Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2024 – 05:37 PM EST

PDB ID	:	4KSS
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:

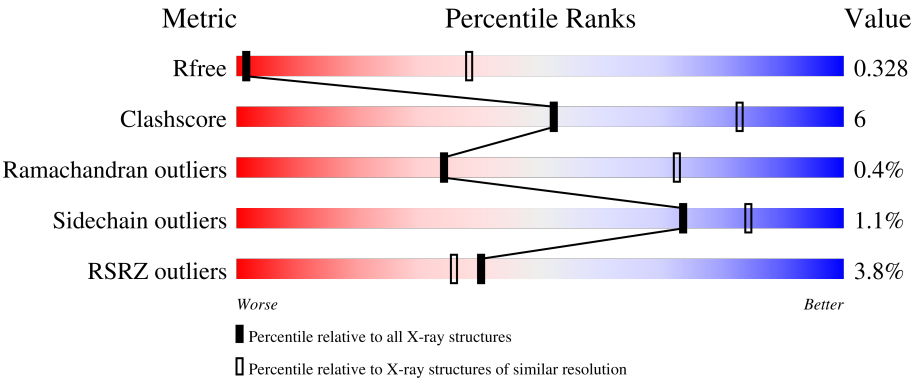
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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}	130704	1004 (10.00-3.90)
Clashscore	141614	1069 (10.00-3.90)
Ramachandran outliers	138981	1002 (10.00-3.90)
Sidechain outliers	138945	1002 (10.00-3.86)
RSRZ outliers	127900	1004 (9.50-3.80)

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 <=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	4% 83% 7% • 10%
1	B	581	3% 83% 6% • 10%
1	C	581	3% 83% 6% • 10%
1	D	581	4% 83% 6% • 10%
1	E	581	3% 84% 5% • 10%

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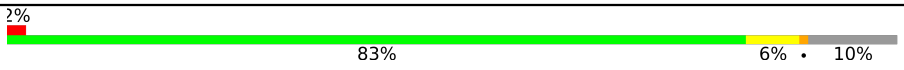
Mol	Chain	Length	Quality of chain
1	F	581	

2 Entry composition (i)

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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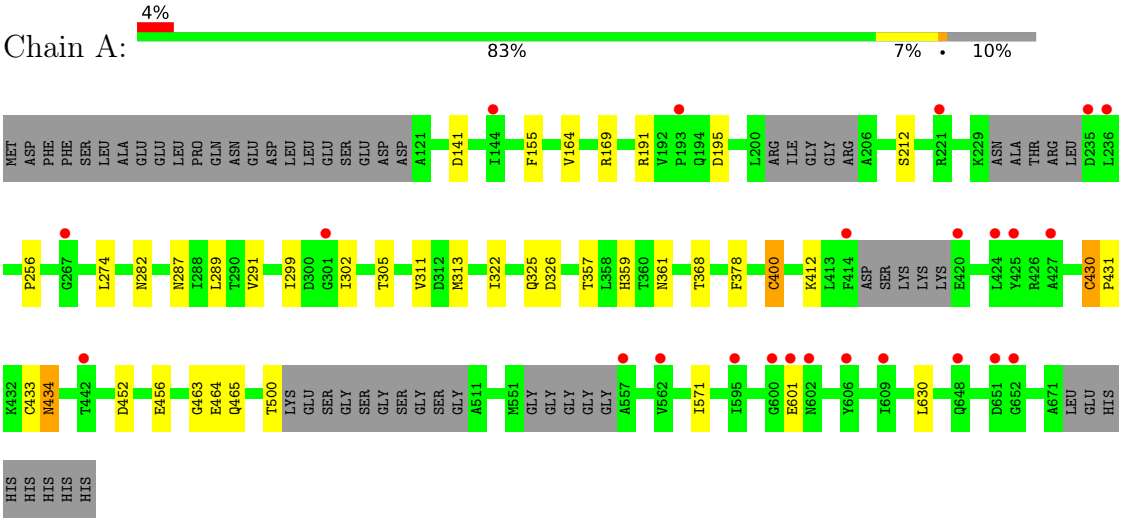
Chain	Residue	Modelled	Actual	Comment	Reference
D	674	HIS	-	expression tag	UNP Q02UZ4
D	675	HIS	-	expression tag	UNP Q02UZ4
D	676	HIS	-	expression tag	UNP Q02UZ4
D	677	HIS	-	expression tag	UNP Q02UZ4
D	678	HIS	-	expression tag	UNP Q02UZ4
D	679	HIS	-	expression tag	UNP Q02UZ4
E	99	MET	-	expression tag	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.

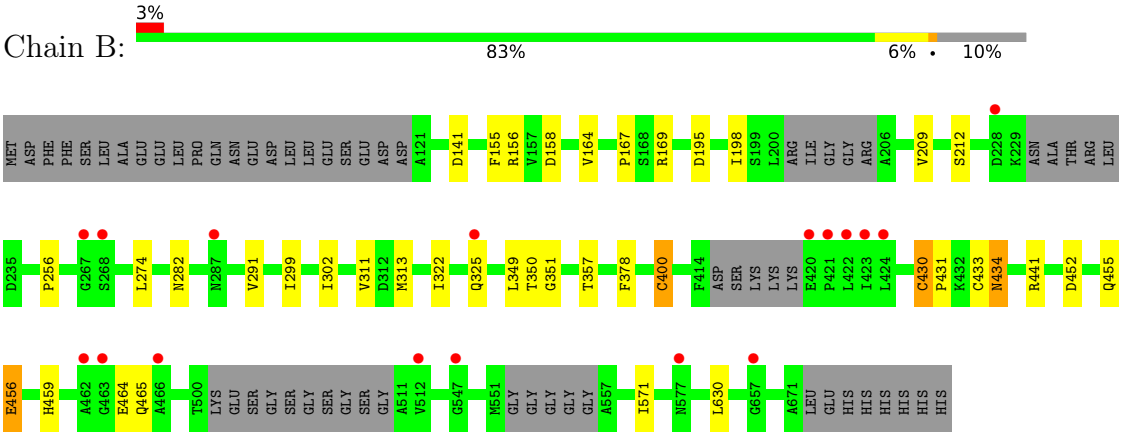
• Molecule 1: Type II secretion system protein E, hemolysin-coregulated protein

Chain A:



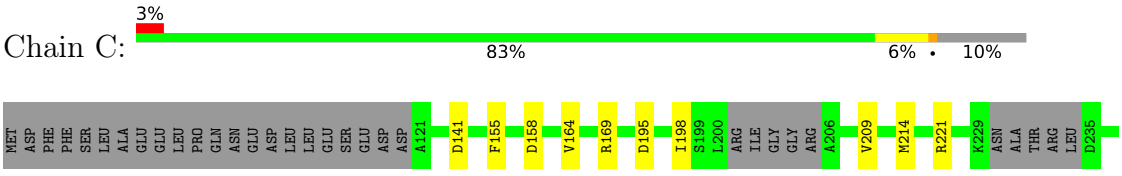
• Molecule 1: Type II secretion system protein E, hemolysin-coregulated protein

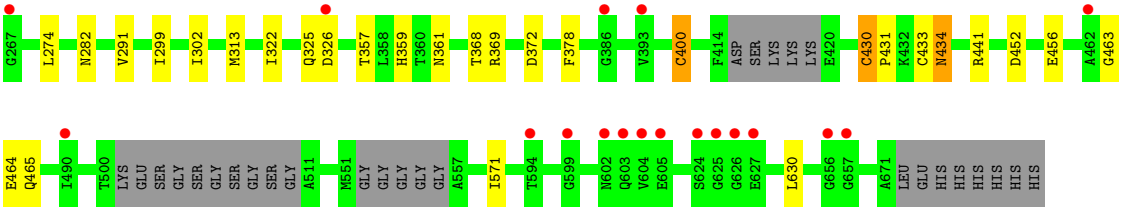
Chain B:

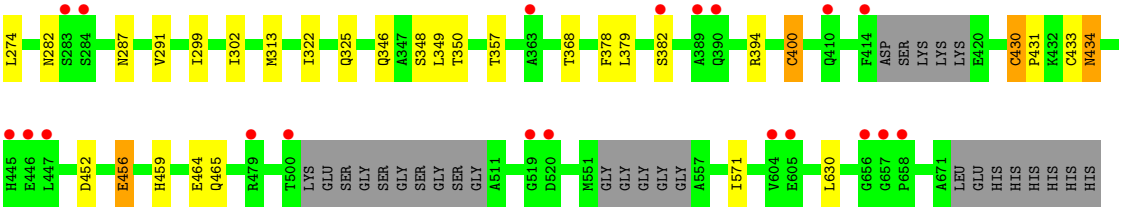


• Molecule 1: Type II secretion system protein E, hemolysin-coregulated protein

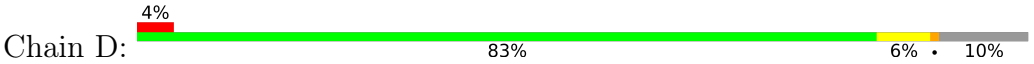
Chain C:



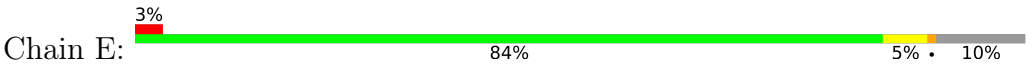


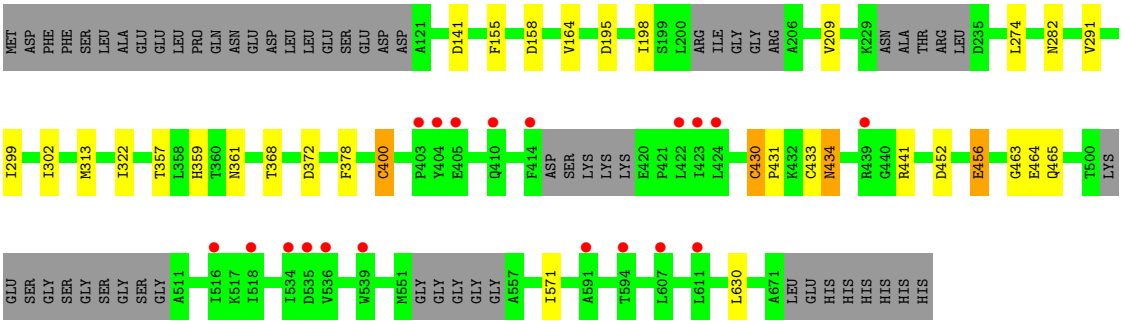


• Molecule 1: Type II secretion system protein E, hemolysin-coregulated protein

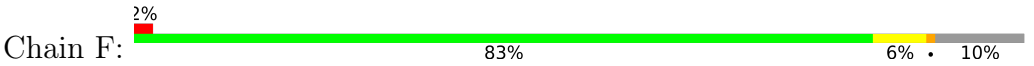


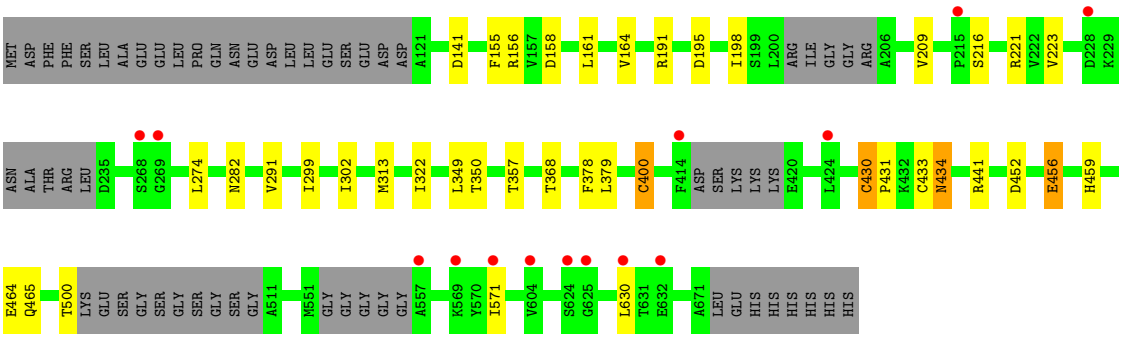
• Molecule 1: Type II secretion system protein E, hemolysin-coregulated protein





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





4 Data and refinement statistics (i)

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 49.95 – 7.58	Depositor EDS
% Data completeness (in resolution range)	99.0 (50.00-7.58) 99.6 (49.95-7.58)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.22 (at 7.37Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.349 , 0.360 0.328 , 0.328	Depositor DCC
R_{free} test set	308 reflections (4.69%)	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)	0.27 , 109.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.26	0/4074	0.47	2/5491 (0.0%)
1	B	0.26	0/4074	0.47	2/5491 (0.0%)
1	C	0.26	0/4074	0.47	2/5491 (0.0%)
1	D	0.26	0/4074	0.47	2/5491 (0.0%)
1	E	0.26	0/4074	0.47	2/5491 (0.0%)
1	F	0.26	0/4074	0.47	2/5491 (0.0%)
All	All	0.26	0/24444	0.47	12/32946 (0.0%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	430	CYS	CA-CB-SG	7.34	127.22	114.00
1	F	430	CYS	CA-CB-SG	7.33	127.19	114.00
1	C	430	CYS	CA-CB-SG	7.32	127.17	114.00
1	B	430	CYS	CA-CB-SG	7.31	127.16	114.00
1	E	430	CYS	CA-CB-SG	7.31	127.15	114.00
1	A	430	CYS	CA-CB-SG	7.29	127.13	114.00
1	E	400	CYS	CA-CB-SG	6.47	125.64	114.00
1	F	400	CYS	CA-CB-SG	6.46	125.63	114.00
1	A	400	CYS	CA-CB-SG	6.44	125.60	114.00
1	B	400	CYS	CA-CB-SG	6.44	125.59	114.00
1	C	400	CYS	CA-CB-SG	6.43	125.57	114.00
1	D	400	CYS	CA-CB-SG	6.42	125.55	114.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4021	0	4099	70	0
1	B	4021	0	4099	59	0
1	C	4021	0	4097	76	0
1	D	4021	0	4098	80	0
1	E	4021	0	4099	55	0
1	F	4021	0	4099	70	0
All	All	24126	0	24591	269	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 6.

All (269) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:430:CYS:HG	1:A:431:PRO:HD2	1.30	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:B:430:CYS:HG	1:B:431:PRO:HD2	1.28	0.90
1:C:430:CYS:HG	1:C:431:PRO:HD2	1.30	0.90
1:F:158:ASP:O	1:F:441:ARG:NH1	2.05	0.90
1:F:430:CYS:HG	1:F:431:PRO:HD2	1.32	0.90
1:A:463:GLY:CA	1:B:459:HIS:CE1	2.54	0.89
1:D:400:CYS:HG	1:D:430:CYS:HB3	1.38	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:A:400:CYS:HG	1:A:430:CYS:HB3	1.38	0.85
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:A:465:GLN:CD	1:B:452:ASP:O	2.16	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:465:GLN:CD	1:D:456:GLU:HB2	1.95	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
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:E:400:CYS:HG	1:E:430:CYS:HB3	1.49	0.76
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:C:463:GLY:C	1:D:459:HIS:CE1	2.59	0.76
1:D:464:GLU:HG3	1:E:378:PHE:HE1	1.50	0.75
1:F:400:CYS:HG	1:F:430:CYS:HB3	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:C:400:CYS:HG	1:C:430:CYS:HB3	1.47	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:B:400:CYS:HG	1:B:430:CYS:HB3	1.52	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:158:ASP:O	1:C:441:ARG:NH2	2.25	0.69
1:A:465:GLN:OE1	1:B:452:ASP:O	2.11	0.69
1:A:378:PHE:CZ	1:F:368:THR:HG23	2.27	0.69
1:D:400:CYS:HG	1:D:430:CYS:CB	2.06	0.68
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
1:E:400:CYS:SG	1:E:433:CYS:HB3	2.34	0.67
1:B:400:CYS:SG	1:B:433:CYS:HB3	2.34	0.67
1:A:400:CYS:HG	1:A:430:CYS:CB	2.06	0.67
1:E:464:GLU:HG3	1:F:378:PHE:HE1	0.75	0.67
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:C:465:GLN:CD	1:D:456:GLU:CB	2.64	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: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:C:372:ASP:CG	1:D:379:LEU:HD21	2.20	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:C:464:GLU:CD	1:D:378:PHE:CZ	2.73	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:463:GLY:HA3	1:D:459:HIS:ND1	2.15	0.59
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:B:400:CYS:SG	1:B:430:CYS:CB	2.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:400:CYS:HG	1:E:430:CYS:CB	2.18	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
1:C:400:CYS:HG	1:C:430:CYS:CB	2.16	0.54
1:F:400:CYS:HG	1:F:430:CYS:CB	2.19	0.54
1:A:325:GLN:OE1	1:F:223:VAL:CG2	2.55	0.54
1:C:158:ASP:C	1:C:441:ARG:NH2	2.61	0.53
1:A:325:GLN:HB3	1:F:221:ARG:HH21	1.74	0.53
1:C:465:GLN:CD	1:D:452:ASP:O	2.47	0.52
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:E:465:GLN:HE22	1:F:456:GLU:H	1.58	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:500:THR:C	1:B:256:PRO:HG2	2.33	0.47
1:B:400:CYS:HG	1:B:430:CYS:CB	2.21	0.47
1:B:156:ARG:NE	1:C:326:ASP:OD2	2.48	0.47
1:D:368:THR:HG21	1:E:378:PHE:CZ	2.50	0.47
1:A:305:THR:HG23	1:F:216:SER:HA	1.96	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:465:GLN:NE2	1:B:455:GLN:C	2.70	0.42
1:E:372:ASP:CG	1:F:379:LEU:HD21	2.40	0.42
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:B:465:GLN:CD	1:C:452:ASP:O	2.53	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: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:A:256:PRO:HG2	1:F:500:THR:C	2.41	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: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: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 (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	509/581 (88%)	490 (96%)	17 (3%)	2 (0%)	34	72
1	B	509/581 (88%)	488 (96%)	19 (4%)	2 (0%)	34	72
1	C	509/581 (88%)	490 (96%)	17 (3%)	2 (0%)	34	72
1	D	509/581 (88%)	490 (96%)	17 (3%)	2 (0%)	34	72
1	E	509/581 (88%)	490 (96%)	17 (3%)	2 (0%)	34	72
1	F	509/581 (88%)	484 (95%)	23 (4%)	2 (0%)	34	72
All	All	3054/3486 (88%)	2932 (96%)	110 (4%)	12 (0%)	34	72

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 (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	444/491 (90%)	439 (99%)	5 (1%)	73 84
1	B	444/491 (90%)	438 (99%)	6 (1%)	67 80
1	C	444/491 (90%)	439 (99%)	5 (1%)	73 84
1	D	444/491 (90%)	440 (99%)	4 (1%)	78 87
1	E	444/491 (90%)	440 (99%)	4 (1%)	78 87
1	F	444/491 (90%)	440 (99%)	4 (1%)	78 87
All	All	2664/2946 (90%)	2636 (99%)	28 (1%)	73 84

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	141	ASP
1	A	169	ARG
1	A	195	ASP
1	A	313	MET
1	A	456	GLU
1	B	141	ASP
1	B	167	PRO
1	B	169	ARG
1	B	195	ASP
1	B	313	MET
1	B	456	GLU
1	C	141	ASP
1	C	169	ARG
1	C	195	ASP
1	C	313	MET
1	C	456	GLU
1	D	141	ASP
1	D	195	ASP
1	D	313	MET
1	D	456	GLU
1	E	141	ASP
1	E	195	ASP
1	E	313	MET
1	E	456	GLU
1	F	141	ASP
1	F	195	ASP
1	F	313	MET
1	F	456	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	246	HIS
1	A	390	GLN
1	A	459	HIS
1	A	465	GLN
1	A	470	HIS
1	B	218	HIS
1	B	246	HIS
1	B	390	GLN
1	B	459	HIS
1	B	470	HIS
1	B	563	GLN
1	C	246	HIS
1	C	390	GLN
1	C	459	HIS
1	C	470	HIS
1	C	563	GLN
1	D	246	HIS
1	D	325	GLN
1	D	346	GLN
1	D	390	GLN
1	D	459	HIS
1	D	465	GLN
1	D	470	HIS
1	D	563	GLN
1	D	670	GLN
1	E	246	HIS
1	E	346	GLN
1	E	390	GLN
1	E	459	HIS
1	E	465	GLN
1	E	470	HIS
1	F	143	HIS
1	F	246	HIS
1	F	346	GLN
1	F	390	GLN
1	F	459	HIS
1	F	465	GLN
1	F	470	HIS
1	F	670	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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%)	0.41	24 (4%)	32	30	119, 174, 258, 384	0
1	B	521/581 (89%)	0.29	17 (3%)	46	41	75, 139, 253, 363	0
1	C	521/581 (89%)	0.46	18 (3%)	44	39	88, 170, 268, 376	0
1	D	521/581 (89%)	0.41	26 (4%)	28	28	69, 160, 262, 407	0
1	E	521/581 (89%)	0.36	19 (3%)	42	38	69, 153, 250, 404	0
1	F	521/581 (89%)	0.35	14 (2%)	54	48	89, 155, 247, 400	0
All	All	3126/3486 (89%)	0.38	118 (3%)	40	36	69, 161, 259, 407	0

All (118) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	446	GLU	4.7
1	C	605	GLU	4.6
1	C	625	GLY	4.5
1	A	557	ALA	4.2
1	F	268	SER	3.9
1	F	228	ASP	3.8
1	B	421	PRO	3.6
1	B	463	GLY	3.6
1	C	603	GLN	3.6
1	C	626	GLY	3.5
1	C	604	VAL	3.5
1	C	602	ASN	3.5
1	E	424	LEU	3.4
1	B	423	ILE	3.3
1	F	557	ALA	3.3
1	D	658	PRO	3.3
1	E	423	ILE	3.1
1	D	228	ASP	3.1
1	A	427	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	414	PHE	3.1
1	B	547	GLY	3.1
1	F	215	PRO	3.1
1	D	605	GLU	3.1
1	B	422	LEU	3.0
1	D	657	GLY	3.0
1	D	447	LEU	3.0
1	A	601	GLU	3.0
1	B	462	ALA	3.0
1	E	422	LEU	2.9
1	A	235	ASP	2.9
1	D	235	ASP	2.9
1	F	269	GLY	2.9
1	D	268	SER	2.8
1	D	389	ALA	2.8
1	A	301	GLY	2.8
1	A	442	THR	2.7
1	D	656	GLY	2.7
1	E	410	GLN	2.7
1	F	571	ILE	2.7
1	E	439	ARG	2.7
1	E	414	PHE	2.7
1	C	624	SER	2.7
1	D	206	ALA	2.7
1	C	627	GLU	2.6
1	A	602	ASN	2.6
1	C	490	ILE	2.6
1	F	604	VAL	2.6
1	D	604	VAL	2.6
1	A	221	ARG	2.6
1	E	535	ASP	2.5
1	F	624	SER	2.5
1	E	518	ILE	2.5
1	D	363	ALA	2.5
1	A	424	LEU	2.5
1	A	648	GLN	2.5
1	D	520	ASP	2.5
1	C	657	GLY	2.5
1	D	519	GLY	2.5
1	B	267	GLY	2.4
1	B	657	GLY	2.4
1	C	656	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	609	ILE	2.4
1	A	600	GLY	2.4
1	D	269	GLY	2.4
1	D	382	SER	2.4
1	E	536	VAL	2.4
1	E	403	PRO	2.4
1	A	420	GLU	2.4
1	B	228	ASP	2.4
1	A	144	ILE	2.4
1	E	594	THR	2.4
1	F	625	GLY	2.4
1	E	591	ALA	2.3
1	C	267	GLY	2.3
1	C	386	GLY	2.3
1	C	594	THR	2.3
1	F	569	LYS	2.3
1	D	271	SER	2.3
1	D	283	SER	2.3
1	B	268	SER	2.3
1	A	595	ILE	2.3
1	E	405	GLU	2.3
1	D	410	GLN	2.3
1	B	325	GLN	2.2
1	A	652	GLY	2.2
1	E	607	LEU	2.2
1	B	512	VAL	2.2
1	A	193	PRO	2.2
1	E	611	LEU	2.2
1	E	534	ILE	2.2
1	F	414	PHE	2.2
1	F	630	LEU	2.2
1	E	516	ILE	2.2
1	E	404	TYR	2.2
1	C	393	VAL	2.1
1	D	284	SER	2.1
1	C	462	ALA	2.1
1	A	651	ASP	2.1
1	D	390	GLN	2.1
1	A	606	TYR	2.1
1	D	479	ARG	2.1
1	D	414	PHE	2.1
1	A	236	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	424	LEU	2.1
1	D	445	HIS	2.1
1	B	577	ASN	2.1
1	A	562	VAL	2.1
1	B	420	GLU	2.1
1	C	599	GLY	2.1
1	A	425	TYR	2.1
1	B	466	ALA	2.1
1	F	632	GLU	2.1
1	D	500	THR	2.0
1	A	267	GLY	2.0
1	C	326	ASP	2.0
1	E	539	TRP	2.0
1	B	287	ASN	2.0
1	F	424	LEU	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 monosaccharides 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.