Full wwPDB X-ray Structure Validation Report (i)

Feb 19, 2024 – 06:31 PM EST

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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

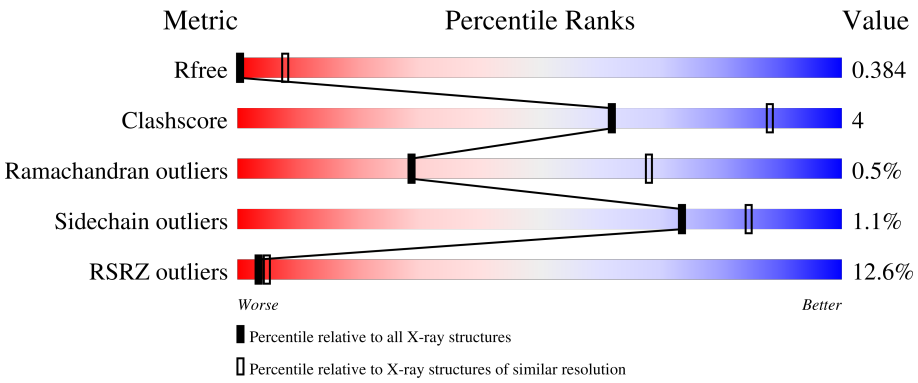
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 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}	130704	1005 (4.62-3.78)
Clashscore	141614	1044 (4.60-3.80)
Ramachandran outliers	138981	1000 (4.60-3.80)
Sidechain outliers	138945	1007 (4.62-3.78)
RSRZ outliers	127900	1063 (4.70-3.70)

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	583	13% 82% 7% • 11%
1	B	583	10% 82% 7% • 11%
1	C	583	10% 83% 6% • 11%

2 Entry composition (i)

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
			Total	C	N	O	S			
1	A	521	4021	2508	724	767	22	0	0	0
1	B	521	4021	2508	724	767	22	0	0	0
1	C	521	4021	2508	724	767	22	0	0	0

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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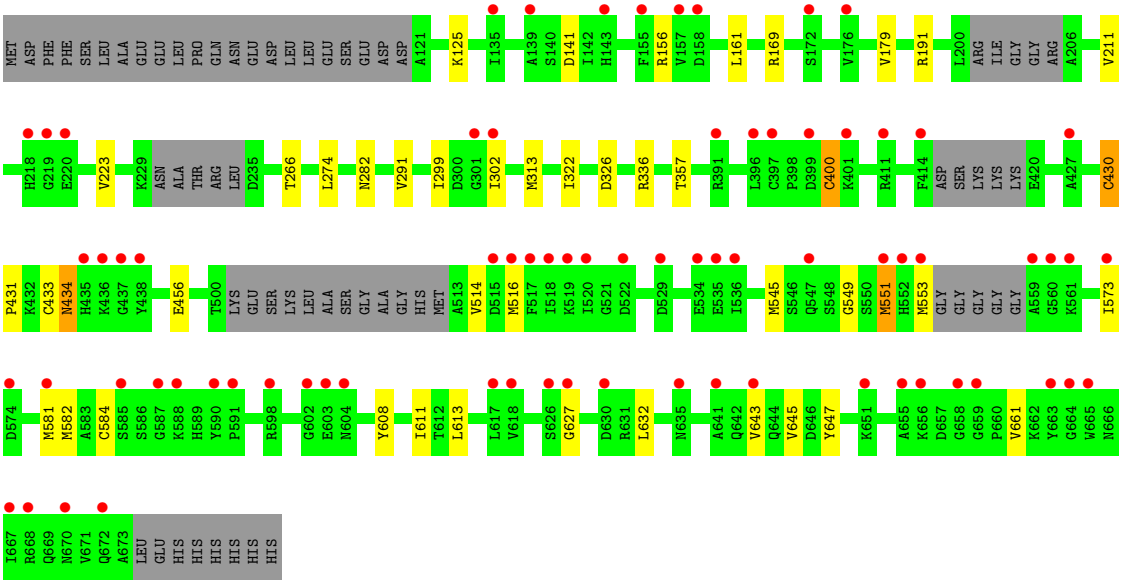
Chain	Residue	Modelled	Actual	Comment	Reference
B	508	GLY	-	linker	UNP P37093
B	509	ALA	-	linker	UNP P37093
B	510	GLY	-	linker	UNP P37093
B	511	HIS	-	linker	UNP P37093
B	674	LEU	-	expression tag	UNP Q02UZ4
B	675	GLU	-	expression tag	UNP Q02UZ4
B	676	HIS	-	expression tag	UNP Q02UZ4
B	677	HIS	-	expression 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

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.

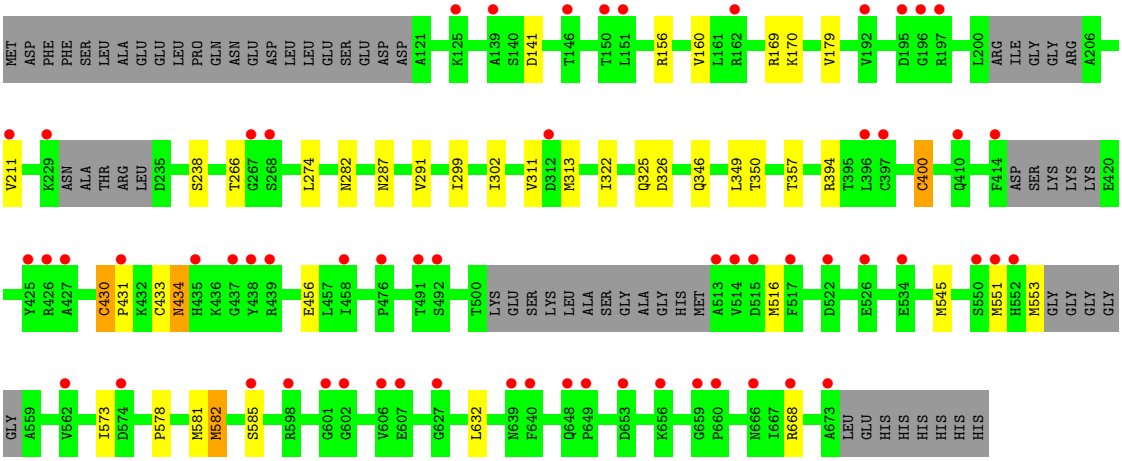
• Molecule 1: Type II secretion system protein E, Hemolysin-coregulated protein

Chain A:



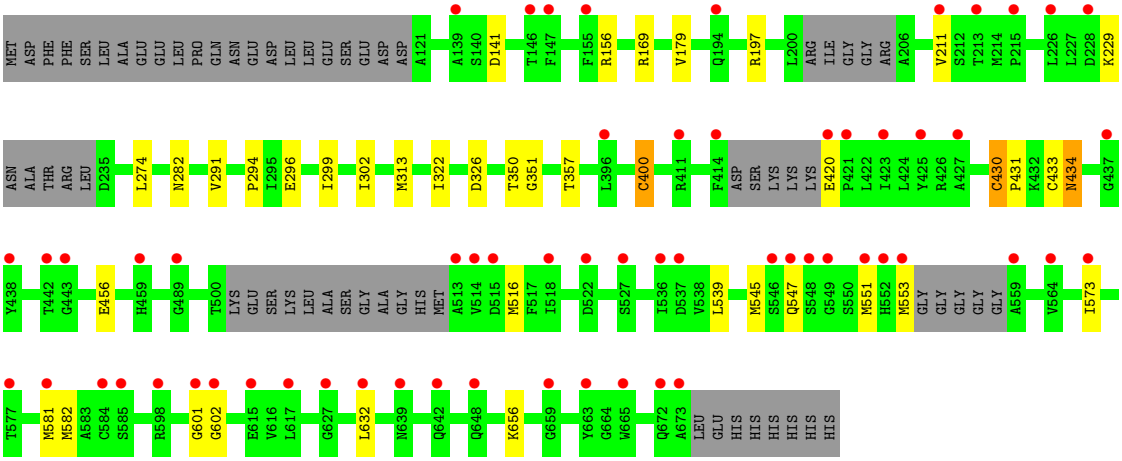
• Molecule 1: Type II secretion system protein E, Hemolysin-coregulated protein

Chain B:



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

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 21 21	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
$< I/\sigma(I) >$ [1]	1.59 (at 3.76Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.384 , 0.376 0.389 , 0.384	Depositor DCC
R_{free} test set	1107 reflections (5.13%)	wwPDB-VP
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
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	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.*

[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 (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	0.38	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(^{o})	Ideal(^{o})
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 (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	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:160:VAL:HG23	1:B:394:ARG:HD3	1.91	0.50
1:B:266:THR:HB	1:C:351:GLY:HA3	1.93	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:A:336:ARG:HH11	1:B:346:GLN:CG	2.23	0.45
1:B:160:VAL:CG2	1:B:394:ARG:CD	2.78	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:161:LEU:HD11	1:B:287:ASN:HB2	1.99	0.44
1:A:400:CYS:SG	1:A:433:CYS:CB	3.05	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:299:ILE:HG21	1:C:302:ILE:HD12	1.99	0.43
1:C:420:GLU:CD	1:C:602:GLY:HA3	2.36	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:299:ILE:HG21	1:A:302:ILE:HD12	2.00	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:514:VAL:HG21	1:B:632:LEU:HD11	2.01	0.43
1:A:608:TYR:OH	1:B:632:LEU:HD12	2.19	0.43
1:A:647:TYR:HB3	1:B:578:PRO:HB3	2.00	0.43
1:A:661:VAL:HB	1:B:578:PRO:HB2	2.01	0.43
1:B:266:THR:OG1	1:C:350:THR:HA	2.16	0.43
1:B:299:ILE:HG21	1:B:302:ILE:HD12	1.99	0.43
1:A:551:MET:O	1:B:668:ARG:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:266:THR:CB	1:C:350:THR:C	2.81	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:A:613:LEU:HD23	1:A:643:VAL:HG23	2.02	0.41
1:B:573:ILE:HD12	1:B:632:LEU:CB	2.49	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%)	25	64
1	B	509/583 (87%)	487 (96%)	20 (4%)	2 (0%)	34	72
1	C	509/583 (87%)	490 (96%)	17 (3%)	2 (0%)	34	72
All	All	1527/1749 (87%)	1463 (96%)	57 (4%)	7 (0%)	29	68

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%)	78	87
1	B	444/493 (90%)	438 (99%)	6 (1%)	67	80
1	C	444/493 (90%)	440 (99%)	4 (1%)	78	87
All	All	1332/1479 (90%)	1318 (99%)	14 (1%)	73	84

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

Sometimes 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 (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 monosaccharides 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 (i)

6.1 Protein, DNA and RNA chains (i)

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%)	0.71	75 (14%)	2	3	49, 135, 243, 274	0
1	B	521/583 (89%)	0.66	61 (11%)	4	5	40, 146, 221, 255	0
1	C	521/583 (89%)	0.63	61 (11%)	4	5	44, 137, 219, 296	0
All	All	1563/1749 (89%)	0.67	197 (12%)	3	5	40, 138, 234, 296	0

All (197) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	437	GLY	10.4
1	A	518	ILE	8.7
1	A	617	LEU	6.9
1	B	396	LEU	6.8
1	C	514	VAL	6.6
1	A	519	LYS	6.4
1	C	549	GLY	6.3
1	A	598	ARG	6.1
1	C	421	PRO	6.0
1	B	607	GLU	5.9
1	B	660	PRO	5.9
1	A	437	GLY	5.2
1	A	664	GLY	5.2
1	B	598	ARG	5.1
1	A	560	GLY	5.1
1	B	196	GLY	5.1
1	A	517	PHE	5.1
1	A	536	ILE	5.1
1	C	673	ALA	4.9
1	A	641	ALA	4.9
1	A	139	ALA	4.8
1	A	626	SER	4.8
1	C	513	ALA	4.6

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Mol	Chain	Res	Type	RSRZ
1	C	548	SER	4.6
1	B	601	GLY	4.5
1	B	562	VAL	4.4
1	B	534	GLU	4.3
1	A	602	GLY	4.3
1	B	522	ASP	4.1
1	A	396	LEU	4.1
1	B	514	VAL	4.1
1	A	515	ASP	4.1
1	B	438	TYR	4.0
1	B	513	ALA	3.9
1	C	147	PHE	3.9
1	B	437	GLY	3.8
1	A	535	GLU	3.8
1	C	601	GLY	3.8
1	B	414	PHE	3.8
1	B	585	SER	3.8
1	A	585	SER	3.8
1	B	162	ARG	3.7
1	B	229	LYS	3.6
1	B	551	MET	3.6
1	C	584	CYS	3.6
1	C	438	TYR	3.6
1	C	396	LEU	3.6
1	C	146	THR	3.6
1	C	615	GLU	3.6
1	A	573	ILE	3.5
1	A	522	ASP	3.5
1	A	516	MET	3.5
1	B	627	GLY	3.5
1	B	139	ALA	3.5
1	C	228	ASP	3.5
1	A	438	TYR	3.5
1	A	672	GLN	3.4
1	B	517	PHE	3.4
1	B	552	HIS	3.4
1	A	534	GLU	3.4
1	A	587	GLY	3.4
1	A	670	ASN	3.4
1	C	559	ALA	3.3
1	A	655	ALA	3.3
1	B	312	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	491	THR	3.3
1	A	414	PHE	3.2
1	A	603	GLU	3.2
1	A	643	VAL	3.2
1	B	151	LEU	3.2
1	B	515	ASP	3.2
1	A	302	ILE	3.2
1	C	602	GLY	3.2
1	A	561	LYS	3.1
1	A	529	ASP	3.1
1	C	617	LEU	3.1
1	A	411	ARG	3.1
1	A	574	ASP	3.1
1	C	665	TRP	3.1
1	B	648	GLN	3.0
1	B	659	GLY	3.0
1	A	520	ILE	3.0
1	C	639	ASN	3.0
1	C	564	VAL	3.0
1	C	427	ALA	3.0
1	A	547	GLN	2.9
1	C	443	GLY	2.9
1	C	546	SER	2.9
1	B	666	ASN	2.9
1	C	537	ASP	2.9
1	A	665	TRP	2.9
1	A	658	GLY	2.9
1	C	527	SER	2.9
1	C	627	GLY	2.9
1	B	649	PRO	2.8
1	A	220	GLU	2.8
1	B	425	TYR	2.8
1	C	420	GLU	2.8
1	B	195	ASP	2.8
1	C	423	ILE	2.7
1	B	673	ALA	2.7
1	A	552	HIS	2.7
1	C	573	ILE	2.7
1	C	663	TYR	2.7
1	C	552	HIS	2.7
1	B	640	PHE	2.7
1	A	397	CYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	150	THR	2.6
1	A	651	LYS	2.6
1	A	618	VAL	2.6
1	C	414	PHE	2.6
1	C	632	LEU	2.6
1	A	158	ASP	2.6
1	C	442	THR	2.6
1	C	577	THR	2.6
1	A	667	ILE	2.5
1	B	427	ALA	2.5
1	B	526	GLU	2.5
1	C	547	GLN	2.5
1	B	656	LYS	2.5
1	C	155	PHE	2.5
1	A	219	GLY	2.5
1	A	635	ASN	2.5
1	C	459	HIS	2.5
1	B	668	ARG	2.5
1	B	397	CYS	2.5
1	C	585	SER	2.5
1	C	518	ILE	2.5
1	C	226	LEU	2.5
1	B	410	GLN	2.4
1	A	218	HIS	2.4
1	C	659	GLY	2.4
1	A	157	VAL	2.4
1	A	663	TYR	2.4
1	C	194	GLN	2.4
1	A	399	ASP	2.4
1	B	192	VAL	2.3
1	A	427	ALA	2.3
1	C	411	ARG	2.3
1	A	155	PHE	2.3
1	C	425	TYR	2.3
1	A	436	LYS	2.3
1	B	125	LYS	2.3
1	C	672	GLN	2.3
1	A	551	MET	2.3
1	B	492	SER	2.3
1	B	211	VAL	2.3
1	B	268	SER	2.3
1	B	458	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	401	LYS	2.3
1	C	215	PRO	2.3
1	A	604	ASN	2.3
1	B	476	PRO	2.3
1	C	213	THR	2.3
1	B	550	SER	2.2
1	B	146	THR	2.2
1	A	659	GLY	2.2
1	C	536	ILE	2.2
1	C	522	ASP	2.2
1	B	639	ASN	2.2
1	A	590	TYR	2.2
1	C	139	ALA	2.2
1	C	551	MET	2.2
1	A	176	VAL	2.2
1	A	581	MET	2.2
1	A	668	ARG	2.2
1	C	489	GLY	2.2
1	A	553	MET	2.2
1	C	553	MET	2.2
1	A	301	GLY	2.2
1	A	391	ARG	2.2
1	B	653	ASP	2.2
1	B	431	PRO	2.1
1	B	439	ARG	2.1
1	B	606	VAL	2.1
1	A	559	ALA	2.1
1	A	627	GLY	2.1
1	B	574	ASP	2.1
1	A	588	LYS	2.1
1	A	656	LYS	2.1
1	A	591	PRO	2.1
1	B	602	GLY	2.1
1	B	426	ARG	2.1
1	A	435	HIS	2.1
1	B	197	ARG	2.1
1	C	642	GLN	2.1
1	A	172	SER	2.1
1	A	143	HIS	2.1
1	C	648	GLN	2.1
1	C	581	MET	2.1
1	C	211	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	267	GLY	2.1
1	A	630	ASP	2.1
1	A	135	ILE	2.1
1	B	435	HIS	2.1
1	C	515	ASP	2.0
1	C	598	ARG	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.