



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:59 PM UTC

PDB ID : 4KSS / pdb_00004kss
Title : Crystal Structure of Vibrio cholerae ATPase GspsE Hexamer
Authors : Hol, W.G.; Turley, S.; Lu, C.Y.; Park, Y.J.
Deposited on : 2013-05-17
Resolution : 7.58 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:

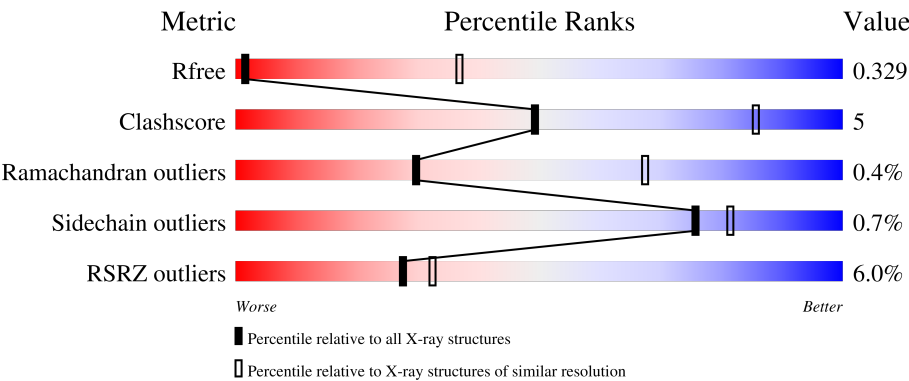
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 7.58 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	1167 (10.00-4.00)
Clashscore	190562	1000 (10.00-4.06)
Ramachandran outliers	187476	1054 (10.00-4.00)
Sidechain outliers	187428	1017 (10.00-4.00)
RSRZ outliers	180081	1161 (10.00-4.00)

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	A	581	5% 83% 6% 10%
1	B	581	4% 83% 6% 10%
1	C	581	4% 83% 6% 10%
1	D	581	7% 83% 6% 10%
1	E	581	5% 84% 5% 10%

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Mol	Chain	Length	Quality of chain
1	F	581	8% 83% 6% • 10%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 24126 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 Type II secretion system protein E, hemolysin-coregulated protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	521	Total	C	N	O	S	0	0	0
			4021	2508	724	767	22			
1	B	521	Total	C	N	O	S	0	0	0
			4021	2508	724	767	22			
1	C	521	Total	C	N	O	S	0	0	0
			4021	2508	724	767	22			
1	D	521	Total	C	N	O	S	0	0	0
			4021	2508	724	767	22			
1	E	521	Total	C	N	O	S	0	0	0
			4021	2508	724	767	22			
1	F	521	Total	C	N	O	S	0	0	0
			4021	2508	724	767	22			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	99	MET	-	expression tag	UNP P37093
A	504	GLY	-	linker	UNP P37093
A	505	SER	-	linker	UNP P37093
A	506	GLY	-	linker	UNP P37093
A	507	SER	-	linker	UNP P37093
A	508	GLY	-	linker	UNP P37093
A	509	SER	-	linker	UNP P37093
A	510	GLY	-	linker	UNP P37093
A	672	LEU	-	expression tag	UNP Q02UZ4
A	673	GLU	-	expression tag	UNP Q02UZ4
A	674	HIS	-	expression tag	UNP Q02UZ4
A	675	HIS	-	expression tag	UNP Q02UZ4
A	676	HIS	-	expression tag	UNP Q02UZ4
A	677	HIS	-	expression tag	UNP Q02UZ4
A	678	HIS	-	expression tag	UNP Q02UZ4
A	679	HIS	-	expression tag	UNP Q02UZ4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	99	MET	-	expression tag	UNP P37093
B	504	GLY	-	linker	UNP P37093
B	505	SER	-	linker	UNP P37093
B	506	GLY	-	linker	UNP P37093
B	507	SER	-	linker	UNP P37093
B	508	GLY	-	linker	UNP P37093
B	509	SER	-	linker	UNP P37093
B	510	GLY	-	linker	UNP P37093
B	672	LEU	-	expression tag	UNP Q02UZ4
B	673	GLU	-	expression tag	UNP Q02UZ4
B	674	HIS	-	expression tag	UNP Q02UZ4
B	675	HIS	-	expression tag	UNP Q02UZ4
B	676	HIS	-	expression tag	UNP Q02UZ4
B	677	HIS	-	expression tag	UNP Q02UZ4
B	678	HIS	-	expression tag	UNP Q02UZ4
B	679	HIS	-	expression tag	UNP Q02UZ4
C	99	MET	-	expression tag	UNP P37093
C	504	GLY	-	linker	UNP P37093
C	505	SER	-	linker	UNP P37093
C	506	GLY	-	linker	UNP P37093
C	507	SER	-	linker	UNP P37093
C	508	GLY	-	linker	UNP P37093
C	509	SER	-	linker	UNP P37093
C	510	GLY	-	linker	UNP P37093
C	672	LEU	-	expression tag	UNP Q02UZ4
C	673	GLU	-	expression tag	UNP Q02UZ4
C	674	HIS	-	expression tag	UNP Q02UZ4
C	675	HIS	-	expression tag	UNP Q02UZ4
C	676	HIS	-	expression tag	UNP Q02UZ4
C	677	HIS	-	expression tag	UNP Q02UZ4
C	678	HIS	-	expression tag	UNP Q02UZ4
C	679	HIS	-	expression tag	UNP Q02UZ4
D	99	MET	-	expression tag	UNP P37093
D	504	GLY	-	linker	UNP P37093
D	505	SER	-	linker	UNP P37093
D	506	GLY	-	linker	UNP P37093
D	507	SER	-	linker	UNP P37093
D	508	GLY	-	linker	UNP P37093
D	509	SER	-	linker	UNP P37093
D	510	GLY	-	linker	UNP P37093
D	672	LEU	-	expression tag	UNP Q02UZ4
D	673	GLU	-	expression tag	UNP Q02UZ4

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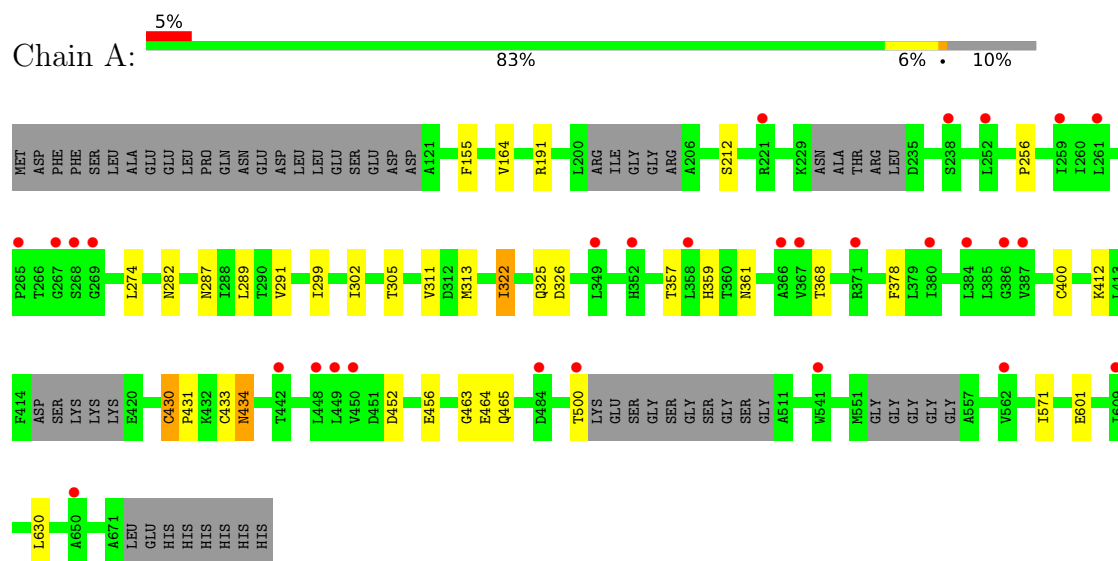
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Chain	Residue	Modelled	Actual	Comment	Reference
D	674	HIS	-	expression tag	UNP Q02UZ4
D	675	HIS	-	expression tag	UNP Q02UZ4
D	676	HIS	-	expression tag	UNP Q02UZ4
D	677	HIS	-	expression tag	UNP Q02UZ4
D	678	HIS	-	expression tag	UNP Q02UZ4
D	679	HIS	-	expression tag	UNP Q02UZ4
E	99	MET	-	expression tag	UNP P37093
E	504	GLY	-	linker	UNP P37093
E	505	SER	-	linker	UNP P37093
E	506	GLY	-	linker	UNP P37093
E	507	SER	-	linker	UNP P37093
E	508	GLY	-	linker	UNP P37093
E	509	SER	-	linker	UNP P37093
E	510	GLY	-	linker	UNP P37093
E	672	LEU	-	expression tag	UNP Q02UZ4
E	673	GLU	-	expression tag	UNP Q02UZ4
E	674	HIS	-	expression tag	UNP Q02UZ4
E	675	HIS	-	expression tag	UNP Q02UZ4
E	676	HIS	-	expression tag	UNP Q02UZ4
E	677	HIS	-	expression tag	UNP Q02UZ4
E	678	HIS	-	expression tag	UNP Q02UZ4
E	679	HIS	-	expression tag	UNP Q02UZ4
F	99	MET	-	expression tag	UNP P37093
F	504	GLY	-	linker	UNP P37093
F	505	SER	-	linker	UNP P37093
F	506	GLY	-	linker	UNP P37093
F	507	SER	-	linker	UNP P37093
F	508	GLY	-	linker	UNP P37093
F	509	SER	-	linker	UNP P37093
F	510	GLY	-	linker	UNP P37093
F	672	LEU	-	expression tag	UNP Q02UZ4
F	673	GLU	-	expression tag	UNP Q02UZ4
F	674	HIS	-	expression tag	UNP Q02UZ4
F	675	HIS	-	expression tag	UNP Q02UZ4
F	676	HIS	-	expression tag	UNP Q02UZ4
F	677	HIS	-	expression tag	UNP Q02UZ4
F	678	HIS	-	expression tag	UNP Q02UZ4
F	679	HIS	-	expression tag	UNP Q02UZ4

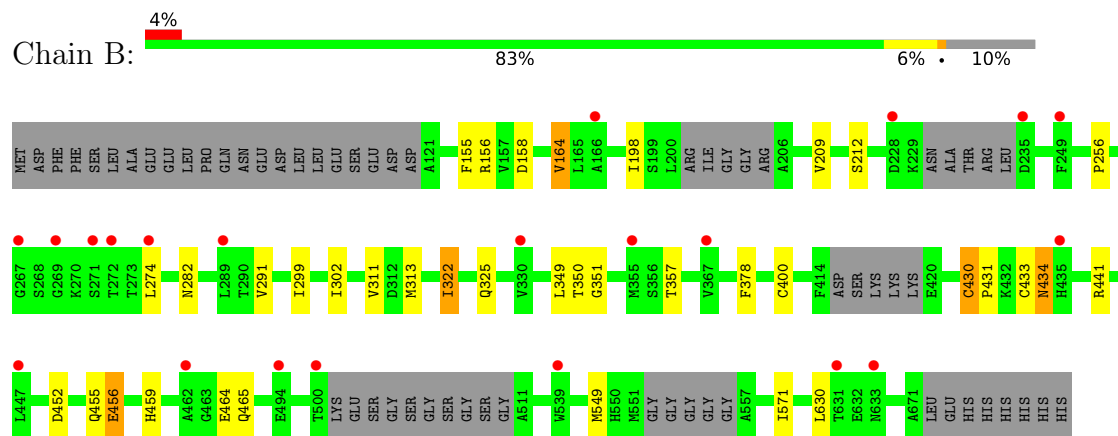
3 Residue-property plots [i](#)

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.

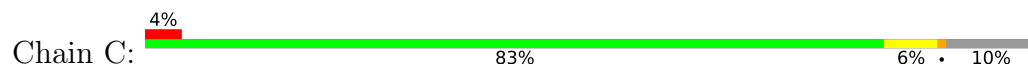
- Molecule 1: Type II secretion system protein E, hemolysin-coregulated protein

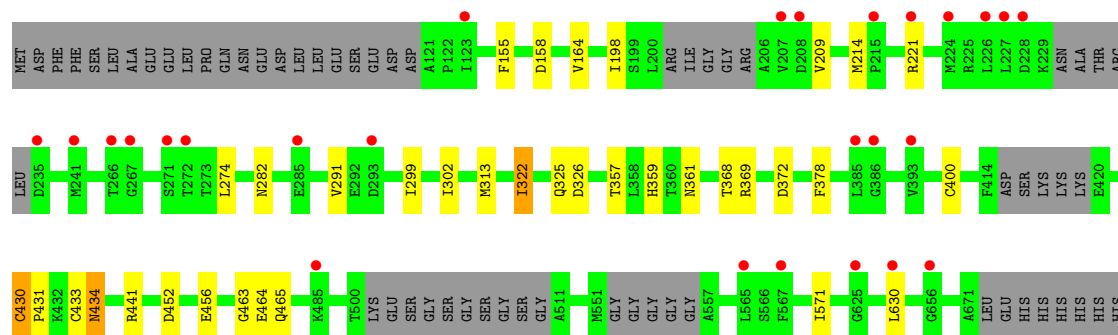


- Molecule 1: Type II secretion system protein E, hemolysin-coregulated protein

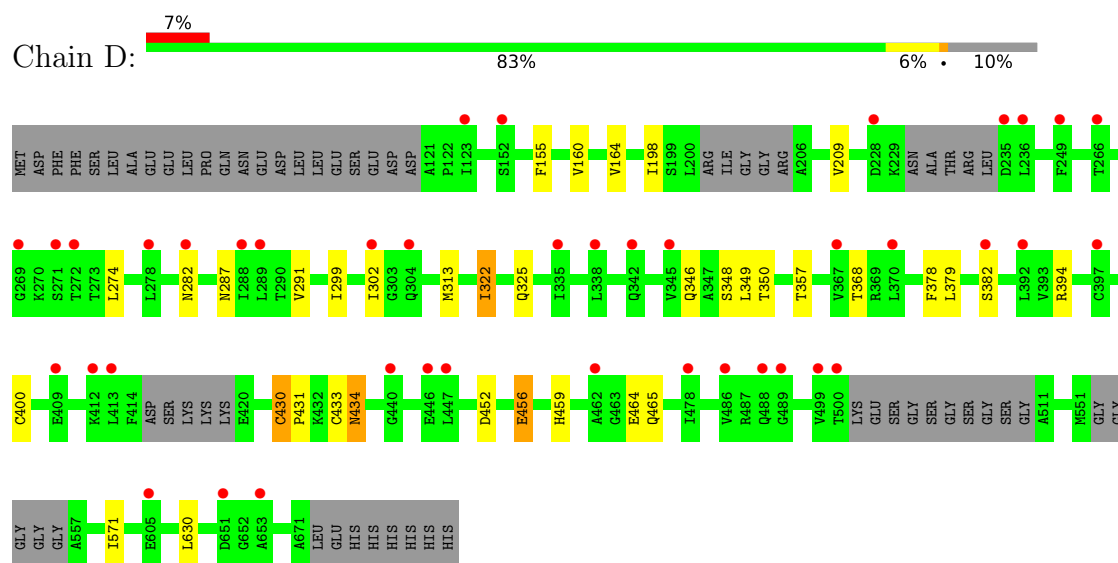


- Molecule 1: Type II secretion system protein E, hemolysin-coregulated protein

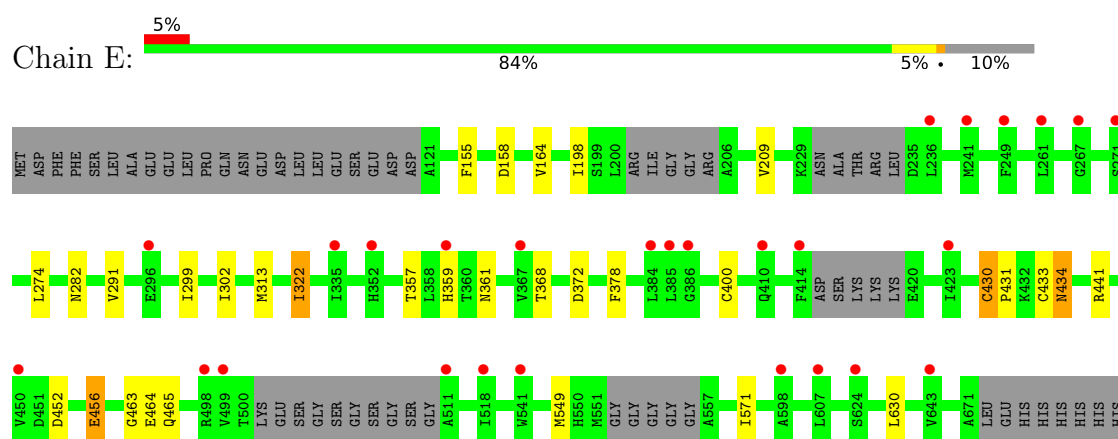




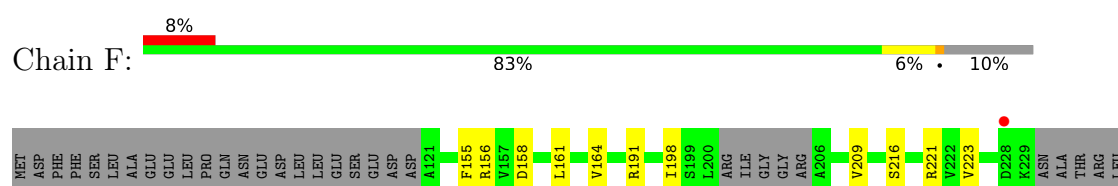
- Molecule 1: Type II secretion system protein E, hemolysin-coregulated protein

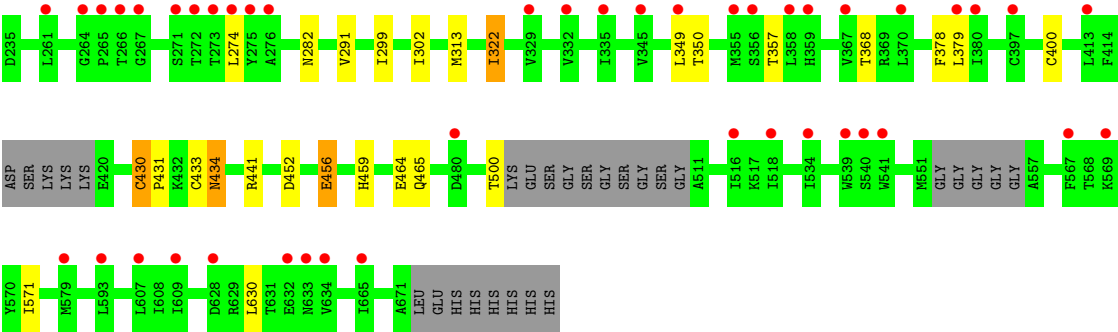


- Molecule 1: Type II secretion system protein E, hemolysin-coregulated protein



- Molecule 1: Type II secretion system protein E, hemolysin-coregulated protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α , β , γ	205.06Å 205.06Å 234.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 7.58 50.00 – 7.58	Depositor EDS
% Data completeness (in resolution range)	99.0 (50.00-7.58) 99.1 (50.00-7.58)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.22 (at 7.37Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.349 , 0.360 0.328 , 0.329	Depositor DCC
R_{free} test set	308 reflections (4.64%)	wwPDB-VP
Wilson B-factor (Å ²)	281.2	Xtriage
Anisotropy	0.061	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 235.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.71	EDS
Total number of atoms	24126	wwPDB-VP
Average B, all atoms (Å ²)	166.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.06% 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	0.40	0/4074	0.65	1/5491 (0.0%)
1	B	0.40	0/4074	0.65	1/5491 (0.0%)
1	C	0.40	0/4074	0.65	1/5491 (0.0%)
1	D	0.40	0/4074	0.65	1/5491 (0.0%)
1	E	0.40	0/4074	0.65	1/5491 (0.0%)
1	F	0.40	0/4074	0.65	1/5491 (0.0%)
All	All	0.40	0/24444	0.65	6/32946 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	430	CYS	CA-CB-SG	5.57	127.22	114.40
1	F	430	CYS	CA-CB-SG	5.56	127.19	114.40
1	C	430	CYS	CA-CB-SG	5.55	127.17	114.40
1	B	430	CYS	CA-CB-SG	5.55	127.16	114.40
1	E	430	CYS	CA-CB-SG	5.54	127.15	114.40
1	A	430	CYS	CA-CB-SG	5.53	127.13	114.40

There are no chirality outliers.

There are no planarity outliers.

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	4021	0	4099	68	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	4021	0	4099	57	0
1	C	4021	0	4097	75	0
1	D	4021	0	4098	81	0
1	E	4021	0	4099	55	0
1	F	4021	0	4099	68	0
All	All	24126	0	24591	262	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 5.

All (262) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:464:GLU:CG	1:D:378:PHE:HE1	1.07	1.66
1:C:463:GLY:CA	1:D:459:HIS:CE1	1.92	1.50
1:C:464:GLU:HG3	1:D:378:PHE:CE1	0.97	1.50
1:C:463:GLY:HA2	1:D:459:HIS:CE1	1.47	1.47
1:E:464:GLU:HG3	1:F:378:PHE:CE1	1.47	1.45
1:C:464:GLU:CG	1:D:378:PHE:CE1	1.82	1.44
1:D:430:CYS:SG	1:D:431:PRO:HD2	1.63	1.39
1:A:430:CYS:SG	1:A:431:PRO:HD2	1.63	1.37
1:B:430:CYS:SG	1:B:431:PRO:HD2	1.63	1.37
1:E:430:CYS:SG	1:E:431:PRO:HD2	1.63	1.37
1:F:430:CYS:SG	1:F:431:PRO:HD2	1.63	1.36
1:C:430:CYS:SG	1:C:431:PRO:HD2	1.63	1.36
1:A:464:GLU:HG3	1:B:378:PHE:CE1	1.61	1.33
1:C:464:GLU:HG3	1:D:378:PHE:CZ	1.72	1.23
1:A:326:ASP:OD2	1:F:156:ARG:NE	1.76	1.18
1:E:430:CYS:SG	1:E:431:PRO:CD	2.33	1.17
1:F:430:CYS:SG	1:F:431:PRO:CD	2.33	1.17
1:D:430:CYS:SG	1:D:431:PRO:CD	2.33	1.16
1:B:430:CYS:SG	1:B:431:PRO:CD	2.33	1.16
1:A:430:CYS:SG	1:A:431:PRO:CD	2.33	1.15
1:C:430:CYS:SG	1:C:431:PRO:CD	2.33	1.15
1:C:463:GLY:HA3	1:D:459:HIS:CE1	1.77	1.14
1:B:158:ASP:O	1:B:441:ARG:NH2	1.81	1.12
1:E:464:GLU:CG	1:F:378:PHE:HE1	1.62	1.12
1:B:465:GLN:NE2	1:C:452:ASP:O	1.83	1.11
1:A:400:CYS:SG	1:A:430:CYS:HB3	2.00	1.01
1:F:400:CYS:SG	1:F:430:CYS:HB3	2.00	1.01
1:B:400:CYS:SG	1:B:430:CYS:HB3	2.01	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:400:CYS:SG	1:C:430:CYS:HB3	2.00	1.00
1:D:400:CYS:SG	1:D:430:CYS:HB3	2.00	1.00
1:E:400:CYS:SG	1:E:430:CYS:HB3	2.00	1.00
1:C:463:GLY:HA2	1:D:459:HIS:HE1	1.26	0.99
1:E:464:GLU:CG	1:F:378:PHE:CE1	2.41	0.99
1:A:311:VAL:HG11	1:F:191:ARG:HB3	1.43	0.98
1:C:464:GLU:CG	1:D:378:PHE:CZ	2.38	0.96
1:A:452:ASP:O	1:F:465:GLN:NE2	1.99	0.95
1:A:464:GLU:HG3	1:B:378:PHE:CZ	2.01	0.95
1:C:465:GLN:OE1	1:D:456:GLU:HB2	1.67	0.94
1:A:464:GLU:CG	1:B:378:PHE:HE1	1.80	0.94
1:C:463:GLY:HA2	1:D:459:HIS:NE2	1.81	0.94
1:E:430:CYS:HG	1:E:431:PRO:HD2	0.90	0.94
1:A:463:GLY:HA2	1:B:459:HIS:CE1	2.02	0.93
1:C:463:GLY:CA	1:D:459:HIS:NE2	2.31	0.93
1:C:368:THR:HG23	1:D:378:PHE:CE2	2.04	0.92
1:D:430:CYS:HG	1:D:431:PRO:HD2	0.90	0.92
1:C:464:GLU:HG2	1:D:378:PHE:HE1	1.32	0.92
1:F:158:ASP:HB3	1:F:441:ARG:NH1	1.85	0.91
1:C:465:GLN:CD	1:D:456:GLU:HB2	1.95	0.90
1:F:158:ASP:O	1:F:441:ARG:NH1	2.05	0.90
1:A:463:GLY:CA	1:B:459:HIS:CE1	2.54	0.89
1:A:465:GLN:CD	1:B:452:ASP:O	2.16	0.88
1:C:464:GLU:HG2	1:D:378:PHE:CE1	2.02	0.87
1:C:464:GLU:H	1:D:459:HIS:CE1	1.93	0.87
1:A:465:GLN:HE22	1:B:456:GLU:N	1.74	0.86
1:E:464:GLU:HG3	1:F:378:PHE:CZ	2.10	0.86
1:A:464:GLU:CG	1:B:378:PHE:CE1	2.51	0.86
1:A:465:GLN:NE2	1:B:456:GLU:N	2.23	0.86
1:D:368:THR:HG23	1:E:378:PHE:CZ	2.11	0.84
1:D:368:THR:HG23	1:E:378:PHE:CE2	2.13	0.84
1:A:465:GLN:NE2	1:B:452:ASP:O	2.11	0.83
1:C:464:GLU:N	1:D:459:HIS:CE1	2.46	0.83
1:E:463:GLY:HA2	1:F:459:HIS:CE1	2.14	0.83
1:C:368:THR:HG23	1:D:378:PHE:HE2	1.44	0.82
1:A:464:GLU:HG3	1:B:378:PHE:HE1	1.06	0.81
1:C:463:GLY:C	1:D:459:HIS:CE1	2.59	0.80
1:C:359:HIS:O	1:D:350:THR:HG22	1.83	0.79
1:E:463:GLY:CA	1:F:459:HIS:CE1	2.66	0.79
1:F:158:ASP:O	1:F:441:ARG:NH2	2.15	0.79
1:E:368:THR:HG23	1:F:378:PHE:CE2	2.17	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:465:GLN:HE22	1:B:456:GLU:H	1.28	0.78
1:C:464:GLU:OE2	1:D:378:PHE:HZ	1.66	0.78
1:C:464:GLU:OE2	1:D:382:SER:HB3	1.84	0.77
1:C:464:GLU:OE2	1:D:378:PHE:CZ	2.37	0.77
1:B:158:ASP:HB3	1:B:441:ARG:NH1	2.00	0.76
1:A:378:PHE:HE1	1:F:464:GLU:HG3	1.48	0.76
1:D:464:GLU:HG3	1:E:378:PHE:HE1	1.50	0.75
1:C:463:GLY:CA	1:D:459:HIS:HE1	1.86	0.75
1:C:368:THR:CG2	1:D:378:PHE:CE2	2.70	0.75
1:A:430:CYS:SG	1:A:431:PRO:HD3	2.27	0.74
1:A:463:GLY:HA2	1:B:459:HIS:HE1	1.52	0.74
1:D:430:CYS:O	1:D:434:ASN:N	2.21	0.74
1:A:430:CYS:O	1:A:434:ASN:N	2.21	0.74
1:D:368:THR:CG2	1:E:378:PHE:CZ	2.70	0.74
1:A:378:PHE:CE2	1:F:368:THR:HG23	2.22	0.74
1:C:368:THR:CG2	1:D:378:PHE:HE2	1.99	0.74
1:F:158:ASP:HB3	1:F:441:ARG:CZ	2.18	0.74
1:B:430:CYS:SG	1:B:431:PRO:HD3	2.27	0.73
1:C:463:GLY:HA3	1:D:459:HIS:NE2	2.01	0.73
1:F:430:CYS:SG	1:F:431:PRO:HD3	2.27	0.73
1:B:430:CYS:O	1:B:434:ASN:N	2.21	0.73
1:A:463:GLY:HA3	1:B:459:HIS:CE1	2.23	0.73
1:F:158:ASP:O	1:F:441:ARG:CZ	2.37	0.73
1:E:430:CYS:O	1:E:434:ASN:N	2.21	0.72
1:A:325:GLN:OE1	1:F:223:VAL:HG23	1.89	0.72
1:C:430:CYS:O	1:C:434:ASN:N	2.21	0.72
1:F:430:CYS:O	1:F:434:ASN:N	2.21	0.72
1:C:464:GLU:CB	1:D:378:PHE:HE1	1.97	0.72
1:D:430:CYS:SG	1:D:431:PRO:HD3	2.27	0.72
1:E:430:CYS:SG	1:E:431:PRO:HD3	2.27	0.72
1:C:430:CYS:SG	1:C:431:PRO:HD3	2.27	0.72
1:B:158:ASP:HB3	1:B:441:ARG:CZ	2.20	0.71
1:C:465:GLN:CD	1:D:456:GLU:CB	2.64	0.69
1:C:158:ASP:O	1:C:441:ARG:NH2	2.25	0.69
1:A:378:PHE:CZ	1:F:368:THR:HG23	2.27	0.69
1:A:465:GLN:OE1	1:B:452:ASP:O	2.11	0.69
1:A:412:LYS:HE2	1:A:601:GLU:OE2	1.93	0.68
1:F:400:CYS:SG	1:F:433:CYS:HB3	2.34	0.68
1:D:400:CYS:SG	1:D:433:CYS:HB3	2.34	0.68
1:A:400:CYS:SG	1:A:433:CYS:HB3	2.34	0.67
1:C:400:CYS:SG	1:C:433:CYS:HB3	2.34	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:400:CYS:SG	1:E:433:CYS:HB3	2.34	0.67
1:F:400:CYS:HG	1:F:430:CYS:HB3	1.57	0.67
1:B:400:CYS:SG	1:B:433:CYS:HB3	2.34	0.67
1:D:400:CYS:HG	1:D:430:CYS:HB3	1.57	0.67
1:E:464:GLU:HG3	1:F:378:PHE:HE1	0.75	0.67
1:C:372:ASP:CG	1:D:379:LEU:HD21	2.20	0.66
1:C:464:GLU:N	1:D:459:HIS:HE1	1.94	0.66
1:C:368:THR:OG1	1:D:378:PHE:CZ	2.49	0.65
1:C:464:GLU:OE2	1:D:382:SER:CB	2.44	0.65
1:E:465:GLN:HE22	1:F:456:GLU:N	1.94	0.65
1:D:465:GLN:NE2	1:E:452:ASP:O	2.29	0.65
1:C:464:GLU:CD	1:D:378:PHE:CZ	2.73	0.65
1:B:212:SER:O	1:C:325:GLN:NE2	2.29	0.63
1:C:372:ASP:OD2	1:D:379:LEU:HD21	1.98	0.63
1:A:326:ASP:OD2	1:F:156:ARG:CD	2.45	0.63
1:E:465:GLN:NE2	1:F:456:GLU:N	2.47	0.63
1:D:368:THR:CG2	1:E:378:PHE:CE2	2.82	0.62
1:A:361:ASN:OD1	1:B:351:GLY:HA2	1.99	0.62
1:A:368:THR:HG23	1:B:378:PHE:CE2	2.35	0.62
1:A:500:THR:O	1:B:256:PRO:HG2	1.99	0.62
1:E:400:CYS:HG	1:E:430:CYS:HB3	1.65	0.61
1:A:400:CYS:SG	1:A:430:CYS:CB	2.85	0.61
1:E:400:CYS:SG	1:E:430:CYS:CB	2.85	0.60
1:A:378:PHE:CE1	1:F:464:GLU:HG3	2.35	0.59
1:F:400:CYS:SG	1:F:430:CYS:CB	2.85	0.59
1:C:158:ASP:C	1:C:441:ARG:NH2	2.61	0.59
1:C:463:GLY:HA3	1:D:459:HIS:ND1	2.15	0.59
1:C:400:CYS:HG	1:C:430:CYS:HB3	1.68	0.58
1:E:463:GLY:HA3	1:F:459:HIS:CE1	2.38	0.58
1:E:465:GLN:NE2	1:F:452:ASP:O	2.37	0.58
1:A:400:CYS:HG	1:A:430:CYS:HB3	1.70	0.57
1:B:400:CYS:SG	1:B:430:CYS:CB	2.85	0.57
1:C:465:GLN:CD	1:D:452:ASP:O	2.47	0.57
1:E:368:THR:HG23	1:F:378:PHE:HE2	1.70	0.57
1:C:400:CYS:SG	1:C:430:CYS:CB	2.85	0.57
1:A:464:GLU:CG	1:B:378:PHE:CZ	2.83	0.56
1:A:359:HIS:O	1:B:350:THR:HG22	2.06	0.56
1:D:400:CYS:SG	1:D:430:CYS:CB	2.85	0.55
1:A:378:PHE:CZ	1:F:368:THR:CG2	2.89	0.55
1:E:359:HIS:O	1:F:350:THR:HG22	2.07	0.55
1:E:464:GLU:OE2	1:F:378:PHE:HZ	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:GLN:OE1	1:F:223:VAL:CG2	2.55	0.54
1:A:325:GLN:HB3	1:F:221:ARG:HH21	1.74	0.53
1:E:368:THR:CG2	1:F:378:PHE:CE2	2.90	0.52
1:A:400:CYS:SG	1:A:433:CYS:SG	3.08	0.52
1:B:400:CYS:SG	1:B:433:CYS:SG	3.08	0.52
1:C:400:CYS:SG	1:C:433:CYS:SG	3.08	0.52
1:A:465:GLN:NE2	1:B:455:GLN:HB2	2.25	0.52
1:A:500:THR:C	1:B:256:PRO:HG2	2.33	0.52
1:E:465:GLN:HE22	1:F:456:GLU:H	1.58	0.52
1:C:464:GLU:CD	1:D:378:PHE:HZ	2.13	0.52
1:A:361:ASN:ND2	1:B:349:LEU:O	2.42	0.52
1:F:400:CYS:SG	1:F:433:CYS:SG	3.08	0.52
1:E:400:CYS:SG	1:E:433:CYS:SG	3.08	0.51
1:F:158:ASP:CB	1:F:441:ARG:CZ	2.88	0.51
1:D:400:CYS:SG	1:D:433:CYS:SG	3.08	0.51
1:C:369:ARG:NH1	1:D:346:GLN:NE2	2.59	0.50
1:A:287:ASN:HB2	1:F:161:LEU:HD11	1.93	0.50
1:D:465:GLN:HE22	1:E:456:GLU:HB2	1.76	0.50
1:D:571:ILE:HD12	1:D:630:LEU:HB2	1.94	0.50
1:F:291:VAL:HG23	1:F:322:ILE:HD12	1.94	0.50
1:C:291:VAL:HG23	1:C:322:ILE:HD12	1.94	0.49
1:D:291:VAL:HG23	1:D:322:ILE:HD12	1.94	0.49
1:A:291:VAL:HG23	1:A:322:ILE:HD12	1.94	0.49
1:A:465:GLN:NE2	1:B:455:GLN:C	2.70	0.49
1:B:291:VAL:HG23	1:B:322:ILE:HD12	1.94	0.49
1:B:571:ILE:HD12	1:B:630:LEU:HB2	1.95	0.49
1:C:155:PHE:CD2	1:C:164:VAL:HG11	2.48	0.49
1:E:291:VAL:HG23	1:E:322:ILE:HD12	1.94	0.49
1:A:500:THR:O	1:B:256:PRO:CG	2.61	0.48
1:C:464:GLU:H	1:D:459:HIS:HE1	1.46	0.48
1:A:368:THR:HG23	1:B:378:PHE:HE2	1.78	0.48
1:E:361:ASN:ND2	1:F:349:LEU:O	2.46	0.48
1:C:571:ILE:HD12	1:C:630:LEU:HB2	1.95	0.48
1:A:311:VAL:HG11	1:F:191:ARG:CB	2.31	0.48
1:A:465:GLN:HE21	1:B:455:GLN:CB	2.27	0.48
1:B:158:ASP:O	1:B:441:ARG:CZ	2.58	0.48
1:A:378:PHE:CE2	1:F:368:THR:CG2	2.94	0.47
1:E:463:GLY:HA2	1:F:459:HIS:HE1	1.75	0.47
1:B:156:ARG:NE	1:C:326:ASP:OD2	2.48	0.47
1:E:372:ASP:CG	1:F:379:LEU:HD21	2.40	0.47
1:D:368:THR:HG21	1:E:378:PHE:CZ	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:THR:HG23	1:F:216:SER:HA	1.96	0.46
1:B:465:GLN:CD	1:C:452:ASP:O	2.53	0.46
1:A:256:PRO:HG2	1:F:500:THR:O	2.16	0.46
1:C:214:MET:HB2	1:D:325:GLN:NE2	2.30	0.46
1:E:465:GLN:HE22	1:F:456:GLU:HB2	1.81	0.46
1:E:571:ILE:HD12	1:E:630:LEU:HB2	1.97	0.46
1:A:326:ASP:O	1:F:156:ARG:NH2	2.49	0.46
1:D:368:THR:CG2	1:E:378:PHE:HZ	2.26	0.46
1:A:191:ARG:HB3	1:B:311:VAL:HG11	1.97	0.46
1:A:256:PRO:HG2	1:F:500:THR:C	2.41	0.46
1:C:361:ASN:ND2	1:D:348:SER:O	2.49	0.46
1:C:368:THR:OG1	1:D:378:PHE:HZ	1.98	0.46
1:C:464:GLU:CB	1:D:378:PHE:CE1	2.84	0.46
1:E:465:GLN:NE2	1:F:456:GLU:HB2	2.31	0.45
1:A:361:ASN:OD1	1:B:351:GLY:CA	2.63	0.45
1:D:160:VAL:HG21	1:D:394:ARG:CZ	2.45	0.45
1:A:571:ILE:HD12	1:A:630:LEU:HB2	1.99	0.45
1:C:463:GLY:HA3	1:D:459:HIS:CD2	2.51	0.45
1:E:291:VAL:CG2	1:E:322:ILE:HD12	2.47	0.45
1:A:400:CYS:SG	1:A:433:CYS:CB	3.05	0.45
1:D:291:VAL:CG2	1:D:322:ILE:HD12	2.47	0.45
1:D:155:PHE:CD2	1:D:164:VAL:HG11	2.51	0.45
1:B:400:CYS:SG	1:B:433:CYS:CB	3.04	0.45
1:C:291:VAL:CG2	1:C:322:ILE:HD12	2.47	0.45
1:C:369:ARG:HH11	1:D:346:GLN:HE22	1.64	0.44
1:D:299:ILE:HG21	1:D:302:ILE:HD12	1.99	0.44
1:B:155:PHE:CD2	1:B:164:VAL:HG11	2.52	0.44
1:E:368:THR:CG2	1:F:378:PHE:HE2	2.30	0.44
1:E:400:CYS:SG	1:E:433:CYS:CB	3.04	0.44
1:C:361:ASN:ND2	1:D:349:LEU:O	2.50	0.44
1:F:291:VAL:CG2	1:F:322:ILE:HD12	2.47	0.44
1:F:299:ILE:HG21	1:F:302:ILE:HD12	1.99	0.44
1:B:464:GLU:HG3	1:C:378:PHE:HE1	1.83	0.44
1:E:299:ILE:HG21	1:E:302:ILE:HD12	1.99	0.44
1:E:464:GLU:CG	1:F:378:PHE:CZ	2.88	0.44
1:A:155:PHE:CD2	1:A:164:VAL:HG11	2.53	0.44
1:B:299:ILE:HG21	1:B:302:ILE:HD12	2.00	0.44
1:A:465:GLN:NE2	1:B:455:GLN:CB	2.81	0.44
1:C:299:ILE:HG21	1:C:302:ILE:HD12	2.00	0.44
1:A:299:ILE:HG21	1:A:302:ILE:HD12	1.99	0.44
1:B:291:VAL:CG2	1:B:322:ILE:HD12	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:400:CYS:SG	1:C:433:CYS:CB	3.04	0.44
1:A:291:VAL:CG2	1:A:322:ILE:HD12	2.47	0.43
1:F:571:ILE:HD12	1:F:630:LEU:HB2	2.00	0.43
1:A:212:SER:O	1:B:325:GLN:NE2	2.48	0.43
1:A:289:LEU:HD21	1:F:221:ARG:CZ	2.48	0.43
1:C:221:ARG:NH2	1:D:287:ASN:HD21	2.17	0.43
1:E:464:GLU:OE2	1:F:378:PHE:CZ	2.70	0.43
1:F:198:ILE:HB	1:F:209:VAL:HG22	2.01	0.43
1:E:155:PHE:CD2	1:E:164:VAL:HG11	2.55	0.42
1:F:155:PHE:CD2	1:F:164:VAL:HG11	2.53	0.42
1:D:400:CYS:SG	1:D:433:CYS:CB	3.04	0.42
1:D:464:GLU:HG3	1:E:378:PHE:CE1	2.41	0.42
1:D:198:ILE:HB	1:D:209:VAL:HG22	2.02	0.41
1:A:274:LEU:HD11	1:A:357:THR:HG23	2.02	0.41
1:D:400:CYS:HG	1:D:430:CYS:CB	2.27	0.41
1:F:400:CYS:SG	1:F:433:CYS:CB	3.04	0.41
1:C:464:GLU:N	1:D:459:HIS:ND1	2.67	0.41
1:D:274:LEU:HD11	1:D:357:THR:HG23	2.02	0.41
1:F:274:LEU:HD11	1:F:357:THR:HG23	2.02	0.41
1:E:198:ILE:HB	1:E:209:VAL:HG22	2.02	0.41
1:C:198:ILE:HB	1:C:209:VAL:HG22	2.03	0.41
1:E:549:MET:HE2	1:E:549:MET:HA	2.03	0.41
1:B:274:LEU:HD11	1:B:357:THR:HG23	2.03	0.40
1:C:369:ARG:NH1	1:D:346:GLN:HE22	2.19	0.40
1:B:549:MET:HE2	1:B:549:MET:HA	2.04	0.40
1:E:158:ASP:O	1:E:441:ARG:NH2	2.54	0.40
1:B:198:ILE:HB	1:B:209:VAL:HG22	2.03	0.40
1:C:274:LEU:HD11	1:C:357:THR:HG23	2.02	0.40
1:E:274:LEU:HD11	1:E:357:THR:HG23	2.02	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	509/581 (88%)	490 (96%)	17 (3%)	2 (0%)	30	67
1	B	509/581 (88%)	488 (96%)	19 (4%)	2 (0%)	30	67
1	C	509/581 (88%)	490 (96%)	17 (3%)	2 (0%)	30	67
1	D	509/581 (88%)	490 (96%)	17 (3%)	2 (0%)	30	67
1	E	509/581 (88%)	490 (96%)	17 (3%)	2 (0%)	30	67
1	F	509/581 (88%)	484 (95%)	23 (4%)	2 (0%)	30	67
All	All	3054/3486 (88%)	2932 (96%)	110 (4%)	12 (0%)	30	67

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	282	ASN
1	B	282	ASN
1	C	282	ASN
1	D	282	ASN
1	E	282	ASN
1	F	282	ASN
1	A	434	ASN
1	B	434	ASN
1	C	434	ASN
1	D	434	ASN
1	E	434	ASN
1	F	434	ASN

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	444/491 (90%)	441 (99%)	3 (1%)	76	81
1	B	444/491 (90%)	440 (99%)	4 (1%)	70	79
1	C	444/491 (90%)	441 (99%)	3 (1%)	76	81
1	D	444/491 (90%)	441 (99%)	3 (1%)	76	81
1	E	444/491 (90%)	441 (99%)	3 (1%)	76	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	444/491 (90%)	441 (99%)	3 (1%)	76	81
All	All	2664/2946 (90%)	2645 (99%)	19 (1%)	76	81

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	313	MET
1	A	322	ILE
1	A	456	GLU
1	B	164	VAL
1	B	313	MET
1	B	322	ILE
1	B	456	GLU
1	C	313	MET
1	C	322	ILE
1	C	456	GLU
1	D	313	MET
1	D	322	ILE
1	D	456	GLU
1	E	313	MET
1	E	322	ILE
1	E	456	GLU
1	F	313	MET
1	F	322	ILE
1	F	456	GLU

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	143	HIS
1	A	246	HIS
1	A	287	ASN
1	A	306	GLN
1	A	359	HIS
1	A	390	GLN
1	A	465	GLN
1	A	577	ASN
1	A	646	GLN
1	B	143	HIS
1	B	218	HIS
1	B	246	HIS

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Mol	Chain	Res	Type
1	B	287	ASN
1	B	306	GLN
1	B	359	HIS
1	B	390	GLN
1	B	459	HIS
1	B	577	ASN
1	B	646	GLN
1	C	143	HIS
1	C	246	HIS
1	C	287	ASN
1	C	306	GLN
1	C	359	HIS
1	C	390	GLN
1	C	563	GLN
1	C	577	ASN
1	C	646	GLN
1	D	143	HIS
1	D	246	HIS
1	D	287	ASN
1	D	306	GLN
1	D	325	GLN
1	D	346	GLN
1	D	390	GLN
1	D	459	HIS
1	D	465	GLN
1	D	577	ASN
1	D	646	GLN
1	D	670	GLN
1	E	143	HIS
1	E	246	HIS
1	E	306	GLN
1	E	325	GLN
1	E	346	GLN
1	E	390	GLN
1	E	465	GLN
1	E	577	ASN
1	E	646	GLN
1	F	143	HIS
1	F	246	HIS
1	F	287	ASN
1	F	306	GLN
1	F	346	GLN

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Mol	Chain	Res	Type
1	F	359	HIS
1	F	390	GLN
1	F	459	HIS
1	F	465	GLN
1	F	577	ASN
1	F	646	GLN
1	F	668	ASN
1	F	670	GLN

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	521/581 (89%)	0.29	29 (5%)	30	34	119, 174, 258, 384	0
1	B	521/581 (89%)	0.22	21 (4%)	42	41	75, 139, 253, 363	0
1	C	521/581 (89%)	0.20	26 (4%)	34	35	88, 170, 268, 376	0
1	D	521/581 (89%)	0.34	41 (7%)	18	25	69, 160, 262, 407	0
1	E	521/581 (89%)	0.22	27 (5%)	33	35	69, 153, 250, 404	0
1	F	521/581 (89%)	0.35	45 (8%)	16	23	89, 155, 247, 400	0
All	All	3126/3486 (89%)	0.27	189 (6%)	27	32	69, 161, 259, 407	0

All (189) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	384	LEU	7.7
1	A	450	VAL	5.7
1	F	335	ILE	5.5
1	A	384	LEU	5.3
1	F	609	ILE	5.2
1	D	413	LEU	5.1
1	D	271	SER	4.9
1	C	293	ASP	4.5
1	D	651	ASP	4.5
1	C	227	LEU	4.1
1	F	379	LEU	4.1
1	B	249	PHE	4.1
1	A	541	TRP	4.0
1	D	288	ILE	4.0
1	A	386	GLY	4.0
1	C	226	LEU	4.0
1	D	446	GLU	3.9
1	A	366	ALA	3.9
1	A	352	HIS	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	252	LEU	3.8
1	F	539	TRP	3.8
1	A	448	LEU	3.8
1	B	447	LEU	3.7
1	A	500	THR	3.7
1	A	261	LEU	3.6
1	C	224	MET	3.6
1	F	356	SER	3.6
1	E	607	LEU	3.6
1	F	593	LEU	3.6
1	E	598	ALA	3.5
1	C	267	GLY	3.5
1	B	166	ALA	3.5
1	E	386	GLY	3.4
1	D	382	SER	3.4
1	A	221	ARG	3.4
1	E	249	PHE	3.4
1	E	296	GLU	3.4
1	D	289	LEU	3.4
1	F	413	LEU	3.4
1	C	241	MET	3.3
1	F	272	THR	3.3
1	A	650	ALA	3.3
1	A	449	LEU	3.3
1	F	273	THR	3.3
1	A	269	GLY	3.3
1	D	342	GLN	3.3
1	E	511	ALA	3.3
1	B	271	SER	3.3
1	D	605	GLU	3.3
1	E	241	MET	3.3
1	D	272	THR	3.3
1	F	271	SER	3.2
1	D	338	LEU	3.2
1	F	267	GLY	3.2
1	D	235	ASP	3.2
1	E	236	LEU	3.2
1	C	207	VAL	3.2
1	D	500	THR	3.1
1	C	266	THR	3.1
1	D	266	THR	3.1
1	D	367	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	F	345	VAL	3.1
1	C	221	ARG	3.0
1	C	565	LEU	3.0
1	C	285	GLU	3.0
1	C	215	PRO	3.0
1	F	518	ILE	2.9
1	F	665	ILE	2.9
1	E	423	ILE	2.9
1	E	541	TRP	2.9
1	A	259	ILE	2.9
1	A	349	LEU	2.9
1	F	607	LEU	2.9
1	D	397	CYS	2.9
1	A	238	SER	2.9
1	C	271	SER	2.9
1	B	274	LEU	2.9
1	D	447	LEU	2.8
1	B	500	THR	2.8
1	C	567	PHE	2.8
1	D	278	LEU	2.8
1	A	609	ILE	2.8
1	E	367	VAL	2.8
1	C	208	ASP	2.8
1	F	540	SER	2.8
1	E	261	LEU	2.8
1	B	355	MET	2.7
1	B	631	THR	2.7
1	D	489	GLY	2.7
1	E	352	HIS	2.7
1	A	367	VAL	2.7
1	B	330	VAL	2.7
1	D	302	ILE	2.7
1	A	562	VAL	2.7
1	B	235	ASP	2.7
1	B	267	GLY	2.6
1	F	264	GLY	2.6
1	C	386	GLY	2.6
1	B	289	LEU	2.6
1	F	359	HIS	2.6
1	B	462	ALA	2.6
1	D	345	VAL	2.6
1	D	152	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	484	ASP	2.6
1	E	643	VAL	2.6
1	D	440	GLY	2.6
1	B	228	ASP	2.5
1	C	123	ILE	2.5
1	D	478	ILE	2.5
1	F	579	MET	2.5
1	E	271	SER	2.5
1	A	267	GLY	2.5
1	F	355	MET	2.5
1	F	358	LEU	2.5
1	F	541	TRP	2.5
1	D	249	PHE	2.5
1	D	282	ASN	2.5
1	F	265	PRO	2.5
1	F	516	ILE	2.5
1	D	335	ILE	2.5
1	F	332	VAL	2.5
1	F	275	TYR	2.5
1	F	266	THR	2.4
1	C	656	GLY	2.4
1	D	269	GLY	2.4
1	C	485	LYS	2.4
1	A	268	SER	2.4
1	B	494	GLU	2.4
1	A	265	PRO	2.4
1	C	385	LEU	2.4
1	D	370	LEU	2.4
1	F	274	LEU	2.4
1	E	267	GLY	2.4
1	E	518	ILE	2.3
1	F	261	LEU	2.3
1	C	228	ASP	2.3
1	F	632	GLU	2.3
1	B	539	TRP	2.3
1	E	498	ARG	2.3
1	C	625	GLY	2.3
1	D	123	ILE	2.3
1	B	269	GLY	2.3
1	F	276	ALA	2.3
1	F	370	LEU	2.3
1	C	235	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	569	LYS	2.2
1	D	499	VAL	2.2
1	E	385	LEU	2.2
1	A	371	ARG	2.2
1	A	442	THR	2.2
1	B	367	VAL	2.2
1	E	624	SER	2.2
1	D	304	GLN	2.2
1	A	387	VAL	2.2
1	E	499	VAL	2.2
1	F	480	ASP	2.2
1	E	359	HIS	2.2
1	D	392	LEU	2.2
1	D	412	LYS	2.2
1	C	393	VAL	2.1
1	F	397	CYS	2.1
1	F	228	ASP	2.1
1	B	633	ASN	2.1
1	E	450	VAL	2.1
1	F	634	VAL	2.1
1	D	488	GLN	2.1
1	D	236	LEU	2.1
1	F	367	VAL	2.1
1	F	380	ILE	2.1
1	F	534	ILE	2.1
1	F	567	PHE	2.1
1	D	228	ASP	2.1
1	F	628	ASP	2.1
1	B	272	THR	2.1
1	D	653	ALA	2.1
1	E	335	ILE	2.1
1	E	410	GLN	2.1
1	C	630	LEU	2.1
1	D	462	ALA	2.1
1	F	633	ASN	2.1
1	D	409	GLU	2.1
1	C	272	THR	2.0
1	F	329	VAL	2.0
1	F	349	LEU	2.0
1	A	380	ILE	2.0
1	B	435	HIS	2.0
1	D	486	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	358	LEU	2.0
1	E	414	PHE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.