



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:10 PM GMT

PDB ID : 4KSR
Title : Crystal Structure of the Vibrio cholerae ATPase GspE Hexamer
Authors : Hol, W.G.; Turley, S.; Lu, C.Y.; Park, Y.J.; Marionni, S.T.; Lee, K.; Patrick, M.; Sandkvist, M.; Bush, M.; Shah, R.
Deposited on : 2013-05-17
Resolution : 4.20 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

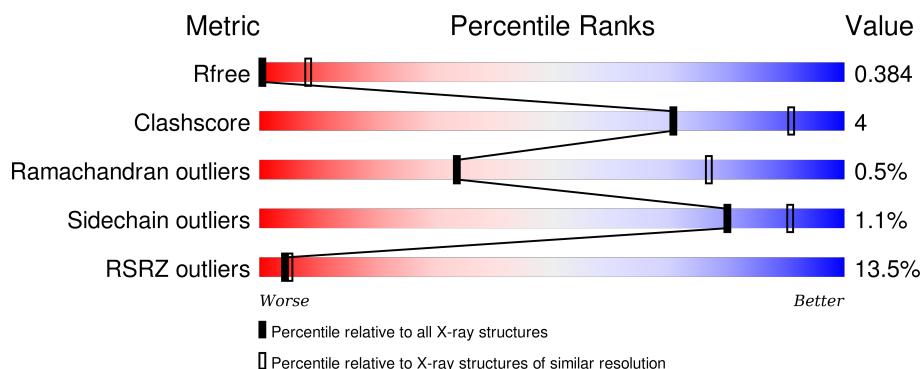
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.20 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	1039 (4.80-3.60)
Clashscore	102246	1140 (4.80-3.60)
Ramachandran outliers	100387	1083 (4.80-3.60)
Sidechain outliers	100360	1067 (4.80-3.60)
RSRZ outliers	91569	1042 (4.80-3.60)

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	583	
1	B	583	
1	C	583	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 12063 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			

There are 51 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	99	MET	-	EXPRESSION TAG	UNP P37093
A	504	LYS	-	LINKER	UNP P37093
A	505	LEU	-	LINKER	UNP P37093
A	506	ALA	-	LINKER	UNP P37093
A	507	SER	-	LINKER	UNP P37093
A	508	GLY	-	LINKER	UNP P37093
A	509	ALA	-	LINKER	UNP P37093
A	510	GLY	-	LINKER	UNP P37093
A	511	HIS	-	LINKER	UNP P37093
A	674	LEU	-	EXPRESSION TAG	UNP Q02UZ4
A	675	GLU	-	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
A	680	HIS	-	EXPRESSION TAG	UNP Q02UZ4
A	681	HIS	-	EXPRESSION TAG	UNP Q02UZ4
B	99	MET	-	EXPRESSION TAG	UNP P37093
B	504	LYS	-	LINKER	UNP P37093
B	505	LEU	-	LINKER	UNP P37093
B	506	ALA	-	LINKER	UNP P37093
B	507	SER	-	LINKER	UNP P37093

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Chain	Residue	Modelled	Actual	Comment	Reference
B	508	GLY	-	LINKER	UNP P37093
B	509	ALA	-	LINKER	UNP P37093
B	510	GLY	-	LINKER	UNP P37093
B	511	HIS	-	LINKER	UNP P37093
B	674	LEU	-	EXPRESSION TAG	UNP Q02UZ4
B	675	GLU	-	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
B	680	HIS	-	EXPRESSION TAG	UNP Q02UZ4
B	681	HIS	-	EXPRESSION TAG	UNP Q02UZ4
C	99	MET	-	EXPRESSION TAG	UNP P37093
C	504	LYS	-	LINKER	UNP P37093
C	505	LEU	-	LINKER	UNP P37093
C	506	ALA	-	LINKER	UNP P37093
C	507	SER	-	LINKER	UNP P37093
C	508	GLY	-	LINKER	UNP P37093
C	509	ALA	-	LINKER	UNP P37093
C	510	GLY	-	LINKER	UNP P37093
C	511	HIS	-	LINKER	UNP P37093
C	674	LEU	-	EXPRESSION TAG	UNP Q02UZ4
C	675	GLU	-	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
C	680	HIS	-	EXPRESSION TAG	UNP Q02UZ4
C	681	HIS	-	EXPRESSION TAG	UNP Q02UZ4

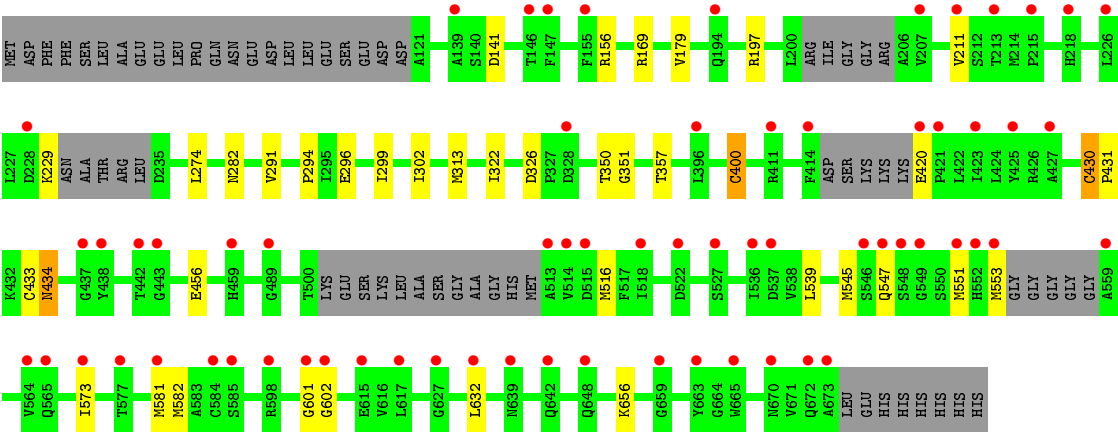
Chain C:

11%

83%

6%

11%



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2 ₁	Depositor
Cell constants a, b, c, α , β , γ	112.47Å 132.91Å 142.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.72 – 4.20 38.69 – 3.78	Depositor EDS
% Data completeness (in resolution range)	98.8 (38.72-4.20) 98.2 (38.69-3.78)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 3.76Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.384 , 0.376 0.389 , 0.384	Depositor DCC
R_{free} test set	828 reflections (5.46%)	DCC
Wilson B-factor (Å ²)	170.3	Xtriage
Anisotropy	0.568	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 83.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Outliers	1 of 21593 reflections (0.005%)	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	12063	wwPDB-VP
Average B, all atoms (Å ²)	138.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% 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	0.38	6/4074 (0.1%)	0.48	2/5491 (0.0%)
1	B	0.38	6/4074 (0.1%)	0.48	2/5491 (0.0%)
1	C	0.38	6/4074 (0.1%)	0.48	2/5491 (0.0%)
All	All	0.38	18/12222 (0.1%)	0.48	6/16473 (0.0%)

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	582	MET	CG-SD	6.52	1.98	1.81
1	C	545	MET	CG-SD	6.38	1.97	1.81
1	C	582	MET	CG-SD	6.32	1.97	1.81
1	A	582	MET	CG-SD	6.30	1.97	1.81
1	A	553	MET	CG-SD	6.29	1.97	1.81
1	C	551	MET	CG-SD	6.29	1.97	1.81
1	A	551	MET	CG-SD	6.28	1.97	1.81
1	B	545	MET	CG-SD	6.27	1.97	1.81
1	B	553	MET	CG-SD	6.27	1.97	1.81
1	C	553	MET	CG-SD	6.26	1.97	1.81
1	A	545	MET	CG-SD	6.26	1.97	1.81
1	B	551	MET	CG-SD	6.25	1.97	1.81
1	B	581	MET	CG-SD	6.25	1.97	1.81
1	C	581	MET	CG-SD	6.25	1.97	1.81
1	A	581	MET	CG-SD	6.24	1.97	1.81
1	B	516	MET	CG-SD	6.23	1.97	1.81
1	C	516	MET	CG-SD	6.10	1.97	1.81
1	A	516	MET	CG-SD	6.10	1.97	1.81

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	430	CYS	CA-CB-SG	7.32	127.18	114.00
1	C	430	CYS	CA-CB-SG	7.31	127.16	114.00
1	A	430	CYS	CA-CB-SG	7.29	127.11	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	400	CYS	CA-CB-SG	6.46	125.63	114.00
1	B	400	CYS	CA-CB-SG	6.45	125.61	114.00
1	C	400	CYS	CA-CB-SG	6.45	125.61	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	44	4
1	B	4021	0	4099	60	2
1	C	4021	0	4099	36	4
All	All	12063	0	12297	107	5

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 4.

All (107) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:430:CYS:SG	1:B:431:PRO:HD2	1.63	1.37
1:A:430:CYS:SG	1:A:431:PRO:HD2	1.63	1.37
1:C:430:CYS:SG	1:C:431:PRO:HD2	1.63	1.36
1:B:266:THR:HG1	1:C:350:THR:C	1.32	1.32
1:B:266:THR:OG1	1:C:350:THR:C	1.74	1.21
1:B:430:CYS:SG	1:B:431:PRO:CD	2.33	1.16
1:C:430:CYS:SG	1:C:431:PRO:CD	2.33	1.16
1:A:430:CYS:SG	1:A:431:PRO:CD	2.33	1.16
1:B:266:THR:OG1	1:C:350:THR:O	1.72	1.02
1:A:400:CYS:SG	1:A:430:CYS:HB3	2.00	1.01
1:C:400:CYS:SG	1:C:430:CYS:HB3	2.00	1.01
1:B:400:CYS:SG	1:B:430:CYS:HB3	2.00	1.00
1:C:430:CYS:HG	1:C:431:PRO:CD	1.73	0.99
1:B:160:VAL:CG2	1:B:394:ARG:HD3	1.93	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:430:CYS:HG	1:A:431:PRO:HD2	0.88	0.94
1:A:336:ARG:HD3	1:B:346:GLN:CD	1.91	0.91
1:C:430:CYS:HG	1:C:431:PRO:HD2	0.78	0.90
1:B:430:CYS:HG	1:B:431:PRO:HD2	1.39	0.85
1:C:420:GLU:OE1	1:C:601:GLY:O	1.96	0.84
1:C:420:GLU:OE2	1:C:602:GLY:HA3	1.78	0.84
1:A:336:ARG:HD3	1:B:346:GLN:NE2	1.94	0.82
1:B:266:THR:OG1	1:C:350:THR:CA	2.28	0.81
1:A:336:ARG:HH11	1:B:346:GLN:HG3	1.45	0.79
1:A:400:CYS:HG	1:A:430:CYS:HB3	1.46	0.79
1:B:160:VAL:HG21	1:B:394:ARG:HD3	1.64	0.78
1:B:400:CYS:HG	1:B:430:CYS:HB3	1.47	0.77
1:A:430:CYS:SG	1:A:431:PRO:HD3	2.27	0.75
1:B:430:CYS:O	1:B:434:ASN:N	2.21	0.73
1:B:430:CYS:SG	1:B:431:PRO:HD3	2.27	0.73
1:B:160:VAL:HG21	1:B:394:ARG:HH11	1.52	0.73
1:C:400:CYS:HG	1:C:430:CYS:HB3	1.52	0.73
1:A:430:CYS:O	1:A:434:ASN:N	2.21	0.72
1:C:430:CYS:O	1:C:434:ASN:N	2.21	0.72
1:A:156:ARG:NE	1:B:326:ASP:OD2	2.22	0.72
1:C:430:CYS:SG	1:C:431:PRO:HD3	2.27	0.72
1:A:336:ARG:NH1	1:B:346:GLN:HG3	2.06	0.71
1:B:266:THR:CB	1:C:350:THR:O	2.39	0.69
1:A:400:CYS:SG	1:A:433:CYS:HB3	2.35	0.67
1:B:400:CYS:SG	1:B:433:CYS:HB3	2.34	0.67
1:C:400:CYS:SG	1:C:433:CYS:HB3	2.34	0.67
1:C:229:LYS:NZ	1:C:296:GLU:O	2.25	0.65
1:B:160:VAL:HG21	1:B:394:ARG:CD	2.26	0.64
1:A:191:ARG:CB	1:B:311:VAL:HG11	2.28	0.63
1:A:191:ARG:HB3	1:B:311:VAL:HG11	1.79	0.63
1:B:400:CYS:SG	1:B:430:CYS:CB	2.85	0.62
1:A:400:CYS:SG	1:A:430:CYS:CB	2.85	0.61
1:A:400:CYS:HG	1:A:430:CYS:CB	2.14	0.60
1:B:400:CYS:HG	1:B:430:CYS:CB	2.16	0.58
1:C:400:CYS:SG	1:C:430:CYS:CB	2.85	0.58
1:A:223:VAL:HG23	1:B:325:GLN:OE1	2.03	0.57
1:B:266:THR:HG1	1:C:350:THR:CA	2.06	0.57
1:B:160:VAL:HG21	1:B:394:ARG:NH1	2.19	0.56
1:B:156:ARG:NE	1:C:326:ASP:OD2	2.42	0.53
1:A:266:THR:HG21	1:B:350:THR:C	2.28	0.53
1:B:573:ILE:HD12	1:B:632:LEU:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:400:CYS:SG	1:C:433:CYS:SG	3.08	0.52
1:C:400:CYS:HG	1:C:430:CYS:CB	2.21	0.52
1:B:400:CYS:SG	1:B:433:CYS:SG	3.08	0.52
1:A:400:CYS:SG	1:A:433:CYS:SG	3.08	0.51
1:B:266:THR:HB	1:C:351:GLY:HA3	1.93	0.50
1:B:160:VAL:HG23	1:B:394:ARG:HD3	1.91	0.50
1:C:291:VAL:HG23	1:C:322:ILE:HD12	1.94	0.49
1:B:291:VAL:HG23	1:B:322:ILE:HD12	1.94	0.49
1:A:573:ILE:HD12	1:A:632:LEU:HB2	1.95	0.49
1:C:420:GLU:CD	1:C:601:GLY:O	2.50	0.49
1:A:266:THR:OG1	1:B:349:LEU:O	2.31	0.49
1:C:573:ILE:HD12	1:C:632:LEU:HB2	1.95	0.48
1:A:291:VAL:HG23	1:A:322:ILE:HD12	1.94	0.48
1:B:179:VAL:HG12	1:B:211:VAL:HG21	1.97	0.47
1:C:179:VAL:HG12	1:C:211:VAL:HG21	1.97	0.46
1:A:336:ARG:NH1	1:B:346:GLN:CG	2.77	0.46
1:A:179:VAL:HG12	1:A:211:VAL:HG21	1.97	0.46
1:B:160:VAL:CG2	1:B:394:ARG:CD	2.78	0.45
1:A:336:ARG:HH11	1:B:346:GLN:CG	2.23	0.45
1:B:291:VAL:CG2	1:B:322:ILE:HD12	2.47	0.45
1:C:197:ARG:NH2	1:C:294:PRO:HG2	2.32	0.45
1:A:291:VAL:CG2	1:A:322:ILE:HD12	2.47	0.45
1:A:400:CYS:SG	1:A:433:CYS:CB	3.05	0.44
1:A:161:LEU:HD11	1:B:287:ASN:HB2	1.99	0.44
1:B:400:CYS:SG	1:B:433:CYS:CB	3.04	0.44
1:A:191:ARG:O	1:B:311:VAL:HG21	2.18	0.44
1:C:420:GLU:CD	1:C:602:GLY:HA3	2.36	0.43
1:C:299:ILE:HG21	1:C:302:ILE:HD12	1.99	0.43
1:A:191:ARG:HB2	1:B:311:VAL:HG11	1.99	0.43
1:C:291:VAL:CG2	1:C:322:ILE:HD12	2.47	0.43
1:C:400:CYS:SG	1:C:433:CYS:CB	3.04	0.43
1:A:608:TYR:O	1:A:647:TYR:HA	2.19	0.43
1:C:197:ARG:NH2	1:C:294:PRO:CG	2.82	0.43
1:A:299:ILE:HG21	1:A:302:ILE:HD12	2.00	0.43
1:A:514:VAL:HG21	1:B:632:LEU:HD11	2.01	0.43
1:A:647:TYR:HB3	1:B:578:PRO:HB3	2.00	0.43
1:A:608:TYR:OH	1:B:632:LEU:HD12	2.19	0.43
1:B:266:THR:OG1	1:C:350:THR:HA	2.16	0.43
1:A:661:VAL:HB	1:B:578:PRO:HB2	2.01	0.43
1:B:299:ILE:HG21	1:B:302:ILE:HD12	1.99	0.43
1:B:266:THR:CB	1:C:350:THR:C	2.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:551:MET:O	1:B:668:ARG:HA	2.20	0.42
1:B:160:VAL:CG2	1:B:394:ARG:NH1	2.81	0.42
1:A:647:TYR:CD1	1:B:578:PRO:HD3	2.54	0.42
1:A:274:LEU:HD11	1:A:357:THR:HG23	2.02	0.42
1:B:573:ILE:HD12	1:B:632:LEU:CB	2.49	0.41
1:A:613:LEU:HD23	1:A:643:VAL:HG23	2.02	0.41
1:B:274:LEU:HD11	1:B:357:THR:HG23	2.02	0.41
1:C:274:LEU:HD11	1:C:357:THR:HG23	2.02	0.41
1:A:611:ILE:HG23	1:A:645:VAL:HG22	2.03	0.41
1:A:336:ARG:HD3	1:B:346:GLN:OE1	2.19	0.40
1:A:223:VAL:CG2	1:B:325:GLN:OE1	2.70	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:ASP:OD2	1:C:156:ARG:NE[2_555]	1.73	0.47
1:A:125:LYS:NZ	1:B:170:LYS:NZ[3_554]	1.89	0.31
1:B:238:SER:OG	1:C:656:LYS:NZ[3_454]	2.04	0.16
1:A:584:CYS:O	1:C:547:GLN:NE2[2_555]	2.08	0.12
1:A:627:GLY:N	1:C:539:LEU:O[2_555]	2.16	0.04

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	509/583 (87%)	486 (96%)	20 (4%)	3 (1%)	30	74
1	B	509/583 (87%)	487 (96%)	20 (4%)	2 (0%)	39	80
1	C	509/583 (87%)	490 (96%)	17 (3%)	2 (0%)	39	80
All	All	1527/1749 (87%)	1463 (96%)	57 (4%)	7 (0%)	34	77

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	282	ASN
1	B	282	ASN
1	C	282	ASN
1	A	434	ASN
1	B	434	ASN
1	C	434	ASN
1	A	549	GLY

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	444/493 (90%)	440 (99%)	4 (1%)	84	93
1	B	444/493 (90%)	438 (99%)	6 (1%)	74	89
1	C	444/493 (90%)	440 (99%)	4 (1%)	84	93
All	All	1332/1479 (90%)	1318 (99%)	14 (1%)	80	91

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	141	ASP
1	A	169	ARG
1	A	313	MET
1	A	456	GLU
1	B	141	ASP
1	B	169	ARG
1	B	313	MET
1	B	456	GLU
1	B	582	MET
1	B	585	SER
1	C	141	ASP
1	C	169	ARG
1	C	313	MET
1	C	456	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	246	HIS
1	A	390	GLN
1	A	465	GLN
1	A	470	HIS
1	A	565	GLN
1	B	246	HIS
1	B	390	GLN
1	B	459	HIS
1	B	465	GLN
1	B	470	HIS
1	C	246	HIS
1	C	390	GLN
1	C	459	HIS
1	C	465	GLN
1	C	470	HIS
1	C	565	GLN
1	C	604	ASN
1	C	648	GLN
1	C	672	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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	521/583 (89%)	0.79	78 (14%) 3 4	49, 135, 243, 274	0
1	B	521/583 (89%)	0.73	67 (12%) 5 5	40, 146, 221, 255	0
1	C	521/583 (89%)	0.70	66 (12%) 5 6	44, 137, 219, 296	0
All	All	1563/1749 (89%)	0.74	211 (13%) 4 5	40, 138, 234, 296	0

All (211) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	437	GLY	11.0
1	A	518	ILE	9.2
1	A	617	LEU	7.3
1	B	396	LEU	7.3
1	C	514	VAL	7.0
1	C	549	GLY	6.7
1	A	519	LYS	6.5
1	A	598	ARG	6.3
1	B	607	GLU	6.2
1	C	421	PRO	6.1
1	B	660	PRO	6.0
1	A	437	GLY	5.5
1	A	664	GLY	5.5
1	A	536	ILE	5.4
1	A	560	GLY	5.4
1	A	517	PHE	5.4
1	C	673	ALA	5.4
1	B	196	GLY	5.4
1	A	641	ALA	5.4
1	A	139	ALA	5.3
1	B	598	ARG	5.3
1	C	513	ALA	5.1
1	A	626	SER	5.0

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Mol	Chain	Res	Type	RSRZ
1	B	601	GLY	4.8
1	C	548	SER	4.8
1	B	562	VAL	4.6
1	B	534	GLU	4.5
1	A	602	GLY	4.5
1	B	438	TYR	4.4
1	A	396	LEU	4.4
1	B	514	VAL	4.4
1	B	522	ASP	4.3
1	B	513	ALA	4.3
1	A	515	ASP	4.3
1	C	147	PHE	4.1
1	B	437	GLY	4.0
1	C	601	GLY	4.0
1	B	414	PHE	4.0
1	A	535	GLU	4.0
1	C	438	TYR	4.0
1	A	585	SER	3.9
1	B	585	SER	3.9
1	C	396	LEU	3.9
1	B	162	ARG	3.8
1	B	139	ALA	3.8
1	B	551	MET	3.8
1	C	146	THR	3.8
1	A	438	TYR	3.8
1	A	573	ILE	3.8
1	C	615	GLU	3.7
1	A	516	MET	3.7
1	B	627	GLY	3.7
1	B	229	LYS	3.7
1	A	522	ASP	3.7
1	C	584	CYS	3.7
1	C	559	ALA	3.7
1	C	228	ASP	3.7
1	B	517	PHE	3.6
1	A	655	ALA	3.6
1	B	552	HIS	3.6
1	A	587	GLY	3.6
1	A	672	GLN	3.6
1	A	534	GLU	3.5
1	B	491	THR	3.5
1	B	151	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	670	ASN	3.5
1	A	414	PHE	3.4
1	B	312	ASP	3.4
1	A	302	ILE	3.4
1	A	643	VAL	3.4
1	C	602	GLY	3.4
1	B	515	ASP	3.4
1	A	603	GLU	3.4
1	C	617	LEU	3.4
1	C	665	TRP	3.3
1	A	529	ASP	3.3
1	A	574	ASP	3.3
1	C	427	ALA	3.3
1	A	520	ILE	3.2
1	B	659	GLY	3.2
1	A	411	ARG	3.2
1	B	648	GLN	3.2
1	A	561	LYS	3.2
1	C	564	VAL	3.2
1	A	665	TRP	3.1
1	C	639	ASN	3.1
1	C	443	GLY	3.1
1	A	547	GLN	3.1
1	B	425	TYR	3.1
1	A	658	GLY	3.1
1	C	627	GLY	3.1
1	C	537	ASP	3.0
1	C	546	SER	3.0
1	B	673	ALA	3.0
1	B	666	ASN	3.0
1	C	527	SER	3.0
1	C	663	TYR	3.0
1	C	423	ILE	3.0
1	A	220	GLU	3.0
1	C	573	ILE	3.0
1	C	420	GLU	2.9
1	B	649	PRO	2.9
1	B	195	ASP	2.9
1	A	552	HIS	2.9
1	B	640	PHE	2.9
1	C	552	HIS	2.9
1	B	150	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	427	ALA	2.8
1	C	632	LEU	2.8
1	C	414	PHE	2.8
1	A	618	VAL	2.8
1	C	442	THR	2.8
1	A	667	ILE	2.8
1	C	577	THR	2.7
1	A	158	ASP	2.7
1	A	397	CYS	2.7
1	C	155	PHE	2.7
1	B	526	GLU	2.7
1	A	651	LYS	2.7
1	C	226	LEU	2.7
1	C	518	ILE	2.7
1	C	459	HIS	2.7
1	A	219	GLY	2.7
1	C	547	GLN	2.7
1	A	663	TYR	2.7
1	A	218	HIS	2.6
1	C	585	SER	2.6
1	A	635	ASN	2.6
1	C	659	GLY	2.6
1	A	427	ALA	2.6
1	C	425	TYR	2.6
1	B	668	ARG	2.6
1	A	157	VAL	2.6
1	B	656	LYS	2.6
1	B	410	GLN	2.6
1	B	397	CYS	2.5
1	A	399	ASP	2.5
1	B	192	VAL	2.5
1	A	155	PHE	2.5
1	B	458	ILE	2.5
1	C	194	GLN	2.5
1	A	551	MET	2.5
1	B	211	VAL	2.4
1	A	590	TYR	2.4
1	C	139	ALA	2.4
1	C	411	ARG	2.4
1	B	268	SER	2.4
1	C	213	THR	2.4
1	C	672	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	492	SER	2.4
1	C	536	ILE	2.4
1	B	146	THR	2.4
1	B	125	LYS	2.4
1	A	436	LYS	2.4
1	A	659	GLY	2.4
1	A	559	ALA	2.4
1	A	604	ASN	2.4
1	B	550	SER	2.4
1	C	215	PRO	2.4
1	A	401	LYS	2.4
1	C	551	MET	2.3
1	B	476	PRO	2.3
1	C	522	ASP	2.3
1	A	581	MET	2.3
1	A	553	MET	2.3
1	C	489	GLY	2.3
1	C	553	MET	2.3
1	A	176	VAL	2.3
1	A	301	GLY	2.3
1	B	639	ASN	2.3
1	B	653	ASP	2.3
1	B	606	VAL	2.3
1	A	668	ARG	2.3
1	A	627	GLY	2.3
1	B	574	ASP	2.3
1	A	435	HIS	2.3
1	B	602	GLY	2.3
1	A	391	ARG	2.3
1	B	439	ARG	2.3
1	A	135	ILE	2.2
1	C	581	MET	2.2
1	C	211	VAL	2.2
1	A	143	HIS	2.2
1	C	642	GLN	2.2
1	B	267	GLY	2.2
1	B	431	PRO	2.2
1	A	172	SER	2.2
1	B	435	HIS	2.2
1	B	197	ARG	2.2
1	B	426	ARG	2.2
1	A	630	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	648	GLN	2.2
1	A	588	LYS	2.2
1	A	656	LYS	2.2
1	A	591	PRO	2.2
1	C	515	ASP	2.2
1	A	589	HIS	2.2
1	B	641	ALA	2.1
1	B	600	ALA	2.1
1	C	598	ARG	2.1
1	C	207	VAL	2.1
1	C	670	ASN	2.1
1	C	218	HIS	2.1
1	B	191	ARG	2.1
1	C	328	ASP	2.1
1	A	586	SER	2.0
1	B	210	ARG	2.0
1	B	429	GLY	2.0
1	C	565	GLN	2.0
1	B	401	LYS	2.0
1	A	660	PRO	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.