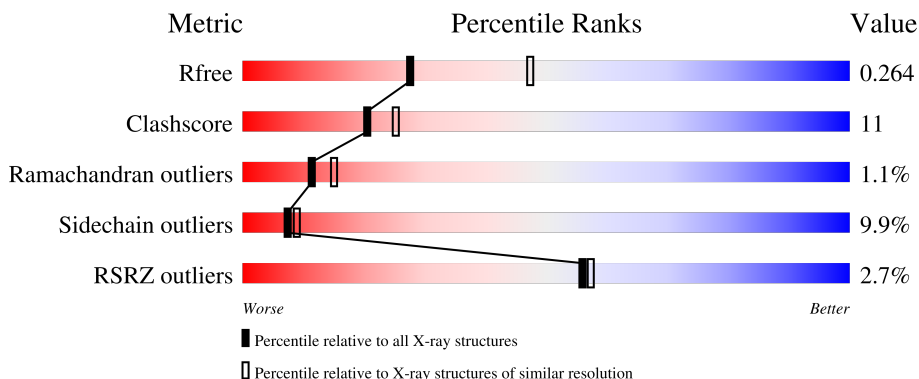
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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	593	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 59%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 17%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 20%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">2% 59% 17% • 20%</p>
1	B	593	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 60%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 16%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 20%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">2% 60% 16% •• 20%</p>
1	C	593	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 60%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 17%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 19%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">3% 60% 17% • 19%</p>
1	D	593	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 59%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 18%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 20%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">2% 59% 18% •• 20%</p>

2 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 14865 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 Protease 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	474	3587	2263	614	702	8	0	0	0
1	B	474	3583	2260	613	702	8	0	0	0
1	C	478	3606	2273	617	708	8	0	0	0
1	D	476	3601	2270	616	707	8	0	0	0

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	26	MET	-	expression tag	UNP P08395
A	27	GLY	-	expression tag	UNP P08395
A	28	SER	-	expression tag	UNP P08395
A	29	SER	-	expression tag	UNP P08395
A	30	HIS	-	expression tag	UNP P08395
A	31	HIS	-	expression tag	UNP P08395
A	32	HIS	-	expression tag	UNP P08395
A	33	HIS	-	expression tag	UNP P08395
A	34	HIS	-	expression tag	UNP P08395
A	35	HIS	-	expression tag	UNP P08395
A	36	SER	-	expression tag	UNP P08395
A	37	SER	-	expression tag	UNP P08395
A	38	GLY	-	expression tag	UNP P08395
A	39	LEU	-	expression tag	UNP P08395
A	40	VAL	-	expression tag	UNP P08395
A	41	PRO	-	expression tag	UNP P08395
A	42	ARG	-	expression tag	UNP P08395
A	43	GLY	-	expression tag	UNP P08395
A	44	SER	-	expression tag	UNP P08395
A	45	HIS	-	expression tag	UNP P08395
A	46	MET	-	expression tag	UNP P08395

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Chain	Residue	Modelled	Actual	Comment	Reference
B	26	MET	-	expression tag	UNP P08395
B	27	GLY	-	expression tag	UNP P08395
B	28	SER	-	expression tag	UNP P08395
B	29	SER	-	expression tag	UNP P08395
B	30	HIS	-	expression tag	UNP P08395
B	31	HIS	-	expression tag	UNP P08395
B	32	HIS	-	expression tag	UNP P08395
B	33	HIS	-	expression tag	UNP P08395
B	34	HIS	-	expression tag	UNP P08395
B	35	HIS	-	expression tag	UNP P08395
B	36	SER	-	expression tag	UNP P08395
B	37	SER	-	expression tag	UNP P08395
B	38	GLY	-	expression tag	UNP P08395
B	39	LEU	-	expression tag	UNP P08395
B	40	VAL	-	expression tag	UNP P08395
B	41	PRO	-	expression tag	UNP P08395
B	42	ARG	-	expression tag	UNP P08395
B	43	GLY	-	expression tag	UNP P08395
B	44	SER	-	expression tag	UNP P08395
B	45	HIS	-	expression tag	UNP P08395
B	46	MET	-	expression tag	UNP P08395
C	26	MET	-	expression tag	UNP P08395
C	27	GLY	-	expression tag	UNP P08395
C	28	SER	-	expression tag	UNP P08395
C	29	SER	-	expression tag	UNP P08395
C	30	HIS	-	expression tag	UNP P08395
C	31	HIS	-	expression tag	UNP P08395
C	32	HIS	-	expression tag	UNP P08395
C	33	HIS	-	expression tag	UNP P08395
C	34	HIS	-	expression tag	UNP P08395
C	35	HIS	-	expression tag	UNP P08395
C	36	SER	-	expression tag	UNP P08395
C	37	SER	-	expression tag	UNP P08395
C	38	GLY	-	expression tag	UNP P08395
C	39	LEU	-	expression tag	UNP P08395
C	40	VAL	-	expression tag	UNP P08395
C	41	PRO	-	expression tag	UNP P08395
C	42	ARG	-	expression tag	UNP P08395
C	43	GLY	-	expression tag	UNP P08395
C	44	SER	-	expression tag	UNP P08395
C	45	HIS	-	expression tag	UNP P08395
C	46	MET	-	expression tag	UNP P08395

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Chain	Residue	Modelled	Actual	Comment	Reference
D	26	MET	-	expression tag	UNP P08395
D	27	GLY	-	expression tag	UNP P08395
D	28	SER	-	expression tag	UNP P08395
D	29	SER	-	expression tag	UNP P08395
D	30	HIS	-	expression tag	UNP P08395
D	31	HIS	-	expression tag	UNP P08395
D	32	HIS	-	expression tag	UNP P08395
D	33	HIS	-	expression tag	UNP P08395
D	34	HIS	-	expression tag	UNP P08395
D	35	HIS	-	expression tag	UNP P08395
D	36	SER	-	expression tag	UNP P08395
D	37	SER	-	expression tag	UNP P08395
D	38	GLY	-	expression tag	UNP P08395
D	39	LEU	-	expression tag	UNP P08395
D	40	VAL	-	expression tag	UNP P08395
D	41	PRO	-	expression tag	UNP P08395
D	42	ARG	-	expression tag	UNP P08395
D	43	GLY	-	expression tag	UNP P08395
D	44	SER	-	expression tag	UNP P08395
D	45	HIS	-	expression tag	UNP P08395
D	46	MET	-	expression tag	UNP P08395

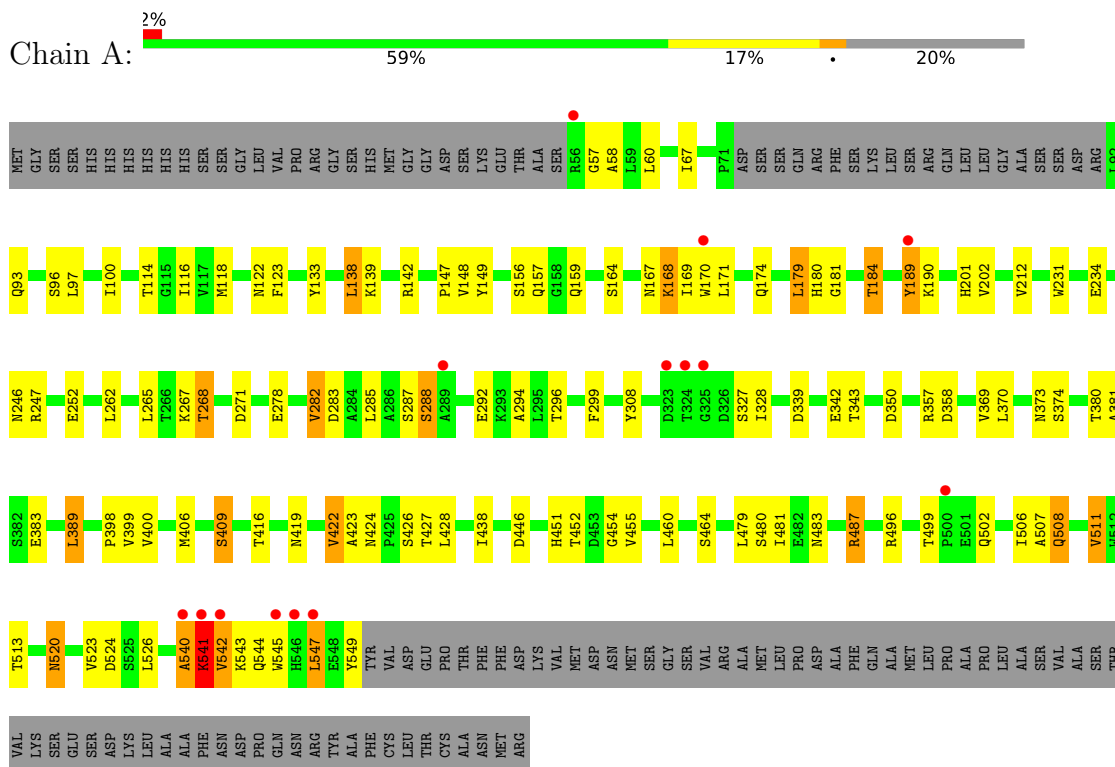
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	116	Total O 116 116	0	0
2	B	127	Total O 127 127	0	0
2	C	144	Total O 144 144	0	0
2	D	101	Total O 101 101	0	0

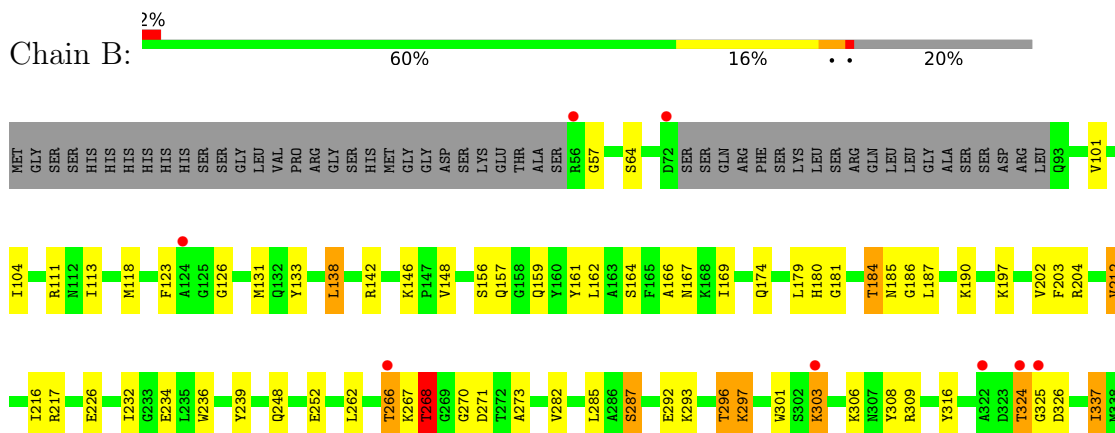
3 Residue-property plots [i](#)

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: Protease 4



- Molecule 1: Protease 4



R496	R540	R541	R542	K543	Q544	W545	H546	L547	E548	Y549	TYR	VAL	ASP	GLU	PRO	THR	PHE	PHE	ASP	LYS	VAL	MET	ASN	ASN	MET	SER	GLY	SER	VAL	ARG	ALA	MET	LEU	PRO	ASP	ALA	ALA	PHE	GLN	ALA	MET	LEU	PRO	ALA	PRO	LEU	ALA	SER
VAL	ALA	SER	THR	VAL	LYS	SER	GLU	SER	ASP	LYS	LEU	ALA	ALA	PHE	ASN	ASP	PRO	GLN	ASN	ARG	TYR	ALA	PHE	CYS	LEU	THR	CYS	ALA	ASN	MET	ARG																	

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	94.17Å 153.49Å 100.66Å 90.00° 104.25° 90.00°	Depositor
Resolution (Å)	50.00 – 2.55 50.00 – 2.55	Depositor EDS
% Data completeness (in resolution range)	96.2 (50.00-2.55) 96.1 (50.00-2.55)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.07 (at 2.54Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.214 , 0.252 0.208 , 0.264	Depositor DCC
R_{free} test set	4338 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	29.4	Xtrriage
Anisotropy	0.551	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 31.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	14865	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.40% 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 i

5.1 Standard geometry i

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	0.93	1/3654 (0.0%)	1.04	8/4960 (0.2%)
1	B	0.93	1/3650 (0.0%)	1.10	11/4956 (0.2%)
1	C	0.96	5/3673 (0.1%)	1.09	10/4988 (0.2%)
1	D	0.90	1/3668 (0.0%)	1.05	7/4979 (0.1%)
All	All	0.93	8/14645 (0.1%)	1.07	36/19883 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	2
All	All	0	5

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	540	ALA	CA-C	10.19	1.57	1.52
1	D	542	VAL	CA-CB	6.82	1.63	1.54
1	C	411	GLY	C-O	-6.08	1.17	1.24
1	C	410	GLY	C-O	-5.79	1.16	1.23
1	C	438	ILE	CA-CB	5.35	1.60	1.54
1	B	541	LYS	N-CA	5.19	1.52	1.46
1	C	511	VAL	CA-CB	5.13	1.60	1.54
1	C	408	ALA	C-O	-5.10	1.17	1.23

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	542	VAL	N-CA-C	9.47	124.87	113.22
1	C	541	LYS	N-CA-C	7.94	118.74	108.34
1	D	541	LYS	N-CA-C	7.69	119.83	108.14
1	D	125	GLY	N-CA-C	6.97	119.15	112.04
1	A	57	GLY	N-CA-C	6.81	118.42	111.95
1	C	542	VAL	N-CA-C	6.72	120.26	113.47
1	C	492	VAL	N-CA-C	-6.48	103.94	111.00
1	B	57	GLY	N-CA-C	6.46	122.37	112.81
1	B	296	THR	N-CA-C	-6.39	102.10	110.53
1	B	146	LYS	CA-C-N	-6.39	114.05	120.31
1	B	146	LYS	C-N-CA	-6.39	114.05	120.31
1	C	339	ASP	N-CA-C	6.27	119.10	111.82
1	B	542	VAL	N-CA-C	6.23	122.30	109.34
1	C	70	LYS	CA-C-N	6.18	127.56	119.84
1	C	70	LYS	C-N-CA	6.18	127.56	119.84
1	D	458	SER	CA-C-N	-6.17	113.26	119.56
1	D	458	SER	C-N-CA	-6.17	113.26	119.56
1	A	422	VAL	N-CA-C	6.00	116.56	108.17
1	B	161	TYR	N-CA-C	-5.71	104.75	110.97
1	C	379	VAL	N-CA-C	5.60	116.34	110.62
1	A	541	LYS	N-CA-C	5.41	116.21	108.74
1	A	374	SER	CA-C-N	5.41	125.88	120.04
1	A	374	SER	C-N-CA	5.41	125.88	120.04
1	B	339	ASP	N-CA-C	5.36	118.98	112.23
1	A	189	TYR	CB-CA-C	-5.35	100.83	110.35
1	C	518	LYS	N-CA-C	-5.34	105.13	111.69
1	D	57	GLY	N-CA-C	5.32	120.16	112.81
1	C	546	HIS	N-CA-C	5.23	117.76	109.24
1	B	416	THR	CA-C-N	-5.19	114.47	119.87
1	B	416	THR	C-N-CA	-5.19	114.47	119.87
1	D	421	ILE	N-CA-C	5.14	115.25	107.80
1	C	513	THR	N-CA-C	-5.11	103.78	110.53
1	B	444	SER	N-CA-C	-5.07	105.22	111.40
1	A	540	ALA	N-CA-C	5.04	116.13	108.12
1	B	217	ARG	N-CA-C	5.01	115.92	108.60
1	D	546	HIS	N-CA-C	5.00	117.40	109.24

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	541	LYS	Peptide
1	B	541	LYS	Peptide

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Mol	Chain	Res	Type	Group
1	C	541	LYS	Peptide
1	D	340	GLY	Peptide
1	D	541	LYS	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	3587	0	3550	82	0
1	B	3583	0	3539	92	0
1	C	3606	0	3549	72	0
1	D	3601	0	3559	94	0
2	A	116	0	0	4	0
2	B	127	0	0	3	0
2	C	144	0	0	6	0
2	D	101	0	0	4	0
All	All	14865	0	14197	320	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 (320) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:542:VAL:HG12	1:B:543:LYS:N	1.40	1.18
1:D:403:MET:CE	1:D:423:ALA:HB2	1.72	1.17
1:B:542:VAL:CG1	1:B:543:LYS:N	2.08	1.12
1:B:542:VAL:CG1	1:B:543:LYS:H	1.54	1.10
1:D:403:MET:HE2	1:D:423:ALA:HB2	1.07	1.07
1:C:174:GLN:HG2	2:C:697:HOH:O	1.52	1.06
1:B:469:LEU:HD21	1:B:477:MET:HE1	1.34	1.05
1:B:296:THR:O	1:B:297:LYS:HB3	1.55	1.02
1:B:424:ASN:HD22	1:B:426:SER:H	1.10	0.98
1:D:157:GLN:HE22	1:D:181:GLY:H	1.14	0.94
1:B:469:LEU:HD21	1:B:477:MET:CE	1.97	0.94
1:B:157:GLN:HE22	1:B:181:GLY:H	1.18	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:424:ASN:HD22	1:A:426:SER:H	1.12	0.91
1:B:403:MET:HE2	1:B:423:ALA:HB2	1.50	0.90
1:D:424:ASN:HD22	1:D:426:SER:H	1.13	0.90
1:C:268:THR:HG22	1:C:271:ASP:HB3	1.55	0.88
1:C:499:THR:HG22	1:C:502:GLN:H	1.39	0.87
1:C:268:THR:HG21	1:C:274:LYS:HB2	1.54	0.87
1:B:296:THR:O	1:B:297:LYS:CB	2.22	0.86
1:C:148:VAL:H	1:C:167:ASN:HD22	1.23	0.86
1:D:403:MET:HE2	1:D:423:ALA:CB	2.02	0.85
1:D:271:ASP:OD2	1:D:274:LYS:HB2	1.77	0.84
1:B:148:VAL:H	1:B:167:ASN:HD22	1.23	0.84
1:C:278:GLU:HG2	2:C:667:HOH:O	1.78	0.83
1:D:403:MET:CE	1:D:423:ALA:CB	2.55	0.83
1:C:157:GLN:HE22	1:C:181:GLY:H	1.26	0.82
1:B:424:ASN:ND2	1:B:426:SER:H	1.77	0.82
1:D:131:MET:HE1	1:D:158:GLY:O	1.81	0.81
1:A:409:SER:HB3	2:A:718:HOH:O	1.81	0.81
1:D:157:GLN:NE2	1:D:180:HIS:H	1.80	0.80
1:A:157:GLN:HE22	1:A:181:GLY:H	1.30	0.80
1:B:487:ARG:HH11	1:B:487:ARG:CG	1.95	0.78
1:D:424:ASN:ND2	1:D:426:SER:H	1.82	0.78
1:A:487:ARG:CG	1:A:487:ARG:HH11	1.98	0.77
1:D:148:VAL:H	1:D:167:ASN:HD22	1.31	0.76
1:A:148:VAL:H	1:A:167:ASN:HD22	1.31	0.76
1:A:357:ARG:HH21	1:B:292:GLU:CD	1.92	0.76
1:A:424:ASN:ND2	1:A:426:SER:H	1.83	0.76
1:C:184:THR:HG22	1:D:455:VAL:H	1.50	0.76
1:A:399:VAL:H	1:A:419:ASN:ND2	1.85	0.75
1:C:123:PHE:CZ	1:C:131:MET:HE2	2.22	0.74
1:B:296:THR:HG22	1:B:308:TYR:HB3	1.69	0.74
1:C:292:GLU:O	1:C:296:THR:HG23	1.88	0.74
1:B:487:ARG:HH11	1:B:487:ARG:HG3	1.51	0.74
1:C:268:THR:CG2	1:C:274:LYS:HB2	2.17	0.74
1:A:399:VAL:H	1:A:419:ASN:HD22	1.36	0.73
1:A:296:THR:HG22	1:A:308:TYR:HB3	1.71	0.73
1:C:168:LYS:HE3	1:C:170:TRP:CZ2	2.24	0.72
1:B:540:ALA:C	1:B:541:LYS:HD3	2.15	0.72
1:B:104:ILE:HD13	1:B:138:LEU:HD13	1.71	0.72
1:A:455:VAL:H	1:B:184:THR:HG22	1.53	0.71
1:C:157:GLN:NE2	1:C:180:HIS:H	1.88	0.71
1:B:542:VAL:HG12	1:B:543:LYS:H	0.66	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:292:GLU:CD	1:D:357:ARG:HH21	2.00	0.69
1:C:515:GLN:HG3	2:C:638:HOH:O	1.94	0.68
1:A:157:GLN:NE2	1:A:180:HIS:H	1.91	0.68
1:C:424:ASN:ND2	1:C:426:SER:H	1.92	0.68
1:C:424:ASN:HD22	1:C:426:SER:H	1.42	0.67
1:B:202:VAL:HG21	1:B:216:ILE:CG2	2.25	0.67
1:B:469:LEU:CD2	1:B:477:MET:HE1	2.20	0.67
1:D:399:VAL:H	1:D:419:ASN:ND2	1.94	0.65
1:B:424:ASN:HD22	1:B:426:SER:N	1.89	0.65
1:A:339:ASP:HA	1:A:381:ALA:HB2	1.79	0.64
1:D:148:VAL:H	1:D:167:ASN:ND2	1.96	0.64
1:D:403:MET:HE3	1:D:427:THR:HG21	1.79	0.63
1:D:541:LYS:HD3	1:D:542:VAL:HG23	1.81	0.63
1:B:499:THR:OG1	1:B:502:GLN:HG2	1.98	0.63
1:C:359:ALA:HB1	1:C:365:VAL:HG11	1.80	0.63
1:C:126:GLY:H	1:C:131:MET:HE3	1.64	0.63
1:B:301:TRP:HE1	1:B:303:LYS:HZ2	1.46	0.62
1:A:157:GLN:HE22	1:A:180:HIS:H	1.48	0.62
1:A:452:THR:HG22	1:B:187:LEU:HD23	1.82	0.62
1:A:487:ARG:HH11	1:A:487:ARG:HG2	1.64	0.62
1:A:184:THR:HG22	1:C:455:VAL:H	1.63	0.62
1:A:424:ASN:HD22	1:A:426:SER:N	1.92	0.61
1:B:202:VAL:HG21	1:B:216:ILE:HG23	1.80	0.61
1:A:398:PRO:HA	1:A:419:ASN:HD21	1.65	0.61
1:C:399:VAL:H	1:C:419:ASN:HD22	1.49	0.61
1:A:373:ASN:HA	1:A:406:MET:O	2.02	0.60
1:C:434:ILE:HG23	1:C:481:ILE:HD13	1.83	0.60
1:C:123:PHE:HZ	1:C:131:MET:HE2	1.66	0.60
1:D:153:GLU:HA	1:D:172:SER:HB2	1.84	0.60
1:A:268:THR:HG21	1:A:271:ASP:O	2.01	0.60
1:B:386:ARG:HG2	1:B:417:PRO:HG3	1.82	0.60
1:A:545:TRP:CZ3	1:A:547:LEU:HD23	2.36	0.60
1:B:292:GLU:O	1:B:296:THR:HG23	2.02	0.59
1:A:148:VAL:H	1:A:167:ASN:ND2	2.01	0.59
1:B:399:VAL:H	1:B:419:ASN:HD22	1.49	0.59
1:A:398:PRO:HA	1:A:419:ASN:ND2	2.17	0.59
1:C:268:THR:CG2	1:C:271:ASP:HB3	2.30	0.59
1:A:327:SER:HB3	1:A:545:TRP:CE2	2.37	0.59
1:A:479:LEU:HD21	1:B:270:GLY:HA2	1.85	0.59
1:B:403:MET:HE1	1:B:429:THR:HG21	1.84	0.59
1:B:373:ASN:HA	1:B:406:MET:O	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:126:GLY:N	1:C:131:MET:HE3	2.18	0.59
1:B:157:GLN:NE2	1:B:180:HIS:H	2.01	0.59
1:C:274:LYS:O	1:C:278:GLU:HG3	2.03	0.59
1:B:541:LYS:HD3	1:B:541:LYS:N	2.18	0.58
1:D:123:PHE:HE2	1:D:131:MET:HE3	1.68	0.58
1:B:303:LYS:HZ2	1:B:303:LYS:HA	1.68	0.58
1:D:344:GLN:CG	1:D:345:GLY:H	2.15	0.58
1:D:419:ASN:HD22	1:D:419:ASN:H	1.50	0.57
1:D:228:ASP:HA	1:D:231:TRP:NE1	2.19	0.57
1:C:171:LEU:HB2	1:C:282:VAL:HG21	1.85	0.57
1:B:123:PHE:CE2	1:B:131:MET:HE2	2.40	0.57
1:D:292:GLU:O	1:D:296:THR:HG22	2.06	0.56
1:A:171:LEU:HB2	1:A:282:VAL:HG21	1.87	0.56
1:A:369:VAL:HA	1:A:400:VAL:O	2.06	0.55
1:D:252:GLU:O	1:D:252:GLU:HG3	2.06	0.55
1:C:270:GLY:HA2	1:D:479:LEU:HD21	1.88	0.55
1:D:383:GLU:CD	1:D:487:ARG:HH12	2.15	0.55
1:D:210:SER:O	1:D:213:GLU:HG3	2.07	0.55
1:B:126:GLY:H	1:B:131:MET:HE3	1.71	0.54
1:C:268:THR:HG21	1:C:274:LYS:CB	2.32	0.54
1:A:370:LEU:HD22	1:A:389:LEU:HD21	1.89	0.54
1:C:373:ASN:HA	1:C:406:MET:O	2.07	0.54
1:D:520:ASN:C	1:D:520:ASN:HD22	2.16	0.54
1:B:273:ALA:HB1	1:B:285:LEU:HD22	1.89	0.54
1:B:421:ILE:CG2	1:B:523:VAL:HG22	2.37	0.53
1:A:116:ILE:HB	1:A:148:VAL:HG22	1.90	0.53
1:D:325:GLY:O	1:D:326:ASP:HB2	2.08	0.53
1:C:268:THR:HG23	1:C:274:LYS:HD2	1.89	0.53
1:B:156:SER:H	1:B:159:GLN:NE2	2.06	0.53
1:A:156:SER:H	1:A:159:GLN:NE2	2.06	0.52
1:A:174:GLN:HG2	2:C:632:HOH:O	2.10	0.52
1:B:164:SER:HA	1:B:169:ILE:HD11	1.90	0.52
1:B:541:LYS:HG3	2:B:732:HOH:O	2.10	0.52
1:A:542:VAL:O	1:A:542:VAL:CG1	2.57	0.52
1:C:123:PHE:CE2	1:C:131:MET:HE2	2.44	0.52
1:D:142:ARG:HG2	1:D:167:ASN:HD21	1.74	0.52
1:D:496:ARG:NH2	1:D:524:ASP:OD1	2.43	0.52
1:A:520:ASN:C	1:A:520:ASN:HD22	2.18	0.51
1:A:164:SER:O	1:A:246:ASN:HB3	2.09	0.51
1:D:60:LEU:HB3	1:D:312:SER:HA	1.92	0.51
1:A:496:ARG:HH22	1:A:524:ASP:CG	2.19	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:296:THR:HG22	1:C:308:TYR:HB3	1.91	0.51
1:B:520:ASN:C	1:B:520:ASN:HD22	2.19	0.51
1:D:200:THR:HG21	1:D:215:PHE:HB3	1.92	0.51
1:C:496:ARG:HH22	1:C:524:ASP:CG	2.19	0.51
1:D:416:THR:HG22	1:D:417:PRO:HD3	1.92	0.50
1:D:496:ARG:HH22	1:D:524:ASP:CG	2.19	0.50
1:A:487:ARG:HH11	1:A:487:ARG:HG3	1.76	0.50
1:B:204:ARG:HD3	1:B:212:VAL:HG11	1.94	0.50
1:B:268:THR:HG23	1:B:271:ASP:HB3	1.92	0.50
1:C:520:ASN:C	1:C:520:ASN:HD22	2.20	0.50
1:D:434:ILE:HG12	1:D:481:ILE:HD12	1.92	0.50
1:A:58:ALA:HB2	1:A:299:PHE:CD1	2.45	0.50
1:D:123:PHE:CE2	1:D:131:MET:HE3	2.47	0.50
1:B:467:ARG:HH11	1:D:185:ASN:ND2	2.10	0.50
1:C:56:ARG:HA	1:C:112:ASN:O	2.11	0.50
1:C:64:SER:O	1:C:92:LEU:O	2.30	0.50
1:A:357:ARG:NH1	1:B:306:LYS:O	2.38	0.50
1:B:399:VAL:H	1:B:419:ASN:ND2	2.09	0.49
1:B:543:LYS:HE3	1:B:544:GLN:H	1.76	0.49
1:A:547:LEU:HD12	1:A:549:TYR:CZ	2.47	0.49
1:C:148:VAL:H	1:C:167:ASN:ND2	2.02	0.49
1:C:370:LEU:HD22	1:C:389:LEU:HD21	1.94	0.49
1:A:231:TRP:CD1	1:A:511:VAL:HG22	2.48	0.49
1:B:301:TRP:HE1	1:B:303:LYS:NZ	2.10	0.49
1:B:421:ILE:HG22	1:B:523:VAL:HG22	1.94	0.49
1:A:164:SER:HA	1:A:169:ILE:HD11	1.95	0.49
1:A:399:VAL:N	1:A:419:ASN:HD22	2.07	0.49
1:C:268:THR:CG2	1:C:274:LYS:CB	2.89	0.49
1:C:292:GLU:CD	1:D:357:ARG:NH2	2.69	0.48
1:D:157:GLN:HG3	1:D:179:LEU:HD12	1.95	0.48
1:A:118:MET:HE3	1:A:138:LEU:HD21	1.96	0.48
1:A:189:TYR:O	1:A:190:LYS:C	2.57	0.48
1:B:202:VAL:HG13	1:B:212:VAL:HG21	1.94	0.48
1:B:118:MET:CE	1:B:166:ALA:HB2	2.43	0.48
1:C:267:LYS:C	1:C:269:GLY:H	2.22	0.48
1:C:424:ASN:HD22	1:C:426:SER:N	2.10	0.48
1:B:113:ILE:HD11	1:B:316:TYR:CE1	2.49	0.47
1:B:460:LEU:HD21	1:B:476:MET:HE1	1.95	0.47
1:D:424:ASN:HD22	1:D:426:SER:N	1.95	0.47
1:A:142:ARG:HG2	1:A:167:ASN:HD21	1.79	0.47
1:A:357:ARG:NH2	1:B:292:GLU:CD	2.69	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:344:GLN:HG2	1:D:345:GLY:H	1.79	0.47
1:B:543:LYS:HD2	1:B:543:LYS:HA	1.61	0.47
1:C:467:ARG:NH2	2:C:620:HOH:O	2.46	0.47
1:D:171:LEU:O	1:D:285:LEU:HA	2.14	0.47
1:D:191:SER:O	1:D:195:LYS:HG3	2.15	0.47
1:A:171:LEU:O	1:A:285:LEU:HA	2.13	0.47
1:D:268:THR:HG23	1:D:271:ASP:H	1.80	0.47
1:B:118:MET:HE2	1:B:148:VAL:CG1	2.44	0.47
1:B:266:THR:C	1:B:268:THR:H	2.22	0.47
1:A:149:TYR:CD1	1:A:170:TRP:HZ3	2.32	0.47
1:C:110:ASP:OD1	1:C:110:ASP:C	2.57	0.47
1:D:131:MET:HE2	1:D:162:LEU:HG	1.97	0.47
1:B:236:TRP:O	1:B:239:TYR:HB3	2.15	0.46
1:D:545:TRP:CH2	1:D:547:LEU:HD22	2.50	0.46
1:D:205:VAL:HA	2:D:629:HOH:O	2.14	0.46
1:D:292:GLU:O	1:D:296:THR:CG2	2.64	0.46
1:B:389:LEU:HG	1:B:399:VAL:HG11	1.98	0.46
1:D:199:SER:O	1:D:439:THR:HA	2.15	0.46
1:B:403:MET:HE3	1:B:427:THR:HG21	1.97	0.46
1:D:149:TYR:CD1	1:D:170:TRP:CZ3	3.03	0.46
1:C:156:SER:H	1:C:159:GLN:NE2	2.13	0.46
1:C:202:VAL:HG13	1:C:212:VAL:HG21	1.97	0.46
1:C:452:THR:HG21	1:C:466:THR:OG1	2.16	0.46
1:A:292:GLU:O	1:A:296:THR:HG23	2.16	0.46
1:B:452:THR:HG21	1:B:466:THR:OG1	2.15	0.46
1:A:58:ALA:HB2	1:A:299:PHE:CE1	2.50	0.46
1:B:123:PHE:HE2	1:B:131:MET:HE2	1.81	0.46
1:A:542:VAL:O	1:A:542:VAL:HG13	2.16	0.46
1:D:419:ASN:ND2	1:D:419:ASN:H	2.14	0.45
1:B:454:GLY:HA3	1:D:184:THR:HG22	1.97	0.45
1:D:342:GLU:O	1:D:343:THR:C	2.59	0.45
1:D:104:ILE:HD13	1:D:138:LEU:HD13	1.98	0.45
1:D:380:THR:O	1:D:384:VAL:HG23	2.17	0.45
1:D:541:LYS:HD3	1:D:542:VAL:CG2	2.45	0.45
1:A:268:THR:CG2	1:A:271:ASP:O	2.64	0.45
1:C:539:LEU:O	1:C:540:ALA:HB2	2.16	0.45
1:A:122:ASN:ND2	2:A:682:HOH:O	2.50	0.45
1:A:168:LYS:NZ	1:A:170:TRP:CZ2	2.85	0.45
1:B:403:MET:HE2	1:B:523:VAL:HG21	1.98	0.45
1:D:373:ASN:HA	1:D:406:MET:O	2.17	0.45
1:C:157:GLN:HE22	1:C:181:GLY:N	2.04	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:502:GLN:HG3	2:A:647:HOH:O	2.16	0.44
1:D:339:ASP:OD2	1:D:380:THR:OG1	2.34	0.44
1:B:458:SER:HB3	1:D:180:HIS:O	2.16	0.44
1:C:362:ASP:OD1	1:C:364:LYS:HB2	2.17	0.44
1:D:542:VAL:HG12	1:D:543:LYS:N	2.31	0.44
1:B:542:VAL:HG13	1:B:543:LYS:N	2.22	0.44
1:C:70:LYS:HA	1:C:71:PRO:HD2	1.86	0.44
1:D:545:TRP:CH2	1:D:547:LEU:CD2	3.01	0.44
1:D:262:LEU:HD23	1:D:262:LEU:HA	1.81	0.44
1:D:481:ILE:HD13	1:D:481:ILE:HA	1.83	0.44
1:A:296:THR:HG22	1:A:308:TYR:CB	2.44	0.44
1:D:157:GLN:HE22	1:D:180:HIS:H	1.61	0.44
1:A:268:THR:HG23	1:A:271:ASP:H	1.83	0.44
1:B:467:ARG:HD3	1:D:185:ASN:HD21	1.81	0.44
1:D:324:THR:HB	1:D:545:TRP:CD1	2.52	0.44
1:A:455:VAL:N	1:B:184:THR:HG22	2.27	0.44
1:C:399:VAL:H	1:C:419:ASN:ND2	2.12	0.44
1:B:422:VAL:HG22	2:B:658:HOH:O	2.17	0.44
1:C:168:LYS:HE3	1:C:170:TRP:CH2	2.52	0.44
1:B:268:THR:O	1:B:268:THR:CG2	2.65	0.43
1:B:487:ARG:CG	1:B:487:ARG:NH1	2.68	0.43
1:C:93:GLN:O	1:C:93:GLN:HG3	2.17	0.43
1:D:339:ASP:HA	1:D:381:ALA:HB2	1.99	0.43
1:A:287:SER:O	1:A:288:SER:C	2.61	0.43
1:A:454:GLY:CA	1:B:184:THR:HG22	2.48	0.43
1:C:62:ASP:O	1:C:314:TYR:HE2	2.01	0.43
1:C:220:MET:HE2	1:C:225:ARG:HA	2.00	0.43
1:B:520:ASN:ND2	1:B:522:LEU:HG	2.33	0.43
1:C:96:SER:HB3	1:C:99:ASP:HB2	2.00	0.43
1:C:187:LEU:HD23	1:D:452:THR:HG22	2.00	0.43
1:A:294:ALA:O	2:A:684:HOH:O	2.21	0.43
1:D:156:SER:H	1:D:159:GLN:NE2	2.16	0.43
1:D:209:LYS:HE2	1:D:435:PHE:HD1	1.83	0.43
1:B:326:ASP:O	1:B:544:GLN:HA	2.18	0.43
1:D:72:ASP:OD1	1:D:345:GLY:HA2	2.19	0.43
1:A:201:HIS:HB2	1:A:438:ILE:HB	2.00	0.43
1:C:415:SER:C	1:C:417:PRO:HD2	2.44	0.43
1:D:245:ALA:O	1:D:248:GLN:NE2	2.44	0.43
1:A:499:THR:OG1	1:A:502:GLN:HG2	2.19	0.42
1:D:386:ARG:HG3	1:D:417:PRO:HD3	2.01	0.42
1:D:542:VAL:HG12	1:D:543:LYS:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:ILE:HD12	1:A:544:GLN:HG3	2.02	0.42
1:B:203:PHE:O	1:B:435:PHE:HA	2.19	0.42
1:C:157:GLN:HE22	1:C:180:HIS:H	1.62	0.42
1:C:162:LEU:HD23	1:C:162:LEU:HA	1.87	0.42
1:A:383:GLU:OE2	1:A:487:ARG:NH1	2.52	0.42
1:A:452:THR:HA	1:B:186:GLY:O	2.19	0.42
1:B:324:THR:HG22	1:B:325:GLY:N	2.34	0.42
1:B:480:SER:HA	2:D:674:HOH:O	2.20	0.42
1:B:540:ALA:O	1:B:541:LYS:HB2	2.19	0.42
1:A:423:ALA:O	1:A:526:LEU:HA	2.19	0.42
1:D:67:ILE:HD12	1:D:100:ILE:HD12	2.02	0.42
1:C:451:HIS:HA	2:C:701:HOH:O	2.20	0.42
1:D:252:GLU:HB3	2:D:711:HOH:O	2.19	0.42
1:B:537:ALA:O	1:B:541:LYS:N	2.44	0.42
1:D:162:LEU:HD23	1:D:162:LEU:HA	1.82	0.42
1:D:423:ALA:O	1:D:526:LEU:HA	2.20	0.42
1:A:399:VAL:N	1:A:419:ASN:ND2	2.63	0.42
1:B:101:VAL:HG21	1:B:133:TYR:CD2	2.55	0.42
1:C:192:LEU:HD13	1:D:448:ILE:O	2.19	0.42
1:A:97:LEU:HD11	1:A:133:TYR:HD2	1.85	0.42
1:A:157:GLN:HE21	1:A:179:LEU:HA	1.84	0.42
1:C:409:SER:HB3	1:C:410:GLY:H	1.43	0.42
1:D:217:ARG:HD2	2:D:684:HOH:O	2.18	0.42
1:D:157:GLN:HE22	1:D:181:GLY:N	1.98	0.41
1:D:261:LEU:O	1:D:265:LEU:HB2	2.19	0.41
1:D:420:TYR:CD2	1:D:535:LYS:HG2	2.55	0.41
1:A:540:ALA:C	1:A:541:LYS:HG3	2.45	0.41
1:A:545:TRP:CH2	1:A:547:LEU:HD23	2.55	0.41
1:D:118:MET:CE	1:D:162:LEU:HB3	2.50	0.41
1:A:427:THR:O	1:A:513:THR:HA	2.20	0.41
1:B:477:MET:HE2	1:B:477:MET:HB2	1.97	0.41
1:C:164:SER:HA	1:C:169:ILE:HD11	2.01	0.41
1:B:475:LEU:HD23	1:B:475:LEU:HA	1.70	0.41
1:D:138:LEU:HD12	1:D:138:LEU:HA	1.88	0.41
1:D:92:LEU:O	1:D:93:GLN:CB	2.69	0.41
1:D:268:THR:CG2	1:D:271:ASP:H	2.33	0.41
1:D:487:ARG:CG	1:D:487:ARG:HH11	2.33	0.41
1:C:540:ALA:O	1:C:541:LYS:HD2	2.20	0.41
1:B:142:ARG:HG2	1:B:167:ASN:HD21	1.86	0.41
1:B:148:VAL:H	1:B:167:ASN:ND2	2.03	0.41
1:B:337:ILE:HA	1:B:347:VAL:HB	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:416:THR:N	1:C:417:PRO:HD2	2.36	0.41
1:D:114:THR:O	1:D:147:PRO:HD2	2.21	0.41
1:D:266:THR:C	1:D:268:THR:H	2.28	0.41
1:C:189:TYR:O	1:C:190:LYS:C	2.64	0.41
1:C:343:THR:O	1:C:344:GLN:C	2.63	0.41
1:A:339:ASP:OD2	1:A:380:THR:OG1	2.38	0.41
1:D:149:TYR:CD1	1:D:170:TRP:HZ3	2.38	0.41
1:D:541:LYS:HB2	1:D:542:VAL:HG23	2.02	0.41
1:A:114:THR:O	1:A:147:PRO:HD2	2.21	0.41
1:A:247:ARG:HH22	1:A:283:ASP:CG	2.29	0.41
1:A:268:THR:HG23	1:A:271:ASP:N	2.36	0.41
1:A:507:ALA:O	1:A:508:GLN:C	2.63	0.41
1:C:393:ARG:HA	1:C:397:LYS:O	2.21	0.40
1:A:67:ILE:HG12	1:A:123:PHE:HE1	1.87	0.40
1:A:446:ASP:OD1	1:A:451:HIS:HE1	2.04	0.40
1:B:113:ILE:CD1	1:B:316:TYR:CE1	3.04	0.40
1:B:309:ARG:NH2	2:B:619:HOH:O	2.53	0.40
1:C:148:VAL:O	1:C:167:ASN:HB2	2.22	0.40
1:A:67:ILE:HD12	1:A:100:ILE:CD1	2.52	0.40
1:B:101:VAL:HG21	1:B:133:TYR:CE2	2.57	0.40
1:D:168:LYS:HD3	1:D:170:TRP:CH2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [\(i\)](#)

5.3.1 Protein backbone [\(i\)](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	470/593 (79%)	440 (94%)	28 (6%)	2 (0%)	30	39
1	B	470/593 (79%)	442 (94%)	22 (5%)	6 (1%)	9	12
1	C	474/593 (80%)	447 (94%)	22 (5%)	5 (1%)	11	15
1	D	472/593 (80%)	442 (94%)	22 (5%)	8 (2%)	7	8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1886/2372 (80%)	1771 (94%)	94 (5%)	21 (1%)	11 15

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	508	GLN
1	B	541	LYS
1	B	542	VAL
1	C	324	THR
1	C	540	ALA
1	D	93	GLN
1	D	326	ASP
1	D	344	GLN
1	D	542	VAL
1	A	342	GLU
1	B	297	LYS
1	C	550	TYR
1	D	343	THR
1	B	267	LYS
1	B	287	SER
1	C	71	PRO
1	C	268	THR
1	B	268	THR
1	D	342	GLU
1	D	206	GLY
1	D	349	GLY

5.3.2 Protein sidechains [i](#)

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	374/475 (79%)	335 (90%)	39 (10%)	7 8
1	B	373/475 (78%)	335 (90%)	38 (10%)	7 8
1	C	374/475 (79%)	338 (90%)	36 (10%)	8 9
1	D	376/475 (79%)	341 (91%)	35 (9%)	8 10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1497/1900 (79%)	1349 (90%)	148 (10%)	7 9

All (148) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	LEU
1	A	93	GLN
1	A	96	SER
1	A	138	LEU
1	A	139	LYS
1	A	168	LYS
1	A	179	LEU
1	A	184	THR
1	A	202	VAL
1	A	212	VAL
1	A	234	GLU
1	A	252	GLU
1	A	262	LEU
1	A	265	LEU
1	A	267	LYS
1	A	268	THR
1	A	278	GLU
1	A	282	VAL
1	A	288	SER
1	A	343	THR
1	A	350	ASP
1	A	358	ASP
1	A	389	LEU
1	A	409	SER
1	A	416	THR
1	A	422	VAL
1	A	428	LEU
1	A	460	LEU
1	A	464	SER
1	A	480	SER
1	A	481	ILE
1	A	483	ASN
1	A	487	ARG
1	A	506	ILE
1	A	511	VAL
1	A	520	ASN
1	A	523	VAL

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Mol	Chain	Res	Type
1	A	543	LYS
1	A	547	LEU
1	B	64	SER
1	B	111	ARG
1	B	138	LEU
1	B	162	LEU
1	B	174	GLN
1	B	179	LEU
1	B	184	THR
1	B	185	ASN
1	B	190	LYS
1	B	197	LYS
1	B	212	VAL
1	B	226	GLU
1	B	232	ILE
1	B	234	GLU
1	B	248	GLN
1	B	252	GLU
1	B	262	LEU
1	B	266	THR
1	B	268	THR
1	B	282	VAL
1	B	287	SER
1	B	293	LYS
1	B	303	LYS
1	B	324	THR
1	B	337	ILE
1	B	422	VAL
1	B	428	LEU
1	B	460	LEU
1	B	477	MET
1	B	487	ARG
1	B	511	VAL
1	B	520	ASN
1	B	523	VAL
1	B	541	LYS
1	B	542	VAL
1	B	543	LYS
1	B	544	GLN
1	B	547	LEU
1	C	71	PRO
1	C	93	GLN

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Mol	Chain	Res	Type
1	C	95	ASN
1	C	113	ILE
1	C	138	LEU
1	C	179	LEU
1	C	184	THR
1	C	191	SER
1	C	212	VAL
1	C	216	ILE
1	C	248	GLN
1	C	262	LEU
1	C	265	LEU
1	C	280	LYS
1	C	282	VAL
1	C	293	LYS
1	C	297	LYS
1	C	304	THR
1	C	358	ASP
1	C	364	LYS
1	C	389	LEU
1	C	406	MET
1	C	409	SER
1	C	422	VAL
1	C	460	LEU
1	C	481	ILE
1	C	499	THR
1	C	511	VAL
1	C	520	ASN
1	C	523	VAL
1	C	541	LYS
1	C	542	VAL
1	C	543	LYS
1	C	544	GLN
1	C	547	LEU
1	C	548	GLU
1	D	93	GLN
1	D	111	ARG
1	D	114	THR
1	D	138	LEU
1	D	139	LYS
1	D	174	GLN
1	D	179	LEU
1	D	184	THR

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Mol	Chain	Res	Type
1	D	207	THR
1	D	212	VAL
1	D	232	ILE
1	D	234	GLU
1	D	252	GLU
1	D	262	LEU
1	D	265	LEU
1	D	268	THR
1	D	280	LYS
1	D	282	VAL
1	D	296	THR
1	D	304	THR
1	D	364	LYS
1	D	389	LEU
1	D	416	THR
1	D	419	ASN
1	D	422	VAL
1	D	424	ASN
1	D	460	LEU
1	D	481	ILE
1	D	487	ARG
1	D	511	VAL
1	D	520	ASN
1	D	523	VAL
1	D	541	LYS
1	D	544	GLN
1	D	547	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	122	ASN
1	A	128	GLN
1	A	157	GLN
1	A	159	GLN
1	A	167	ASN
1	A	174	GLN
1	A	185	ASN
1	A	238	ASN
1	A	241	ASN
1	A	259	GLN
1	A	346	ASN

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Mol	Chain	Res	Type
1	A	419	ASN
1	A	424	ASN
1	A	451	HIS
1	A	510	HIS
1	A	520	ASN
1	B	93	GLN
1	B	122	ASN
1	B	157	GLN
1	B	159	GLN
1	B	167	ASN
1	B	238	ASN
1	B	241	ASN
1	B	248	GLN
1	B	259	GLN
1	B	346	ASN
1	B	419	ASN
1	B	424	ASN
1	B	508	GLN
1	B	520	ASN
1	C	112	ASN
1	C	122	ASN
1	C	157	GLN
1	C	159	GLN
1	C	167	ASN
1	C	185	ASN
1	C	237	GLN
1	C	238	ASN
1	C	241	ASN
1	C	253	GLN
1	C	346	ASN
1	C	419	ASN
1	C	424	ASN
1	C	515	GLN
1	C	520	ASN
1	C	544	GLN
1	D	122	ASN
1	D	157	GLN
1	D	159	GLN
1	D	167	ASN
1	D	185	ASN
1	D	238	ASN
1	D	241	ASN

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Mol	Chain	Res	Type
1	D	334	ASN
1	D	346	ASN
1	D	419	ASN
1	D	424	ASN
1	D	508	GLN
1	D	510	HIS
1	D	520	ASN
1	D	544	GLN
1	D	546	HIS

5.3.3 RNA [i](#)

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

6.1 Protein, DNA and RNA chains

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	474/593 (79%)	0.08	14 (2%) 52 54	14, 28, 51, 65	0
1	B	474/593 (79%)	-0.01	12 (2%) 58 59	14, 25, 48, 59	0
1	C	478/593 (80%)	-0.05	16 (3%) 49 50	14, 25, 49, 62	0
1	D	476/593 (80%)	-0.01	9 (1%) 66 66	14, 27, 49, 60	0
All	All	1902/2372 (80%)	0.00	51 (2%) 56 57	14, 26, 49, 65	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	545	TRP	5.6
1	A	324	THR	5.5
1	D	343	THR	5.4
1	D	545	TRP	5.2
1	B	545	TRP	4.8
1	D	325	GLY	4.1
1	B	542	VAL	4.1
1	D	542	VAL	4.1
1	C	91	ARG	3.7
1	A	170	TRP	3.6
1	C	92	LEU	3.6
1	C	545	TRP	3.6
1	D	324	THR	3.5
1	A	540	ALA	3.5
1	C	325	GLY	3.5
1	B	325	GLY	3.4
1	A	289	ALA	3.2
1	C	546	HIS	3.1
1	A	542	VAL	3.1
1	C	324	THR	3.0
1	B	322	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	72	ASP	3.0
1	A	323	ASP	2.9
1	C	551	VAL	2.8
1	C	189	TYR	2.7
1	C	287	SER	2.7
1	A	325	GLY	2.6
1	B	303	LYS	2.6
1	C	542	VAL	2.6
1	C	550	TYR	2.6
1	B	324	THR	2.5
1	A	547	LEU	2.5
1	B	546	HIS	2.5
1	A	500	PRO	2.4
1	A	546	HIS	2.4
1	A	56	ARG	2.4
1	D	546	HIS	2.4
1	C	540	ALA	2.4
1	C	56	ARG	2.3
1	B	266	THR	2.3
1	D	541	LYS	2.3
1	C	301	TRP	2.2
1	D	540	ALA	2.2
1	C	547	LEU	2.2
1	D	73	SER	2.2
1	A	541	LYS	2.2
1	B	124	ALA	2.2
1	C	544	GLN	2.2
1	A	189	TYR	2.1
1	B	549	TYR	2.1
1	B	56	ARG	2.1

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

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.