



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:11 PM GMT

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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

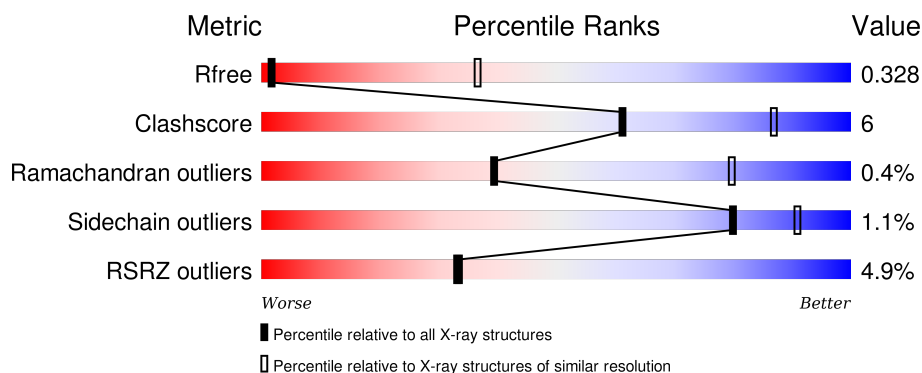
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	91344	1015 (11.50-3.66)
Clashscore	102246	1063 (10.00-3.70)
Ramachandran outliers	100387	1036 (11.50-3.66)
Sidechain outliers	100360	1006 (11.50-3.66)
RSRZ outliers	91569	1014 (11.50-3.66)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>5%</div> <div>83%</div> <div>7%</div> <div>10%</div> </div>
1	B	581	<div> <div>4%</div> <div>83%</div> <div>6%</div> <div>10%</div> </div>
1	C	581	<div> <div>5%</div> <div>83%</div> <div>6%</div> <div>10%</div> </div>
1	D	581	<div> <div>5%</div> <div>83%</div> <div>6%</div> <div>10%</div> </div>
1	E	581	<div> <div>5%</div> <div>84%</div> <div>5%</div> <div>10%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	581	<div><div></div><div>3%</div><div>83%</div><div>6%</div><div>10%</div></div>

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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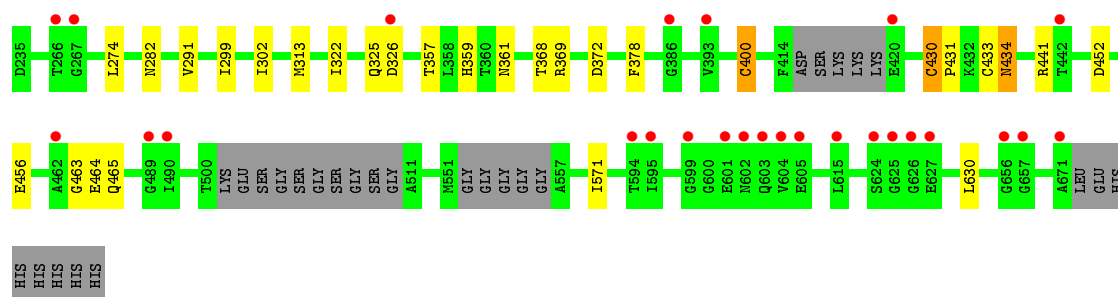
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Chain	Residue	Modelled	Actual	Comment	Reference
B	99	MET	-	EXPRESSION TAG	UNP P37093
B	504	GLY	-	LINKER	UNP P37093
B	505	SER	-	LINKER	UNP P37093
B	506	GLY	-	LINKER	UNP P37093
B	507	SER	-	LINKER	UNP P37093
B	508	GLY	-	LINKER	UNP P37093
B	509	SER	-	LINKER	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

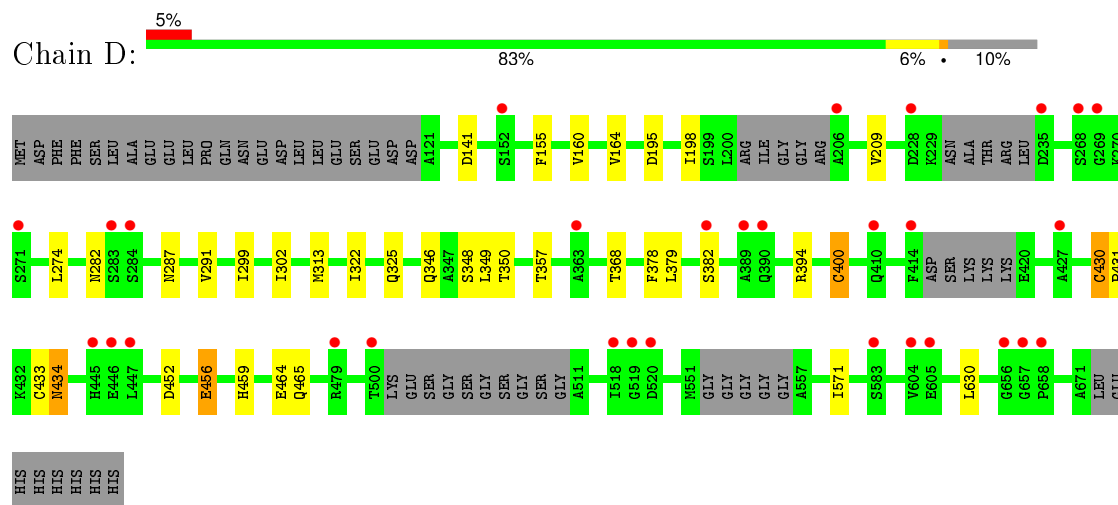
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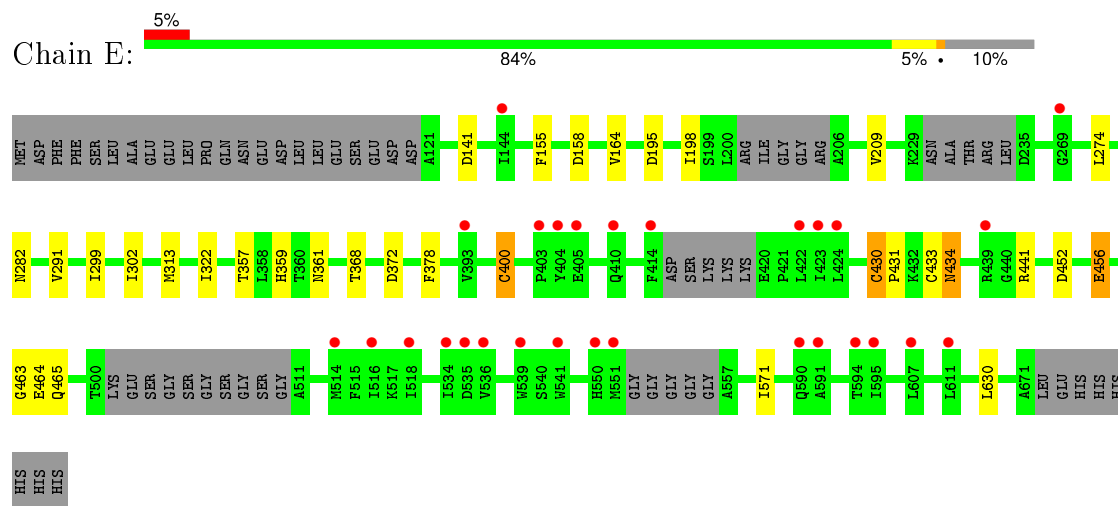
Chain	Residue	Modelled	Actual	Comment	Reference
D	674	HIS	-	EXPRESSION TAG	UNP Q02UZ4
D	675	HIS	-	EXPRESSION TAG	UNP Q02UZ4
D	676	HIS	-	EXPRESSION TAG	UNP Q02UZ4
D	677	HIS	-	EXPRESSION TAG	UNP Q02UZ4
D	678	HIS	-	EXPRESSION TAG	UNP Q02UZ4
D	679	HIS	-	EXPRESSION TAG	UNP Q02UZ4
E	99	MET	-	EXPRESSION TAG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



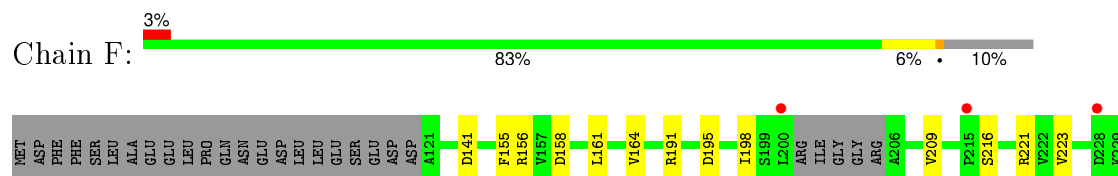
- Molecule 1: Type II secretion system protein E, hemolysin-coregulated protein

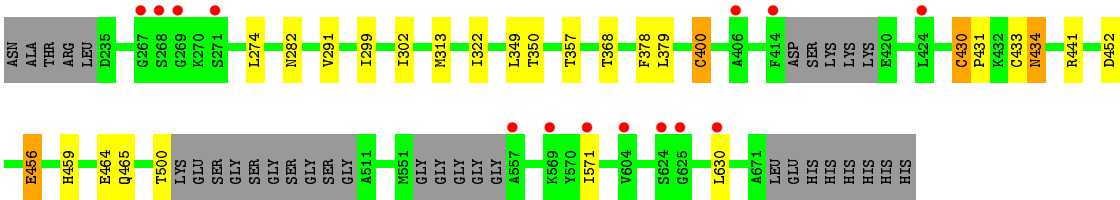


- Molecule 1: Type II secretion system protein E, hemolysin-coregulated protein



- 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	205.06 Å 205.06 Å 234.98 Å 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
$\langle I/\sigma(I) \rangle$ ¹	2.22 (at 7.37 Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.349 , 0.360 0.328 , 0.328	Depositor DCC
R_{free} test set	308 reflections (4.92%)	DCC
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 , 108.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	1 of 6573 reflections (0.015%)	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, 0.375 respectively for untwinned datasets, and 0.333, 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(°)	Ideal(°)
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:464:GLU:HG3	1:D:378:PHE:CE1	0.97	1.50
1:C:463:GLY:CA	1:D:459:HIS:CE1	1.92	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:430:CYS:HG	1:F:431:PRO:HD2	1.32	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: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:E:464:GLU:HG3	1:F:378:PHE:CZ	2.10	0.86
1:A:465:GLN:HE22	1:B:456:GLU:N	1.74	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:F:400:CYS:HG	1:F:430:CYS:HB3	1.50	0.75
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: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:C:368:THR:CG2	1:D:378:PHE:HE2	1.99	0.74
1:A:378:PHE:CE2	1:F:368:THR:HG23	2.22	0.74
1:F:158:ASP:HB3	1:F:441:ARG:CZ	2.18	0.74
1:C:463:GLY:HA3	1:D:459:HIS:NE2	2.01	0.73
1:B:430:CYS:SG	1:B:431:PRO:HD3	2.27	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:C:430:CYS:O	1:C:434:ASN:N	2.21	0.72
1:A:325:GLN:OE1	1:F:223:VAL:HG23	1.89	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:E:400:CYS:SG	1:E:433:CYS:HB3	2.34	0.67
1:C:400:CYS:SG	1:C: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:464:GLU:OE2	1:D:382:SER:CB	2.44	0.65
1:C:368:THR:OG1	1:D:378:PHE:CZ	2.49	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:F:400:CYS:SG	1:F:433:CYS:SG	3.08	0.52
1:A:361:ASN:ND2	1:B:349:LEU:O	2.42	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:C:155:PHE:CD2	1:C:164:VAL:HG11	2.48	0.49
1:B:571:ILE:HD12	1:B:630:LEU:HB2	1.95	0.49
1:E:291:VAL:HG23	1:E:322:ILE:HD12	1.94	0.49
1:C:464:GLU:H	1:D:459:HIS:HE1	1.46	0.48
1:A:500:THR:O	1:B:256:PRO:CG	2.61	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:B:158:ASP:O	1:B:441:ARG:CZ	2.58	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:E:463:GLY:HA2	1:F:459:HIS:HE1	1.75	0.47
1:A:378:PHE:CE2	1:F:368:THR:CG2	2.94	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:E:465:GLN:HE22	1:F:456:GLU:HB2	1.81	0.46
1:A:256:PRO:HG2	1:F:500:THR:O	2.16	0.46
1:E:571:ILE:HD12	1:E:630:LEU:HB2	1.97	0.46
1:C:214:MET:HB2	1:D:325:GLN:NE2	2.30	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:C:368:THR:OG1	1:D:378:PHE:HZ	1.98	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: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: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:B:155:PHE:CD2	1:B:164:VAL:HG11	2.52	0.44
1:F:291:VAL:CG2	1:F:322:ILE:HD12	2.47	0.44
1:C:361:ASN:ND2	1:D:349:LEU:O	2.50	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:E:464:GLU:CG	1:F:378:PHE:CZ	2.88	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:B:299:ILE:HG21	1:B:302:ILE:HD12	2.00	0.44
1:A:155:PHE:CD2	1:A:164:VAL:HG11	2.53	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:B:291:VAL:CG2	1:B:322:ILE:HD12	2.47	0.44
1:A:299:ILE:HG21	1:A:302:ILE:HD12	1.99	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:289:LEU:HD21	1:F:221:ARG:CZ	2.48	0.43
1:A:212:SER:O	1:B:325:GLN:NE2	2.48	0.43
1:E:464:GLU:OE2	1:F:378:PHE:CZ	2.70	0.43
1:C:221:ARG:NH2	1:D:287:ASN:HD21	2.17	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:F:155:PHE:CD2	1:F:164:VAL:HG11	2.53	0.42
1:E:155:PHE:CD2	1:E:164:VAL:HG11	2.55	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:E:274:LEU:HD11	1:E:357:THR:HG23	2.02	0.40
1:C:274:LEU:HD11	1:C: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%)	39	80
1	B	509/581 (88%)	488 (96%)	19 (4%)	2 (0%)	39	80
1	C	509/581 (88%)	490 (96%)	17 (3%)	2 (0%)	39	80
1	D	509/581 (88%)	490 (96%)	17 (3%)	2 (0%)	39	80
1	E	509/581 (88%)	490 (96%)	17 (3%)	2 (0%)	39	80
1	F	509/581 (88%)	484 (95%)	23 (4%)	2 (0%)	39	80
All	All	3054/3486 (88%)	2932 (96%)	110 (4%)	12 (0%)	39	80

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%)	439 (99%)	5 (1%)	80	91
1	B	444/491 (90%)	438 (99%)	6 (1%)	74	89
1	C	444/491 (90%)	439 (99%)	5 (1%)	80	91
1	D	444/491 (90%)	440 (99%)	4 (1%)	84	93
1	E	444/491 (90%)	440 (99%)	4 (1%)	84	93
1	F	444/491 (90%)	440 (99%)	4 (1%)	84	93
All	All	2664/2946 (90%)	2636 (99%)	28 (1%)	80	91

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

Some 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 [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 carbohydrates 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%)	0.50	28 (5%)	29	30	119, 174, 258, 384	0
1	B	521/581 (89%)	0.39	23 (4%)	38	37	75, 139, 253, 363	0
1	C	521/581 (89%)	0.55	27 (5%)	31	31	88, 170, 268, 376	0
1	D	521/581 (89%)	0.50	30 (5%)	26	27	69, 160, 262, 407	0
1	E	521/581 (89%)	0.45	28 (5%)	29	30	69, 153, 250, 404	0
1	F	521/581 (89%)	0.42	17 (3%)	50	46	89, 155, 247, 400	0
All	All	3126/3486 (89%)	0.47	153 (4%)	33	33	69, 161, 259, 407	0

All (153) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	605	GLU	5.0
1	D	446	GLU	4.9
1	C	625	GLY	4.9
1	A	557	ALA	4.7
1	F	268	SER	4.1
1	F	228	ASP	4.1
1	C	603	GLN	3.9
1	C	604	VAL	3.9
1	B	463	GLY	3.8
1	C	626	GLY	3.8
1	C	602	ASN	3.7
1	B	423	ILE	3.6
1	F	557	ALA	3.6
1	E	424	LEU	3.6
1	B	421	PRO	3.5
1	F	215	PRO	3.5
1	A	427	ALA	3.4
1	D	658	PRO	3.4
1	B	547	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	228	ASP	3.4
1	B	462	ALA	3.3
1	E	423	ILE	3.3
1	D	447	LEU	3.3
1	D	389	ALA	3.3
1	D	657	GLY	3.2
1	D	206	ALA	3.2
1	A	414	PHE	3.2
1	B	422	LEU	3.2
1	D	605	GLU	3.1
1	F	269	GLY	3.1
1	A	235	ASP	3.1
1	A	301	GLY	3.1
1	E	422	LEU	3.1
1	D	519	GLY	3.0
1	A	442	THR	3.0
1	A	601	GLU	3.0
1	C	490	ILE	3.0
1	D	268	SER	3.0
1	D	235	ASP	3.0
1	D	656	GLY	2.9
1	A	221	ARG	2.9
1	D	520	ASP	2.9
1	C	624	SER	2.9
1	F	571	ILE	2.9
1	E	414	PHE	2.9
1	C	627	GLU	2.9
1	F	604	VAL	2.8
1	E	410	GLN	2.8
1	E	535	ASP	2.8
1	D	363	ALA	2.8
1	E	594	THR	2.8
1	C	657	GLY	2.8
1	A	144	ILE	2.8
1	A	609	ILE	2.8
1	E	518	ILE	2.7
1	F	624	SER	2.7
1	B	657	GLY	2.7
1	E	439	ARG	2.7
1	A	602	ASN	2.7
1	F	625	GLY	2.7
1	E	536	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	656	GLY	2.7
1	A	420	GLU	2.7
1	C	594	THR	2.6
1	E	591	ALA	2.6
1	B	325	GLN	2.6
1	A	595	ILE	2.6
1	C	267	GLY	2.6
1	D	604	VAL	2.6
1	D	382	SER	2.6
1	D	269	GLY	2.5
1	E	607	LEU	2.5
1	B	267	GLY	2.5
1	A	424	LEU	2.5
1	D	445	HIS	2.5
1	B	228	ASP	2.5
1	A	600	GLY	2.5
1	A	648	GLN	2.5
1	D	283	SER	2.5
1	C	386	GLY	2.5
1	B	512	VAL	2.5
1	C	462	ALA	2.5
1	B	287	ASN	2.5
1	A	606	TYR	2.5
1	E	534	ILE	2.4
1	E	516	ILE	2.4
1	B	268	SER	2.4
1	E	611	LEU	2.4
1	E	403	PRO	2.4
1	A	145	GLU	2.4
1	D	390	GLN	2.4
1	B	424	LEU	2.4
1	D	518	ILE	2.4
1	C	599	GLY	2.4
1	D	271	SER	2.4
1	F	630	LEU	2.4
1	C	393	VAL	2.3
1	D	410	GLN	2.3
1	F	424	LEU	2.3
1	D	284	SER	2.3
1	C	595	ILE	2.3
1	B	577	ASN	2.3
1	C	671	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	479	ARG	2.3
1	F	414	PHE	2.3
1	A	562	VAL	2.3
1	E	404	TYR	2.3
1	A	222	VAL	2.3
1	E	595	ILE	2.3
1	D	414	PHE	2.3
1	D	500	THR	2.3
1	A	193	PRO	2.3
1	E	551	MET	2.3
1	E	405	GLU	2.2
1	F	406	ALA	2.2
1	B	466	ALA	2.2
1	C	266	THR	2.2
1	A	236	LEU	2.2
1	F	569	LYS	2.2
1	B	420	GLU	2.2
1	A	305	THR	2.2
1	A	651	ASP	2.2
1	C	420	GLU	2.2
1	A	425	TYR	2.2
1	E	550	HIS	2.2
1	A	652	GLY	2.2
1	E	539	TRP	2.2
1	C	489	GLY	2.2
1	F	267	GLY	2.1
1	B	435	HIS	2.1
1	B	511	ALA	2.1
1	D	583	SER	2.1
1	D	427	ALA	2.1
1	E	514	MET	2.1
1	C	615	LEU	2.1
1	C	326	ASP	2.1
1	C	601	GLU	2.1
1	B	326	ASP	2.1
1	C	191	ARG	2.1
1	F	271	SER	2.1
1	C	442	THR	2.1
1	E	144	ILE	2.1
1	E	541	TRP	2.1
1	A	267	GLY	2.1
1	E	269	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	393	VAL	2.0
1	B	289	LEU	2.0
1	F	200	LEU	2.0
1	B	269	GLY	2.0
1	B	662	GLY	2.0
1	D	152	SER	2.0
1	E	590	GLN	2.0
1	A	206	ALA	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 carbohydrates 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.