



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:45 AM UTC

PDB ID : 7ZF5 / pdb_00007zf5
Title : SARS-CoV-2 Omicron RBD in complex with Omi-12 and Beta-54 Fabs
Authors : Zhou, D.; Huo, J.; Ren, J.; Stuart, D.I.
Deposited on : 2022-04-01
Resolution : 5.32 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

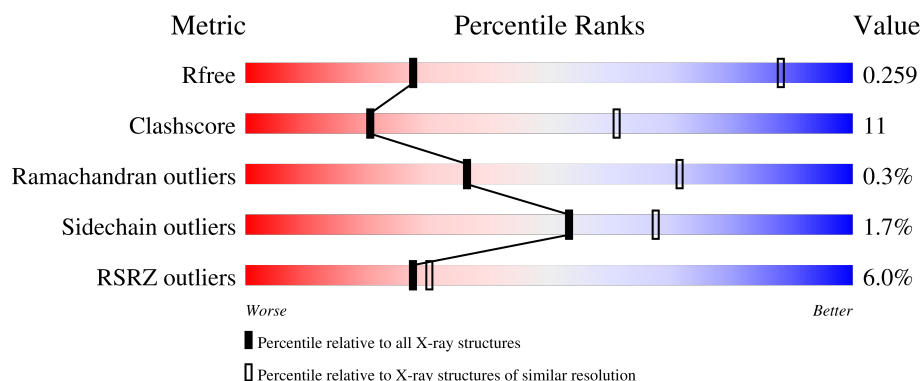
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 5.32 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.



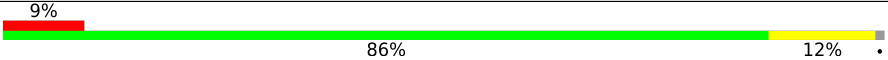
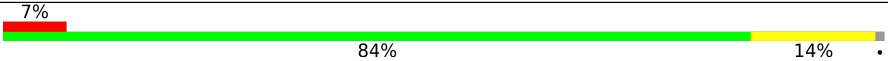
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1045 (6.64-4.00)
Clashscore	190562	1101 (6.64-4.00)
Ramachandran outliers	187476	1008 (6.64-3.96)
Sidechain outliers	187428	1012 (6.70-3.94)
RSRZ outliers	180081	1039 (6.64-4.00)

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

Mol	Chain	Length	Quality of chain
1	B	231	
1	H	231	
2	C	214	
2	L	214	
3	A	202	

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Mol	Chain	Length	Quality of chain
3	E	202	 5% 75% 17% 7%
4	D	228	 4% 78% 19% ..
4	G	228	 6% 78% 20% ..
5	F	215	 9% 86% 12% .
5	I	215	 7% 84% 14% .

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 16314 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 Beta-54 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	229	Total	C	N	O	S	0	0	0
			1706	1080	283	337	6			
1	B	229	Total	C	N	O	S	0	0	0
			1706	1080	283	337	6			

- Molecule 2 is a protein called Beta-54 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	213	Total	C	N	O	S	0	0	0
			1627	1022	270	330	5			
2	C	213	Total	C	N	O	S	0	0	0
			1627	1022	270	330	5			

- Molecule 3 is a protein called Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	187	Total	C	N	O	S	0	0	0
			1502	966	255	273	8			
3	A	187	Total	C	N	O	S	0	0	0
			1502	966	255	273	8			

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	327	HIS	-	expression tag	UNP P0DTC2
E	328	HIS	-	expression tag	UNP P0DTC2
E	329	HIS	-	expression tag	UNP P0DTC2
E	330	HIS	-	expression tag	UNP P0DTC2
E	331	HIS	-	expression tag	UNP P0DTC2
E	332	HIS	-	expression tag	UNP P0DTC2
E	339	ASP	GLY	variant	UNP P0DTC2
E	371	LEU	SER	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
E	373	PRO	SER	variant	UNP P0DTC2
E	375	PHE	SER	variant	UNP P0DTC2
E	417	ASN	LYS	variant	UNP P0DTC2
E	440	LYS	ASN	variant	UNP P0DTC2
E	446	SER	GLY	variant	UNP P0DTC2
E	477	ASN	SER	variant	UNP P0DTC2
E	478	LYS	THR	variant	UNP P0DTC2
E	484	ALA	GLU	variant	UNP P0DTC2
E	493	ARG	GLN	variant	UNP P0DTC2
E	496	SER	GLY	variant	UNP P0DTC2
E	498	ARG	GLN	conflict	UNP P0DTC2
E	501	TYR	ASN	variant	UNP P0DTC2
E	505	HIS	TYR	variant	UNP P0DTC2
E	527	LYS	-	expression tag	UNP P0DTC2
E	528	LYS	-	expression tag	UNP P0DTC2
A	327	HIS	-	expression tag	UNP P0DTC2
A	328	HIS	-	expression tag	UNP P0DTC2
A	329	HIS	-	expression tag	UNP P0DTC2
A	330	HIS	-	expression tag	UNP P0DTC2
A	331	HIS	-	expression tag	UNP P0DTC2
A	332	HIS	-	expression tag	UNP P0DTC2
A	339	ASP	GLY	variant	UNP P0DTC2
A	371	LEU	SER	variant	UNP P0DTC2
A	373	PRO	SER	variant	UNP P0DTC2
A	375	PHE	SER	variant	UNP P0DTC2
A	417	ASN	LYS	variant	UNP P0DTC2
A	440	LYS	ASN	variant	UNP P0DTC2
A	446	SER	GLY	variant	UNP P0DTC2
A	477	ASN	SER	variant	UNP P0DTC2
A	478	LYS	THR	variant	UNP P0DTC2
A	484	ALA	GLU	variant	UNP P0DTC2
A	493	ARG	GLN	variant	UNP P0DTC2
A	496	SER	GLY	variant	UNP P0DTC2
A	498	ARG	GLN	conflict	UNP P0DTC2
A	501	TYR	ASN	variant	UNP P0DTC2
A	505	HIS	TYR	variant	UNP P0DTC2
A	527	LYS	-	expression tag	UNP P0DTC2
A	528	LYS	-	expression tag	UNP P0DTC2

- Molecule 4 is a protein called Omi-12 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	224	Total 1684	C 1054	N 288	O 332	S 10	0	0	0
4	G	224	Total 1684	C 1054	N 288	O 332	S 10	0	0	0

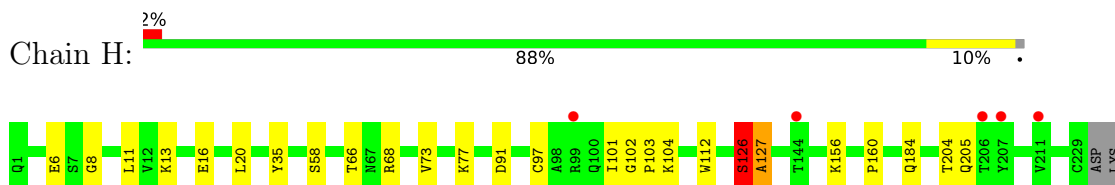
- Molecule 5 is a protein called Omi-12 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	212	Total 1638	C 1026	N 283	O 324	S 5	0	1	0
5	I	212	Total 1638	C 1026	N 283	O 324	S 5	0	1	0

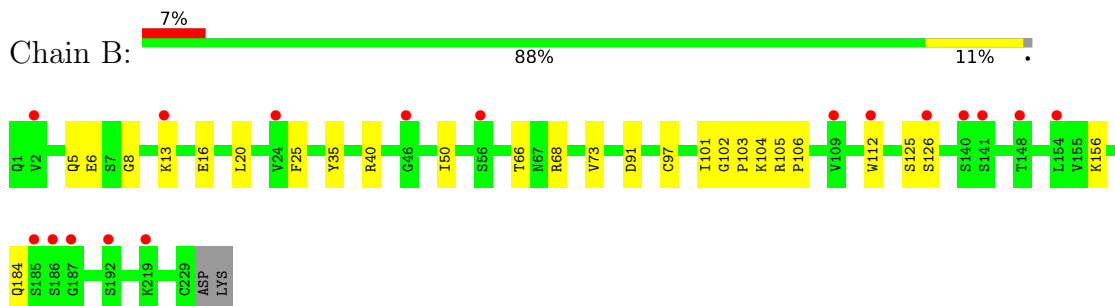
3 Residue-property plots [i](#)

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.

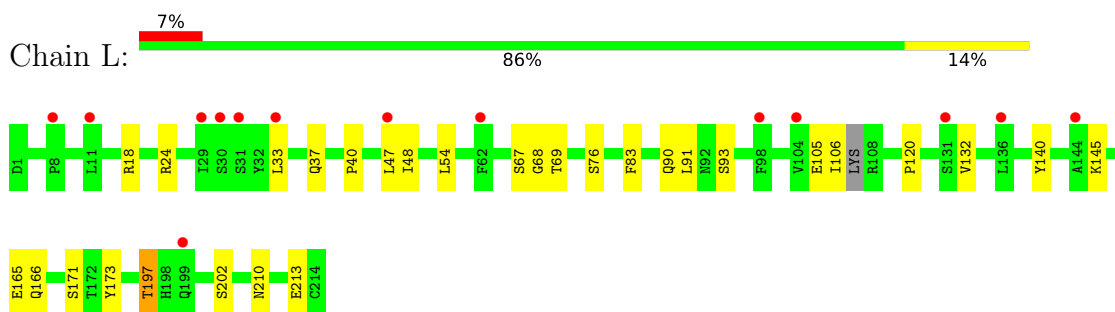
- Molecule 1: Beta-54 heavy chain



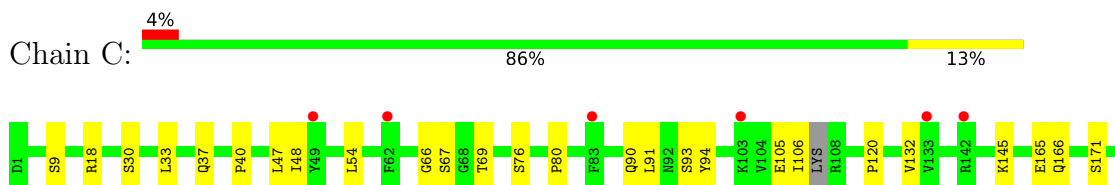
- Molecule 1: Beta-54 heavy chain



- Molecule 2: Beta-54 light chain

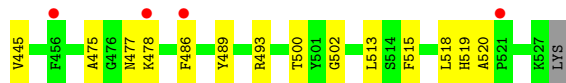
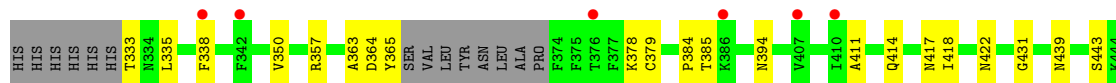
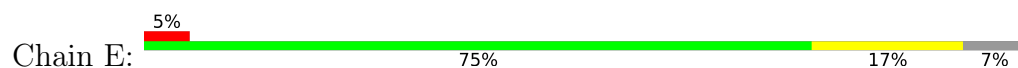


- Molecule 2: Beta-54 light chain

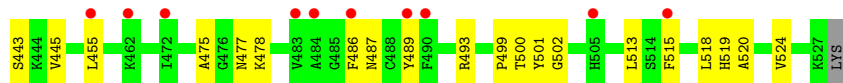
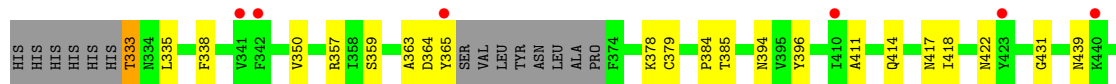
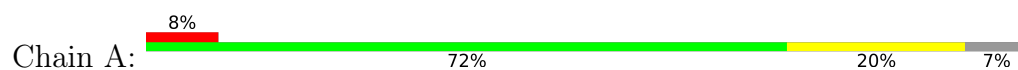




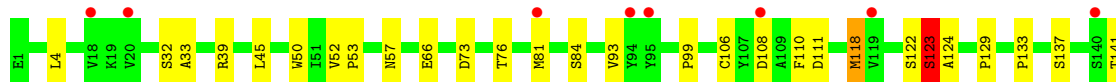
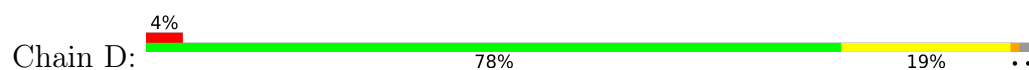
- Molecule 3: Spike protein S1



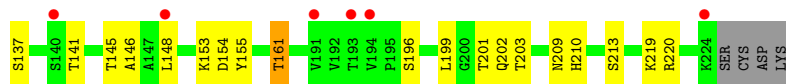
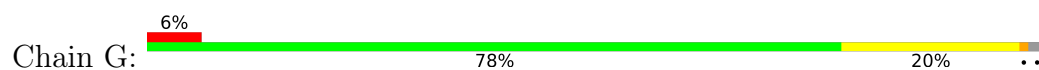
- Molecule 3: Spike protein S1



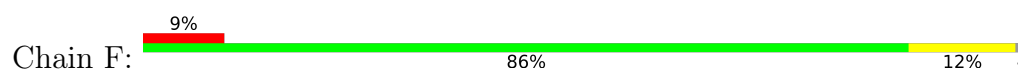
- Molecule 4: Omi-12 heavy chain

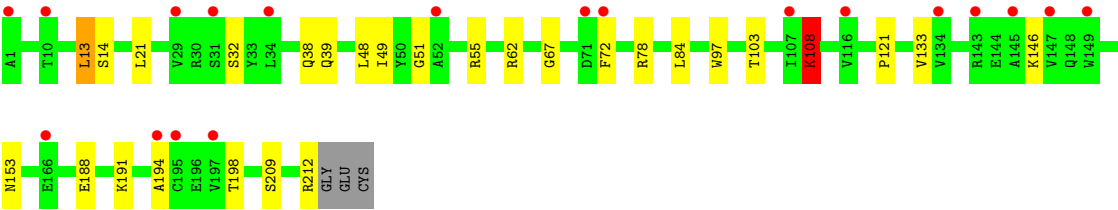


- Molecule 4: Omi-12 heavy chain

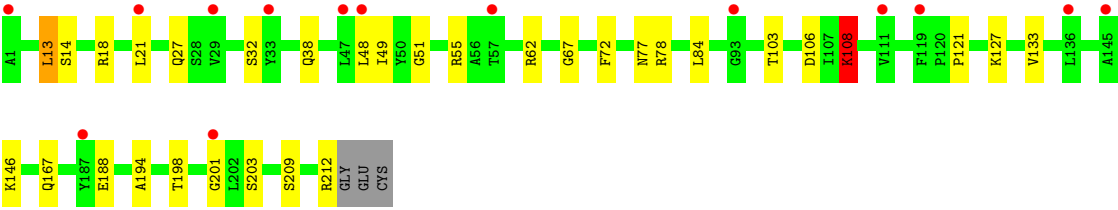
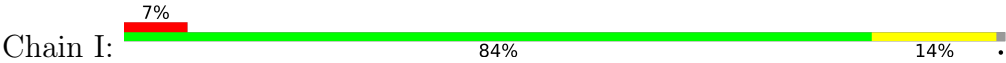


- Molecule 5: Omi-12 light chain





● Molecule 5: Omi-12 light chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	95.49Å 156.01Å 122.09Å 90.00° 90.27° 90.00°	Depositor
Resolution (Å)	95.49 – 5.32 95.49 – 5.33	Depositor EDS
% Data completeness (in resolution range)	50.2 (95.49-5.32) 50.2 (95.49-5.33)	Depositor EDS
R_{merge}	0.51	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 5.41Å)	Xtriage
Refinement program	PHENIX 1.19_4092	Depositor
R, R_{free}	0.249 , 0.256 0.246 , 0.259	Depositor DCC
R_{free} test set	321 reflections (2.48%)	wwPDB-VP
Wilson B-factor (Å ²)	70.6	Xtriage
Anisotropy	1.116	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 146.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.077 for h,-k,-l	Xtriage
F_o, F_c correlation	0.75	EDS
Total number of atoms	16314	wwPDB-VP
Average B, all atoms (Å ²)	130.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.67% 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	B	0.34	1/1752 (0.1%)	0.38	0/2399
1	H	0.19	1/1752 (0.1%)	0.43	3/2399 (0.1%)
2	C	0.22	0/1661	0.35	0/2255
2	L	0.12	0/1661	0.32	0/2255
3	A	0.11	0/1545	0.27	0/2099
3	E	0.12	0/1545	0.26	0/2099
4	D	1.01	1/1724 (0.1%)	0.38	1/2347 (0.0%)
4	G	0.20	1/1724 (0.1%)	0.61	3/2347 (0.1%)
5	F	0.21	1/1677 (0.1%)	0.46	3/2277 (0.1%)
5	I	0.27	1/1677 (0.1%)	0.38	0/2277
All	All	0.38	6/16718 (0.0%)	0.40	10/22754 (0.0%)

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	H	0	1
4	D	0	1
All	All	0	2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	123	SER	C-N	-41.34	0.76	1.33
1	B	126	SER	C-N	-12.99	1.15	1.33
5	I	108	LYS	C-N	9.50	1.45	1.33
5	F	108	LYS	C-N	-6.25	1.25	1.33
1	H	126	SER	C-N	-6.18	1.25	1.33
4	G	123	SER	C-N	-5.12	1.25	1.33

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	123	SER	O-C-N	14.93	142.12	121.97
4	G	123	SER	CA-C-N	-13.66	101.30	122.62
4	G	123	SER	C-N-CA	-13.66	101.30	122.62
5	F	108	LYS	O-C-N	10.62	135.87	122.81
4	D	123	SER	O-C-N	-8.80	111.78	122.34
1	H	126	SER	CA-C-N	-8.20	105.88	121.54
1	H	126	SER	C-N-CA	-8.20	105.88	121.54
5	F	108	LYS	CA-C-N	-7.30	109.99	122.10
5	F	108	LYS	C-N-CA	-7.30	109.99	122.10
1	H	126	SER	O-C-N	5.57	130.47	122.28

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	123	SER	Mainchain
1	H	126	SER	Mainchain

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	B	1706	0	1674	54	2
1	H	1706	0	1674	23	15
2	C	1627	0	1584	38	1
2	L	1627	0	1584	40	2
3	A	1502	0	1425	100	19
3	E	1502	0	1425	79	17
4	D	1684	0	1638	89	10
4	G	1684	0	1639	67	10
5	F	1638	0	1608	31	2
5	I	1638	0	1608	37	18
All	All	16314	0	15859	361	48

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 (361) 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)
2:L:67:SER:HB3	4:D:84:SER:CB	1.48	1.42
3:E:489:TYR:CZ	4:D:53:PRO:HD2	1.57	1.36
4:D:123:SER:C	4:D:124:ALA:CA	1.99	1.35
1:B:103:PRO:O	3:A:500:THR:CB	1.75	1.31
1:B:102:GLY:CA	3:A:500:THR:HG21	1.59	1.30
1:B:104:LYS:HA	3:A:500:THR:O	1.19	1.28
3:E:478:LYS:CD	5:F:32:SER:HB2	1.66	1.23
1:B:102:GLY:HA3	3:A:500:THR:CG2	1.70	1.22
4:D:123:SER:O	4:D:124:ALA:N	1.67	1.21
4:D:123:SER:CA	4:D:124:ALA:N	2.01	1.20
2:L:68:GLY:HA3	4:D:66:GLU:O	1.41	1.20
2:C:69:THR:OG1	4:G:66:GLU:HB2	1.39	1.20
5:I:13:LEU:C	5:I:108:LYS:HB2	1.69	1.18
2:L:69:THR:OG1	4:D:66:GLU:HB2	1.44	1.17
2:C:69:THR:OG1	4:G:66:GLU:CB	1.91	1.17
3:A:489:TYR:CZ	4:G:53:PRO:HD2	1.79	1.17
1:B:103:PRO:O	3:A:500:THR:OG1	1.59	1.16
2:C:67:SER:HB3	4:G:84:SER:CB	1.75	1.16
3:E:486:PHE:CZ	4:D:110:PHE:CZ	2.33	1.15
3:E:475:ALA:O	4:D:106:CYS:HB2	1.42	1.13
3:A:475:ALA:O	4:G:106:CYS:HB2	1.50	1.12
3:A:486:PHE:CE1	4:G:110:PHE:CZ	2.37	1.10
5:I:14:SER:N	5:I:108:LYS:HB2	1.66	1.10
3:E:486:PHE:CE1	4:D:110:PHE:CZ	2.38	1.10
3:E:478:LYS:HD2	5:F:32:SER:HB2	1.31	1.08
3:E:477:ASN:HB2	4:D:108:ASP:HB2	1.30	1.08
3:E:478:LYS:CE	5:F:32:SER:HB2	1.85	1.07
2:C:67:SER:CB	4:G:84:SER:HB3	1.86	1.06
3:E:489:TYR:CE1	4:D:52:VAL:HB	1.92	1.05
3:E:489:TYR:CZ	4:D:53:PRO:CD	2.38	1.05
3:A:489:TYR:CZ	4:G:53:PRO:CD	2.39	1.04
2:L:67:SER:CB	4:D:84:SER:HB2	1.86	1.03
1:B:103:PRO:O	3:A:500:THR:C	2.01	1.03
3:E:478:LYS:HD2	5:F:32:SER:CB	1.89	1.02
3:A:489:TYR:CE1	4:G:53:PRO:HD2	1.96	1.00
1:B:104:LYS:O	3:A:501:TYR:HA	1.61	1.00
4:D:122:SER:OG	4:D:156:PHE:HZ	1.44	0.99
4:D:122:SER:OG	4:D:156:PHE:CZ	2.17	0.97
2:C:67:SER:HB3	4:G:84:SER:HB3	0.98	0.97
2:L:67:SER:HB3	4:D:84:SER:HB2	0.98	0.96
3:E:478:LYS:HG2	4:D:108:ASP:OD1	1.65	0.95
1:B:103:PRO:O	3:A:500:THR:HB	1.64	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:489:TYR:CE2	4:D:53:PRO:HD2	2.01	0.94
3:E:489:TYR:HE1	4:D:52:VAL:HG12	1.31	0.94
1:B:104:LYS:CA	3:A:500:THR:O	2.13	0.94
2:L:67:SER:CB	4:D:84:SER:CB	2.43	0.92
2:L:68:GLY:CA	4:D:66:GLU:O	2.18	0.91
2:C:67:SER:O	4:G:67:ARG:HA	1.71	0.91
2:C:106:ILE:HB	2:C:166:GLN:HE22	1.35	0.91
2:C:67:SER:CB	4:G:84:SER:CB	2.45	0.90
1:B:104:LYS:C	3:A:501:TYR:HA	1.96	0.90
2:C:69:THR:OG1	4:G:66:GLU:HB3	1.71	0.89
3:E:478:LYS:HG2	4:D:108:ASP:CG	1.98	0.89
3:A:487:ASN:ND2	4:G:107:TYR:O	2.06	0.88
2:L:67:SER:HB3	4:D:84:SER:HB3	1.51	0.88
1:H:103:PRO:O	3:E:500:THR:O	1.93	0.87
3:E:489:TYR:CE1	4:D:52:VAL:CB	2.57	0.87
2:C:106:ILE:HB	2:C:166:GLN:NE2	1.90	0.87
1:H:35:TYR:OH	3:E:500:THR:HG23	1.74	0.87
3:E:478:LYS:HE3	5:F:32:SER:HB2	1.55	0.86
3:E:417:ASN:OD1	3:E:418:ILE:HG12	1.75	0.86
4:D:123:SER:O	4:D:124:ALA:CA	2.15	0.86
3:E:486:PHE:CE1	4:D:110:PHE:HZ	1.89	0.86
3:A:493:ARG:NH1	4:G:57:ASN:OD1	2.09	0.85
4:D:123:SER:C	4:D:124:ALA:N	0.76	0.85
3:A:417:ASN:OD1	3:A:418:ILE:HG12	1.75	0.85
3:A:489:TYR:OH	4:G:33:ALA:HB2	1.76	0.84
4:G:203:THR:HG22	4:G:220:ARG:NH2	1.92	0.84
3:E:478:LYS:CE	5:F:32:SER:CB	2.56	0.83
4:D:203:THR:HG22	4:D:220:ARG:NH2	1.92	0.83
3:E:477:ASN:HB2	4:D:108:ASP:CB	2.09	0.82
5:I:14:SER:CA	5:I:108:LYS:HB2	2.08	0.82
1:B:102:GLY:HA3	3:A:500:THR:HG21	0.86	0.82
1:B:103:PRO:O	3:A:500:THR:CA	2.27	0.81
3:E:489:TYR:HE1	4:D:52:VAL:CG1	1.93	0.81
3:A:478:LYS:CD	5:I:32:SER:HB2	2.08	0.81
3:E:477:ASN:CB	4:D:108:ASP:HB2	2.09	0.81
1:B:35:TYR:OH	3:A:499:PRO:HG2	1.80	0.80
5:I:13:LEU:C	5:I:108:LYS:CB	2.54	0.80
2:L:145:LYS:HB3	2:L:197:THR:HG22	1.64	0.80
2:C:145:LYS:HB3	2:C:197:THR:HG22	1.64	0.80
2:L:90:GLN:HE21	2:L:93:SER:H	1.30	0.79
3:E:489:TYR:CE1	4:D:52:VAL:CG1	2.66	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:13:LEU:O	5:I:108:LYS:N	2.13	0.79
2:C:90:GLN:HE21	2:C:93:SER:H	1.30	0.78
4:D:123:SER:O	4:D:124:ALA:HA	1.83	0.78
3:E:478:LYS:HE3	5:F:32:SER:CB	2.15	0.77
1:B:35:TYR:CE2	3:A:445:VAL:HG13	2.19	0.77
1:B:35:TYR:CE1	3:A:445:VAL:HG22	2.19	0.77
1:B:102:GLY:C	3:A:500:THR:HG21	2.11	0.76
3:E:489:TYR:CE2	4:D:53:PRO:CD	2.65	0.76
3:E:489:TYR:CD1	4:D:52:VAL:HB	2.20	0.76
3:E:486:PHE:CE1	4:D:33:ALA:HB3	2.21	0.75
1:H:103:PRO:O	3:E:500:THR:HB	1.86	0.75
2:C:69:THR:HG23	4:G:66:GLU:HA	1.69	0.75
3:A:478:LYS:HE3	5:I:32:SER:HB2	1.68	0.75
5:F:13:LEU:C	5:F:108:LYS:HB2	2.12	0.74
3:E:486:PHE:CZ	4:D:110:PHE:CE1	2.75	0.74
3:A:417:ASN:OD1	3:A:418:ILE:N	2.21	0.74
3:E:417:ASN:OD1	3:E:418:ILE:N	2.21	0.74
1:B:104:LYS:O	3:A:501:TYR:CA	2.36	0.74
5:F:14:SER:N	5:F:108:LYS:HB2	2.04	0.73
1:B:103:PRO:CD	3:A:500:THR:OG1	2.37	0.73
2:L:105:GLU:HG3	2:L:173:TYR:OH	1.89	0.73
1:B:104:LYS:HA	3:A:500:THR:C	2.14	0.73
3:E:489:TYR:CE1	4:D:53:PRO:HD2	2.22	0.72
3:E:489:TYR:CE1	4:D:52:VAL:HG12	2.21	0.71
1:B:35:TYR:OH	3:A:499:PRO:CG	2.38	0.71
5:I:14:SER:N	5:I:108:LYS:CB	2.51	0.71
1:B:103:PRO:C	3:A:500:THR:CB	2.64	0.70
1:H:104:LYS:HA	3:E:500:THR:O	1.92	0.70
3:A:486:PHE:CZ	4:G:110:PHE:CZ	2.79	0.70
3:A:478:LYS:CE	5:I:32:SER:HB2	2.20	0.70
2:C:67:SER:C	4:G:67:ARG:HA	2.17	0.70
1:B:103:PRO:C	3:A:500:THR:HB	2.16	0.69
3:A:478:LYS:HG2	4:G:108:ASP:CG	2.17	0.69
2:L:40:PRO:HB3	2:L:165:GLU:HG3	1.72	0.69
3:E:478:LYS:HE3	5:F:32:SER:CA	2.22	0.69
3:E:489:TYR:OH	4:D:53:PRO:CD	2.39	0.69
1:B:103:PRO:C	3:A:500:THR:OG1	2.36	0.69
4:D:161:THR:HG23	4:D:209:ASN:HB3	1.74	0.69
3:E:489:TYR:OH	4:D:53:PRO:HD3	1.92	0.69
4:D:93:VAL:HG22	4:D:118:MET:HG3	1.75	0.68
4:G:161:THR:HG23	4:G:209:ASN:HB3	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:83:PHE:CD1	2:L:166:GLN:OE1	2.46	0.68
3:A:489:TYR:CE2	4:G:53:PRO:CG	2.77	0.68
2:L:69:THR:HG23	4:D:66:GLU:HA	1.76	0.68
4:D:133:PRO:HD3	4:D:219:LYS:HE3	1.75	0.67
4:G:133:PRO:HD3	4:G:219:LYS:HE3	1.75	0.67
3:A:478:LYS:HE3	5:I:32:SER:CB	2.24	0.66
4:G:93:VAL:HG22	4:G:118:MET:HG3	1.75	0.66
5:I:14:SER:HA	5:I:108:LYS:HB2	1.77	0.66
3:A:455:LEU:HD21	4:G:54:GLY:HA3	1.77	0.66
5:I:13:LEU:O	5:I:108:LYS:HB2	1.96	0.66
3:A:489:TYR:CD1	4:G:52:VAL:HB	2.31	0.65
3:A:489:TYR:CE2	4:G:53:PRO:CD	2.79	0.65
3:E:489:TYR:CE2	4:D:53:PRO:CG	2.80	0.65
5:F:14:SER:CA	5:F:108:LYS:HB2	2.27	0.65
2:C:67:SER:O	4:G:66:GLU:O	2.12	0.65
2:C:67:SER:CB	4:G:84:SER:HB2	2.26	0.64
3:E:486:PHE:CZ	4:D:110:PHE:CE2	2.86	0.64
1:H:103:PRO:O	3:E:500:THR:C	2.41	0.64
1:H:103:PRO:O	3:E:500:THR:CB	2.45	0.64
3:A:489:TYR:CZ	4:G:53:PRO:HD3	2.32	0.64
1:B:104:LYS:O	3:A:502:GLY:N	2.31	0.64
1:H:13:LYS:HB2	1:H:16:GLU:HG3	1.81	0.63
3:E:478:LYS:HG2	4:D:108:ASP:OD2	1.99	0.63
3:A:478:LYS:HD2	5:I:32:SER:CB	2.28	0.62
3:A:478:LYS:HG2	4:G:108:ASP:OD1	1.99	0.62
1:B:103:PRO:CG	3:A:500:THR:OG1	2.48	0.62
2:C:40:PRO:HB3	2:C:165:GLU:HG3	1.81	0.62
5:F:14:SER:HA	5:F:108:LYS:HB2	1.81	0.62
1:H:11:LEU:HB2	1:H:160:PRO:HG3	1.81	0.62
1:B:103:PRO:N	3:A:500:THR:OG1	2.32	0.62
3:E:486:PHE:HD1	4:D:50:TRP:CZ3	2.18	0.61
3:A:486:PHE:CE1	4:G:110:PHE:CE1	2.88	0.61
2:L:90:GLN:NE2	2:L:93:SER:H	1.98	0.61
3:A:489:TYR:CE1	4:G:52:VAL:HB	2.35	0.61
1:H:35:TYR:CZ	3:E:500:THR:HG23	2.35	0.61
3:E:486:PHE:CE1	4:D:33:ALA:CB	2.83	0.61
1:B:13:LYS:HB2	1:B:16:GLU:HG3	1.81	0.61
1:B:68:ARG:NH2	1:B:91:ASP:OD2	2.33	0.61
1:H:68:ARG:NH2	1:H:91:ASP:OD2	2.33	0.61
3:E:478:LYS:CG	5:F:32:SER:HB2	2.29	0.60
1:B:103:PRO:HG2	3:A:500:THR:OG1	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:478:LYS:HD2	5:I:32:SER:HB2	1.84	0.60
5:I:32:SER:HA	5:I:51:GLY:HA2	1.84	0.59
3:A:478:LYS:CG	5:I:32:SER:HB2	2.32	0.59
3:A:489:TYR:CE2	4:G:53:PRO:HD2	2.33	0.59
3:A:478:LYS:HG3	5:I:32:SER:HB2	1.84	0.59
1:B:103:PRO:O	3:A:500:THR:O	2.18	0.59
2:C:69:THR:H	4:G:66:GLU:HB2	1.67	0.59
1:H:156:LYS:NZ	1:H:184:GLN:OE1	2.36	0.58
2:C:67:SER:HB2	4:G:84:SER:HB2	1.85	0.58
5:F:32:SER:HA	5:F:51:GLY:HA2	1.84	0.58
2:C:67:SER:O	4:G:67:ARG:CA	2.49	0.58
2:C:80:PRO:HB3	2:C:171:SER:OG	2.04	0.58
2:C:40:PRO:CB	2:C:165:GLU:HG3	2.34	0.58
2:C:90:GLN:NE2	2:C:93:SER:H	1.98	0.58
3:A:489:TYR:OH	4:G:53:PRO:HD3	2.03	0.58
2:L:69:THR:CB	4:D:66:GLU:HB2	2.34	0.58
1:H:35:TYR:CZ	3:E:500:THR:CG2	2.87	0.57
3:E:486:PHE:HE1	4:D:33:ALA:HB3	1.70	0.57
1:H:103:PRO:HG2	3:E:500:THR:OG1	2.04	0.56
1:B:156:LYS:NZ	1:B:184:GLN:OE1	2.36	0.56
2:C:37:GLN:HB2	2:C:47:LEU:HD11	1.87	0.56
3:A:478:LYS:CE	5:I:32:SER:CB	2.82	0.56
1:B:102:GLY:C	3:A:500:THR:CG2	2.78	0.56
4:D:123:SER:N	4:D:124:ALA:N	2.54	0.56
1:H:126:SER:C	1:H:127:ALA:O	2.48	0.56
3:E:478:LYS:HE2	4:D:108:ASP:OD2	2.06	0.56
3:E:478:LYS:HD2	5:F:32:SER:HB3	1.84	0.56
2:L:67:SER:N	4:D:84:SER:OG	2.40	0.55
2:L:37:GLN:HB2	2:L:47:LEU:HD11	1.87	0.55
3:E:478:LYS:CD	5:F:32:SER:CB	2.50	0.55
1:B:35:TYR:OH	3:A:499:PRO:HD2	2.06	0.55
3:E:486:PHE:HE1	4:D:33:ALA:CB	2.19	0.55
4:D:39:ARG:HB2	4:D:45:LEU:HD23	1.89	0.54
5:I:106:ASP:HB3	5:I:167:GLN:OE1	2.07	0.54
2:L:69:THR:N	4:D:66:GLU:O	2.40	0.54
3:A:439:ASN:O	3:A:443:SER:OG	2.22	0.54
2:L:105:GLU:OE2	2:L:140:TYR:CE2	2.60	0.54
2:C:69:THR:CB	4:G:66:GLU:HB2	2.36	0.53
4:G:39:ARG:HB2	4:G:45:LEU:HD23	1.89	0.53
1:B:35:TYR:CZ	3:A:445:VAL:HG22	2.43	0.53
3:E:493:ARG:NH1	4:D:57:ASN:OD1	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:90:GLN:NE2	2:C:93:SER:O	2.37	0.53
1:H:58:SER:OG	3:E:445:VAL:HG23	2.08	0.53
3:A:357:ARG:HH21	3:A:394:ASN:HD21	1.56	0.53
5:I:14:SER:CA	5:I:108:LYS:CB	2.85	0.53
2:L:83:PHE:CD2	2:L:166:GLN:HB3	2.44	0.53
3:E:439:ASN:O	3:E:443:SER:OG	2.22	0.53
1:B:102:GLY:C	3:A:500:THR:CB	2.82	0.52
3:E:489:TYR:OH	4:D:33:ALA:HB2	2.09	0.52
5:I:13:LEU:HA	5:I:108:LYS:HG3	1.91	0.52
5:I:121:PRO:HD3	5:I:133:VAL:HG22	1.91	0.52
2:L:106:ILE:O	2:L:140:TYR:CE2	2.63	0.52
3:E:486:PHE:CE1	4:D:110:PHE:CE1	2.97	0.52
1:H:126:SER:O	1:H:127:ALA:C	2.48	0.52
3:E:357:ARG:HH21	3:E:394:ASN:HD21	1.56	0.52
2:L:69:THR:HG1	4:D:66:GLU:HB2	1.66	0.52
5:F:121:PRO:HD3	5:F:133:VAL:HG22	1.91	0.52
1:B:103:PRO:N	3:A:500:THR:CB	2.73	0.52
3:A:478:LYS:CD	5:I:32:SER:CB	2.80	0.51
2:C:40:PRO:CG	2:C:165:GLU:HG3	2.40	0.51
3:E:486:PHE:CE2	4:D:110:PHE:CE2	2.98	0.51
1:H:104:LYS:O	3:E:502:GLY:N	2.42	0.51
3:A:486:PHE:CE1	4:G:33:ALA:HB3	2.45	0.51
2:L:90:GLN:NE2	2:L:93:SER:O	2.37	0.51
4:D:203:THR:CG2	4:D:220:ARG:NH2	2.72	0.51
1:B:35:TYR:CZ	3:A:499:PRO:HG2	2.45	0.51
3:A:364:ASP:OD1	3:A:364:ASP:N	2.39	0.50
1:B:68:ARG:HH22	1:B:91:ASP:CG	2.20	0.50
5:I:14:SER:HA	5:I:108:LYS:CB	2.41	0.50
4:G:203:THR:CG2	4:G:220:ARG:NH2	2.72	0.50
4:G:210:HIS:ND1	4:G:213:SER:OG	2.34	0.50
2:L:69:THR:CG2	4:D:66:GLU:HB2	2.42	0.50
1:H:102:GLY:HA3	3:E:500:THR:HG21	1.94	0.49
2:L:69:THR:HG23	4:D:66:GLU:CA	2.42	0.49
3:A:477:ASN:HB2	4:G:108:ASP:HB2	1.94	0.49
1:B:35:TYR:OH	3:A:499:PRO:CD	2.60	0.49
3:E:478:LYS:HE3	5:F:32:SER:HA	1.94	0.49
3:E:486:PHE:HA	4:D:50:TRP:CH2	2.47	0.49
3:A:486:PHE:CD1	4:G:110:PHE:CZ	2.97	0.49
4:D:73:ASP:HB3	4:D:76:THR:HG22	1.95	0.49
1:H:68:ARG:HH22	1:H:91:ASP:CG	2.20	0.49
2:L:106:ILE:H	2:L:166:GLN:HE22	1.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:486:PHE:HB2	5:F:97:TRP:CH2	2.48	0.49
1:B:102:GLY:CA	3:A:500:THR:CG2	2.51	0.49
4:D:196:SER:HA	4:D:199:LEU:HD23	1.95	0.49
1:B:106:PRO:HA	3:A:501:TYR:CZ	2.48	0.48
2:C:67:SER:HB2	4:G:84:SER:CB	2.35	0.48
2:L:106:ILE:HB	2:L:171:SER:HB3	1.95	0.48
1:B:103:PRO:C	3:A:500:THR:HG1	2.13	0.47
4:G:137:SER:O	4:G:141:THR:HG23	2.13	0.47
3:A:486:PHE:HE1	4:G:33:ALA:HB3	1.79	0.47
3:E:478:LYS:CG	4:D:108:ASP:OD1	2.51	0.47
4:D:137:SER:O	4:D:141:THR:HG23	2.13	0.47
4:G:196:SER:HA	4:G:199:LEU:HD23	1.95	0.47
5:F:146:LYS:HB3	5:F:198:THR:HB	1.97	0.47
4:G:73:ASP:HB3	4:G:76:THR:HG22	1.95	0.47
2:C:66:GLY:C	4:G:84:SER:OG	2.58	0.47
2:C:94:TYR:OH	3:A:445:VAL:HG12	2.15	0.47
3:A:486:PHE:CZ	4:G:110:PHE:CE2	3.02	0.47
4:G:122:SER:C	4:G:124:ALA:H	2.23	0.47
2:L:83:PHE:CG	2:L:166:GLN:HB3	2.49	0.47
1:H:8:GLY:HA3	1:H:20:LEU:HD23	1.97	0.47
5:I:49:ILE:HD13	5:I:55:ARG:HA	1.96	0.47
1:B:8:GLY:HA3	1:B:20:LEU:HD23	1.97	0.47
1:B:103:PRO:HD2	3:A:500:THR:OG1	2.14	0.46
3:A:489:TYR:CE2	4:G:53:PRO:HG3	2.50	0.46
1:B:102:GLY:C	3:A:500:THR:HB	2.40	0.46
2:L:68:GLY:C	4:D:66:GLU:O	2.59	0.46
2:L:210:ASN:HB2	2:L:213:GLU:HB2	1.97	0.46
3:A:338:PHE:HE2	3:A:363:ALA:HB1	1.81	0.46
5:I:188:GLU:OE1	5:I:212:ARG:NH1	2.49	0.46
5:F:49:ILE:HD13	5:F:55:ARG:HA	1.97	0.46
5:I:146:LYS:HB3	5:I:198:THR:HB	1.97	0.46
2:L:106:ILE:HB	2:L:166:GLN:NE2	2.31	0.46
3:E:350:VAL:HG22	3:E:422:ASN:HB3	1.98	0.46
2:L:18:ARG:HG3	2:L:76:SER:HA	1.98	0.45
3:E:338:PHE:HE2	3:E:363:ALA:HB1	1.81	0.45
4:D:122:SER:CB	4:D:156:PHE:CZ	2.97	0.45
5:F:188:GLU:OE1	5:F:212:ARG:NH1	2.49	0.45
3:E:364:ASP:OD1	3:E:364:ASP:N	2.39	0.45
3:A:350:VAL:HG22	3:A:422:ASN:HB3	1.98	0.45
3:A:379:CYS:SG	3:A:384:PRO:HG3	2.56	0.45
2:C:210:ASN:HB2	2:C:213:GLU:HB2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:32:SER:OG	4:G:99:PRO:O	2.33	0.45
1:B:103:PRO:CA	3:A:500:THR:OG1	2.65	0.45
2:C:30:SER:OG	4:G:69:THR:HG21	2.17	0.45
3:E:379:CYS:SG	3:E:384:PRO:HG3	2.56	0.45
3:A:478:LYS:HD2	5:I:32:SER:HB3	1.97	0.45
5:I:13:LEU:CA	5:I:108:LYS:HG3	2.47	0.45
1:B:106:PRO:HA	3:A:501:TYR:OH	2.17	0.45
2:C:18:ARG:HG3	2:C:76:SER:HA	1.98	0.45
4:D:122:SER:OG	4:D:156:PHE:CE2	2.68	0.45
3:A:489:TYR:HE1	4:G:52:VAL:HG12	1.81	0.45
3:A:489:TYR:CE1	4:G:52:VAL:CB	3.00	0.44
3:A:486:PHE:CE1	4:G:110:PHE:HZ	2.17	0.44
1:B:105:ARG:C	3:A:501:TYR:CE1	2.95	0.44
3:A:478:LYS:HG2	4:G:108:ASP:OD2	2.16	0.44
3:A:478:LYS:HE3	5:I:32:SER:CA	2.48	0.44
2:C:120:PRO:HD3	2:C:132:VAL:HG22	2.00	0.44
3:A:431:GLY:HA2	3:A:515:PHE:HD2	1.83	0.44
2:L:69:THR:CG2	4:D:66:GLU:CB	2.96	0.44
4:D:210:HIS:ND1	4:D:213:SER:OG	2.34	0.44
5:F:67:GLY:HA3	5:F:72:PHE:HA	2.00	0.43
3:E:486:PHE:HB2	5:F:97:TRP:CZ2	2.54	0.43
4:D:81:MET:HE3	4:D:81:MET:HB3	1.88	0.43
4:D:146:ALA:HB3	4:D:199:LEU:HD21	2.00	0.43
1:B:101:ILE:HG21	1:B:112:TRP:CE2	2.54	0.43
4:D:122:SER:CB	4:D:156:PHE:HZ	2.29	0.43
3:E:486:PHE:HD1	4:D:50:TRP:CE3	2.36	0.43
1:H:101:ILE:HG21	1:H:112:TRP:CE2	2.54	0.43
4:G:146:ALA:HB3	4:G:199:LEU:HD21	2.00	0.43
2:L:83:PHE:CE2	2:L:166:GLN:HB3	2.53	0.43
2:L:120:PRO:HD3	2:L:132:VAL:HG22	2.00	0.43
5:I:67:GLY:HA3	5:I:72:PHE:HA	2.00	0.43
3:E:431:GLY:HA2	3:E:515:PHE:HD2	1.83	0.43
5:I:194:ALA:HB2	5:I:209:SER:HB3	2.01	0.43
1:B:13:LYS:HA	1:B:125:SER:O	2.19	0.42
5:F:194:ALA:HB2	5:F:209:SER:HB3	2.01	0.42
2:L:67:SER:CB	4:D:84:SER:HB3	2.35	0.42
3:E:486:PHE:CD1	5:F:97:TRP:HH2	2.38	0.42
4:D:111:ASP:OD1	4:D:111:ASP:N	2.53	0.42
3:E:411:ALA:HB3	3:E:414:GLN:HG3	2.02	0.42
3:E:486:PHE:HA	4:D:50:TRP:CZ3	2.54	0.42
4:D:39:ARG:NH1	5:F:39:GLN:OE1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:105:GLU:OE2	2:L:140:TYR:HE2	2.00	0.42
5:F:62:ARG:HD2	5:F:78:ARG:O	2.20	0.42
4:G:153:LYS:HG2	4:G:154:ASP:CG	2.45	0.42
1:H:6:GLU:HB3	1:H:97:CYS:SG	2.60	0.42
1:B:6:GLU:HB3	1:B:97:CYS:SG	2.60	0.42
3:A:411:ALA:HB3	3:A:414:GLN:HG3	2.01	0.42
4:D:32:SER:OG	4:D:99:PRO:O	2.33	0.41
2:C:48:ILE:HD13	2:C:54:LEU:HA	2.02	0.41
5:I:62:ARG:HD2	5:I:78:ARG:O	2.20	0.41
4:D:153:LYS:HG2	4:D:154:ASP:CG	2.45	0.41
3:E:478:LYS:HE3	5:F:32:SER:O	2.20	0.41
2:C:69:THR:N	4:G:66:GLU:HB2	2.35	0.41
2:C:105:GLU:HG2	2:C:106:ILE:N	2.35	0.41
5:I:38:GLN:HB2	5:I:48:LEU:HD11	2.03	0.41
1:H:77:LYS:HE2	1:H:77:LYS:HB3	1.88	0.41
5:F:38:GLN:HB2	5:F:48:LEU:HD11	2.03	0.41
4:G:81:MET:HE3	4:G:81:MET:HB3	1.89	0.41
1:B:104:LYS:O	3:A:501:TYR:C	2.64	0.41
4:D:199:LEU:HD13	4:D:199:LEU:HA	1.96	0.41
5:I:13:LEU:C	5:I:108:LYS:CG	2.93	0.41
5:I:18:ARG:NH1	5:I:77:ASN:OD1	2.54	0.41
5:I:21:LEU:HD23	5:I:103:THR:HB	2.02	0.41
3:A:333:THR:O	3:A:333:THR:OG1	2.35	0.41
5:F:21:LEU:HD23	5:F:103:THR:HB	2.02	0.40
4:G:129:PRO:HB3	4:G:155:TYR:HB3	2.03	0.40
2:L:48:ILE:HD13	2:L:54:LEU:HA	2.02	0.40
2:L:105:GLU:HG2	2:L:106:ILE:N	2.35	0.40
2:C:69:THR:OG1	4:G:66:GLU:OE1	2.39	0.40
4:D:129:PRO:HB3	4:D:155:TYR:HB3	2.03	0.40
3:A:359:SER:HA	3:A:524:VAL:HG22	2.04	0.40
1:B:35:TYR:CE1	3:A:499:PRO:HG2	2.56	0.40
1:B:40:ARG:HB3	1:B:50:ILE:HD11	2.03	0.40

All (48) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:378:LYS:CD	3:A:378:LYS:CD[2_445]	0.24	1.96
1:H:204:THR:CA	5:I:127:LYS:CE[2_444]	0.73	1.47
1:H:204:THR:CA	5:I:127:LYS:NZ[2_444]	0.76	1.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:204:THR:CB	5:I:127:LYS:NZ[2_444]	1.04	1.16
4:D:201:THR:O	4:G:201:THR:C[2_445]	1.04	1.16
1:H:204:THR:C	5:I:127:LYS:CE[2_444]	1.09	1.11
3:E:378:LYS:CB	3:A:378:LYS:NZ[2_445]	1.10	1.10
4:D:201:THR:O	4:G:201:THR:O[2_445]	1.10	1.10
1:H:204:THR:C	5:I:127:LYS:CD[2_444]	1.16	1.04
3:E:378:LYS:NZ	3:A:378:LYS:CG[2_445]	1.19	1.01
3:E:378:LYS:CE	3:A:378:LYS:CG[2_445]	1.20	1.00
3:E:378:LYS:CG	3:A:378:LYS:NZ[2_445]	1.23	0.97
3:E:378:LYS:CG	3:A:378:LYS:CE[2_445]	1.23	0.97
3:E:378:LYS:NZ	3:A:378:LYS:CB[2_445]	1.23	0.97
4:D:201:THR:C	4:G:201:THR:O[2_445]	1.23	0.97
1:H:204:THR:O	5:I:127:LYS:CD[2_444]	1.37	0.83
3:E:378:LYS:CD	3:A:378:LYS:CE[2_445]	1.40	0.80
3:E:378:LYS:CD	3:A:378:LYS:CG[2_445]	1.43	0.77
1:H:204:THR:N	5:I:127:LYS:CE[2_444]	1.44	0.76
3:E:378:LYS:CG	3:A:378:LYS:CD[2_445]	1.45	0.75
3:E:378:LYS:CE	3:A:378:LYS:CD[2_445]	1.48	0.72
3:E:365:TYR:O	3:A:385:THR:CG2[2_445]	1.64	0.56
3:E:365:TYR:O	3:A:385:THR:CB[2_445]	1.64	0.56
3:E:385:THR:CG2	3:A:365:TYR:O[2_445]	1.77	0.43
4:D:201:THR:CA	4:G:201:THR:CB[2_445]	1.81	0.39
1:H:205:GLN:N	5:I:127:LYS:CE[2_444]	1.82	0.38
4:D:201:THR:C	4:G:201:THR:C[2_445]	1.82	0.38
1:H:204:THR:CG2	5:I:127:LYS:NZ[2_444]	1.87	0.33
4:D:202:GLN:N	4:G:201:THR:O[2_445]	1.87	0.33
2:L:24:ARG:NH2	5:I:27:GLN:CA[1_655]	1.89	0.31
1:B:5:GLN:OE1	5:I:203:SER:O[1_655]	1.89	0.31
1:H:204:THR:N	5:I:127:LYS:NZ[2_444]	1.90	0.30
4:D:201:THR:CA	4:G:201:THR:CA[2_445]	1.92	0.28
1:H:204:THR:CA	5:I:127:LYS:CD[2_444]	1.93	0.27
4:D:201:THR:O	4:G:202:GLN:N[2_445]	1.93	0.27
3:E:378:LYS:CB	3:A:378:LYS:CE[2_445]	1.99	0.21
4:D:201:THR:CB	4:G:201:THR:CA[2_445]	1.99	0.21
3:E:385:THR:CB	3:A:365:TYR:O[2_445]	2.00	0.20
1:H:205:GLN:N	5:I:127:LYS:CD[2_444]	2.03	0.17
3:E:378:LYS:CE	3:A:378:LYS:CB[2_445]	2.03	0.17
4:D:201:THR:O	4:G:201:THR:CA[2_445]	2.04	0.16
1:H:204:THR:C	5:I:127:LYS:NZ[2_444]	2.09	0.11
1:B:25:PHE:CE1	5:I:201:GLY:O[1_655]	2.11	0.09
1:H:204:THR:CB	5:I:127:LYS:CE[2_444]	2.14	0.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:202:SER:O	2:C:9:SER:OG[1_655]	2.17	0.03
1:H:204:THR:O	5:I:127:LYS:CE[2_444]	2.18	0.02
3:A:357:ARG:NH1	5:F:191:LYS:NZ[1_455]	2.18	0.02
3:A:396:TYR:OH	5:F:153:ASN:ND2[1_455]	2.18	0.02

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	B	227/231 (98%)	213 (94%)	13 (6%)	1 (0%)	30	67
1	H	227/231 (98%)	213 (94%)	12 (5%)	2 (1%)	14	49
2	C	209/214 (98%)	202 (97%)	7 (3%)	0	100	100
2	L	209/214 (98%)	202 (97%)	7 (3%)	0	100	100
3	A	183/202 (91%)	170 (93%)	11 (6%)	2 (1%)	11	45
3	E	183/202 (91%)	170 (93%)	11 (6%)	2 (1%)	11	45
4	D	222/228 (97%)	212 (96%)	10 (4%)	0	100	100
4	G	222/228 (97%)	211 (95%)	11 (5%)	0	100	100
5	F	211/215 (98%)	205 (97%)	6 (3%)	0	100	100
5	I	211/215 (98%)	205 (97%)	6 (3%)	0	100	100
All	All	2104/2180 (96%)	2003 (95%)	94 (4%)	7 (0%)	36	71

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	127	ALA
3	E	519	HIS
3	A	519	HIS
3	E	520	ALA
3	A	520	ALA

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Mol	Chain	Res	Type
1	H	66	THR
1	B	66	THR

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	B	197/200 (98%)	196 (100%)	1 (0%)	81	82
1	H	197/200 (98%)	196 (100%)	1 (0%)	81	82
2	C	185/186 (100%)	182 (98%)	3 (2%)	55	69
2	L	185/186 (100%)	182 (98%)	3 (2%)	55	69
3	A	162/177 (92%)	158 (98%)	4 (2%)	42	61
3	E	162/177 (92%)	158 (98%)	4 (2%)	42	61
4	D	190/195 (97%)	185 (97%)	5 (3%)	40	60
4	G	190/195 (97%)	185 (97%)	5 (3%)	40	60
5	F	184/185 (100%)	181 (98%)	3 (2%)	55	69
5	I	184/185 (100%)	181 (98%)	3 (2%)	55	69
All	All	1836/1886 (97%)	1804 (98%)	32 (2%)	53	67

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	73	VAL
2	L	33	LEU
2	L	91	LEU
2	L	197	THR
1	B	73	VAL
2	C	33	LEU
2	C	91	LEU
2	C	197	THR
3	E	333	THR
3	E	335	LEU
3	E	513	LEU

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Mol	Chain	Res	Type
3	E	518	LEU
3	A	333	THR
3	A	335	LEU
3	A	513	LEU
3	A	518	LEU
4	D	4	LEU
4	D	118	MET
4	D	145	THR
4	D	148	LEU
4	D	161	THR
5	F	13	LEU
5	F	84	LEU
5	F	108	LYS
4	G	4	LEU
4	G	118	MET
4	G	145	THR
4	G	148	LEU
4	G	161	THR
5	I	13	LEU
5	I	84	LEU
5	I	108	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
2	L	37	GLN
2	L	160	GLN
2	L	166	GLN
2	C	160	GLN
4	D	174	HIS
5	F	138	ASN
4	G	174	HIS
5	I	138	ASN

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1
4	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	126:SER	C	127:ALA	N	1.15
1	D	123:SER	C	124:ALA	N	0.76

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	B	229/231 (99%)	0.33	17 (7%)	20	25	62, 131, 220, 270	0
1	H	229/231 (99%)	0.20	5 (2%)	62	51	80, 128, 173, 230	0
2	C	213/214 (99%)	0.35	9 (4%)	40	38	63, 154, 235, 268	0
2	L	213/214 (99%)	0.35	14 (6%)	24	27	79, 120, 156, 175	0
3	A	187/202 (92%)	0.45	16 (8%)	16	21	60, 125, 172, 233	0
3	E	187/202 (92%)	0.31	10 (5%)	32	32	92, 140, 188, 243	0
4	D	224/228 (98%)	0.33	9 (4%)	42	39	66, 125, 187, 276	0
4	G	224/228 (98%)	0.45	14 (6%)	26	29	64, 113, 187, 245	0
5	F	212/215 (98%)	0.45	19 (8%)	15	20	78, 124, 154, 171	1 (0%)
5	I	212/215 (98%)	0.32	14 (6%)	24	27	63, 122, 157, 183	1 (0%)
All	All	2130/2180 (97%)	0.35	127 (5%)	27	30	60, 126, 195, 276	2 (0%)

All (127) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	I	1	ALA	10.0
4	D	108	ASP	7.6
3	A	484	ALA	6.6
1	B	2	VAL	6.3
5	F	1	ALA	5.8
3	A	486	PHE	5.6
2	L	33	LEU	5.5
2	C	62	PHE	5.3
4	D	20	VAL	5.2
1	B	186	SER	5.0
2	C	49	TYR	4.8
5	F	166	GLU	4.7
3	A	515	PHE	4.7

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Mol	Chain	Res	Type	RSRZ
4	G	71	THR	4.7
5	I	93	GLY	4.6
3	E	342	PHE	4.4
1	B	126	SER	4.2
4	G	94	TYR	3.9
2	L	47	LEU	3.9
2	L	98	PHE	3.9
2	L	11	LEU	3.8
4	D	94	TYR	3.8
3	A	410	ILE	3.7
4	G	108	ASP	3.7
4	D	18	VAL	3.7
3	E	486	PHE	3.6
5	I	111	VAL	3.6
1	H	207	TYR	3.5
4	D	81	MET	3.5
2	L	144	ALA	3.5
4	D	203	THR	3.5
5	I	187	TYR	3.4
3	E	456	PHE	3.4
5	F	143	ARG	3.4
5	F	34	LEU	3.3
5	F	116	VAL	3.2
3	A	440	LYS	3.2
3	A	490	PHE	3.2
4	D	140	SER	3.2
5	I	48	LEU	3.2
4	D	119	VAL	3.2
2	L	199	GLN	3.1
1	B	112	TRP	3.1
5	F	72	PHE	3.1
4	G	56	GLY	3.1
2	L	136	LEU	3.1
2	L	62	PHE	3.1
3	E	410	ILE	3.1
5	F	29	VAL	3.0
4	G	136	PRO	3.0
5	F	10	THR	3.0
5	F	149	TRP	2.9
1	H	211	VAL	2.8
5	I	136	LEU	2.8
1	H	99	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
2	C	103	LYS	2.8
3	A	483	VAL	2.7
5	F	71	ASP	2.7
5	F	107	ILE	2.7
3	A	365	TYR	2.7
3	A	341	VAL	2.7
1	B	154	LEU	2.7
5	I	47	LEU	2.7
5	I	33	TYR	2.6
5	F	134	VAL	2.6
5	F	145	ALA	2.6
2	C	186	TYR	2.6
5	I	201	GLY	2.6
1	B	148	THR	2.6
4	G	148	LEU	2.6
1	B	56	SER	2.6
3	E	376	THR	2.6
5	F	52	ALA	2.5
2	L	31	SER	2.5
4	G	193	THR	2.5
1	B	141	SER	2.5
3	E	338	PHE	2.5
5	F	31	SER	2.5
2	L	29	ILE	2.4
4	D	95	TYR	2.4
3	A	462	LYS	2.4
4	G	127	LYS	2.4
5	F	194	ALA	2.4
3	E	478	LYS	2.4
4	G	140	SER	2.4
3	A	505	HIS	2.4
4	G	24	ALA	2.4
5	I	29	VAL	2.4
3	E	386	LYS	2.4
2	L	131	SER	2.4
1	B	187	GLY	2.3
2	C	142	ARG	2.3
5	I	21	LEU	2.3
3	E	521	PRO	2.3
5	I	145	ALA	2.3
4	G	194	VAL	2.3
5	F	197	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
3	A	342	PHE	2.3
2	C	192	TYR	2.2
3	A	423	TYR	2.2
2	L	8	PRO	2.2
5	F	147	VAL	2.2
5	F	195	CYS	2.2
1	B	140	SER	2.2
3	A	472	ILE	2.2
1	B	109	VAL	2.2
4	G	191	VAL	2.2
2	C	180	THR	2.1
2	L	30	SER	2.1
4	G	65	GLN	2.1
1	B	24	VAL	2.1
2	L	104	VAL	2.1
3	A	489	TYR	2.1
1	B	192	SER	2.1
3	E	407	VAL	2.1
1	H	206	THR	2.1
2	C	83	PHE	2.1
1	B	13	LYS	2.1
1	B	46	GLY	2.1
5	I	57	THR	2.1
5	I	119	PHE	2.0
2	C	133	VAL	2.0
4	G	224	LYS	2.0
1	H	144	THR	2.0
1	B	219	LYS	2.0
3	A	455	LEU	2.0
1	B	185	SER	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

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.