Full wwPDB X-ray Structure Validation Report (i)

Oct 11, 2021 – 07:42 AM EDT

PDB ID	:	2RET
Title	:	The crystal structure of a binary complex of two pseudopilins: EpsI and EpsJ from the Type 2 Secretion System of Vibrio vulnificus
Authors	:	Yanez, M.E.; Korotkov, K.V.; Abendroth, J.; Hol, W.G.J.
Deposited on	:	2007-09-27
Resolution	:	2.21 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 following versions of software and data (see references (i)) were used in the production of this report:

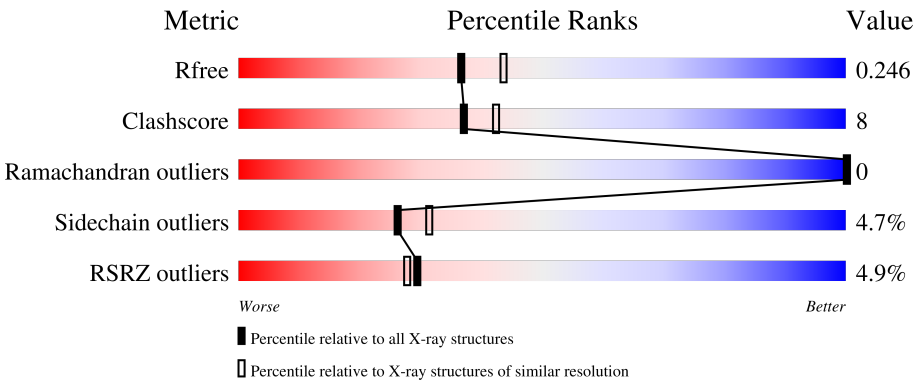
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 2.21 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	5912 (2.24-2.20)
Clashscore	141614	6646 (2.24-2.20)
Ramachandran outliers	138981	6543 (2.24-2.20)
Sidechain outliers	138945	6544 (2.24-2.20)
RSRZ outliers	127900	5797 (2.24-2.20)

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	103	4%, 65%, 15%, •, 18%
1	C	103	5%, 61%, 14%, •, 22%
1	E	103	7%, 66%, 12%, •, 20%
1	G	103	8%, 66%, 13%, 21%
2	B	175	3%, 78%, 12%, •, 9%

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Mol	Chain	Length	Quality of chain
2	D	175	% 77% 10% • 11%
2	F	175	2% 76% 13% • 11%
2	H	175	6% 78% 9% • 10%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 8286 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 Pseudopilin EpsI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	Se			
1	A	84	637	408	103	120	6	0	1	0
1	C	80	608	391	97	114	6	0	1	0
1	E	82	627	402	101	118	6	0	1	0
1	G	81	617	396	99	116	6	0	1	0

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	24	MSE	-	expression tag	UNP Q7MPZ1
A	96	THR	GLU	engineered mutation	UNP Q7MPZ1
A	97	THR	LYS	engineered mutation	UNP Q7MPZ1
A	111	SER	-	expression tag	UNP Q7MPZ1
A	112	GLU	-	expression tag	UNP Q7MPZ1
A	113	ASN	-	expression tag	UNP Q7MPZ1
A	114	LEU	-	expression tag	UNP Q7MPZ1
A	115	TYR	-	expression tag	UNP Q7MPZ1
A	116	PHE	-	expression tag	UNP Q7MPZ1
A	117	GLN	-	expression tag	UNP Q7MPZ1
A	118	GLY	-	expression tag	UNP Q7MPZ1
A	119	GLY	-	expression tag	UNP Q7MPZ1
A	120	GLY	-	expression tag	UNP Q7MPZ1
A	121	HIS	-	expression tag	UNP Q7MPZ1
A	122	HIS	-	expression tag	UNP Q7MPZ1
A	123	HIS	-	expression tag	UNP Q7MPZ1
A	124	HIS	-	expression tag	UNP Q7MPZ1
A	125	HIS	-	expression tag	UNP Q7MPZ1
A	126	HIS	-	expression tag	UNP Q7MPZ1
C	24	MSE	-	expression tag	UNP Q7MPZ1
C	96	THR	GLU	engineered mutation	UNP Q7MPZ1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	97	THR	LYS	engineered mutation	UNP Q7MPZ1
C	111	SER	-	expression tag	UNP Q7MPZ1
C	112	GLU	-	expression tag	UNP Q7MPZ1
C	113	ASN	-	expression tag	UNP Q7MPZ1
C	114	LEU	-	expression tag	UNP Q7MPZ1
C	115	TYR	-	expression tag	UNP Q7MPZ1
C	116	PHE	-	expression tag	UNP Q7MPZ1
C	117	GLN	-	expression tag	UNP Q7MPZ1
C	118	GLY	-	expression tag	UNP Q7MPZ1
C	119	GLY	-	expression tag	UNP Q7MPZ1
C	120	GLY	-	expression tag	UNP Q7MPZ1
C	121	HIS	-	expression tag	UNP Q7MPZ1
C	122	HIS	-	expression tag	UNP Q7MPZ1
C	123	HIS	-	expression tag	UNP Q7MPZ1
C	124	HIS	-	expression tag	UNP Q7MPZ1
C	125	HIS	-	expression tag	UNP Q7MPZ1
C	126	HIS	-	expression tag	UNP Q7MPZ1
E	24	MSE	-	expression tag	UNP Q7MPZ1
E	96	THR	GLU	engineered mutation	UNP Q7MPZ1
E	97	THR	LYS	engineered mutation	UNP Q7MPZ1
E	111	SER	-	expression tag	UNP Q7MPZ1
E	112	GLU	-	expression tag	UNP Q7MPZ1
E	113	ASN	-	expression tag	UNP Q7MPZ1
E	114	LEU	-	expression tag	UNP Q7MPZ1
E	115	TYR	-	expression tag	UNP Q7MPZ1
E	116	PHE	-	expression tag	UNP Q7MPZ1
E	117	GLN	-	expression tag	UNP Q7MPZ1
E	118	GLY	-	expression tag	UNP Q7MPZ1
E	119	GLY	-	expression tag	UNP Q7MPZ1
E	120	GLY	-	expression tag	UNP Q7MPZ1
E	121	HIS	-	expression tag	UNP Q7MPZ1
E	122	HIS	-	expression tag	UNP Q7MPZ1
E	123	HIS	-	expression tag	UNP Q7MPZ1
E	124	HIS	-	expression tag	UNP Q7MPZ1
E	125	HIS	-	expression tag	UNP Q7MPZ1
E	126	HIS	-	expression tag	UNP Q7MPZ1
G	24	MSE	-	expression tag	UNP Q7MPZ1
G	96	THR	GLU	engineered mutation	UNP Q7MPZ1
G	97	THR	LYS	engineered mutation	UNP Q7MPZ1
G	111	SER	-	expression tag	UNP Q7MPZ1
G	112	GLU	-	expression tag	UNP Q7MPZ1
G	113	ASN	-	expression tag	UNP Q7MPZ1

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Chain	Residue	Modelled	Actual	Comment	Reference
G	114	LEU	-	expression tag	UNP Q7MPZ1
G	115	TYR	-	expression tag	UNP Q7MPZ1
G	116	PHE	-	expression tag	UNP Q7MPZ1
G	117	GLN	-	expression tag	UNP Q7MPZ1
G	118	GLY	-	expression tag	UNP Q7MPZ1
G	119	GLY	-	expression tag	UNP Q7MPZ1
G	120	GLY	-	expression tag	UNP Q7MPZ1
G	121	HIS	-	expression tag	UNP Q7MPZ1
G	122	HIS	-	expression tag	UNP Q7MPZ1
G	123	HIS	-	expression tag	UNP Q7MPZ1
G	124	HIS	-	expression tag	UNP Q7MPZ1
G	125	HIS	-	expression tag	UNP Q7MPZ1
G	126	HIS	-	expression tag	UNP Q7MPZ1

- Molecule 2 is a protein called EpsJ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	Se			
2	B	159	1321	839	243	236	3	0	3	0
2	D	155	1285	818	232	232	3	0	1	0
2	F	156	1289	820	234	232	3	0	1	0
2	H	157	1287	819	233	232	3	0	1	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
3	B	1	1	1	0	0
3	F	1	1	1	0	0

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
4	F	1	1	1	0	0
4	H	1	1	1	0	0

- Molecule 5 is water.

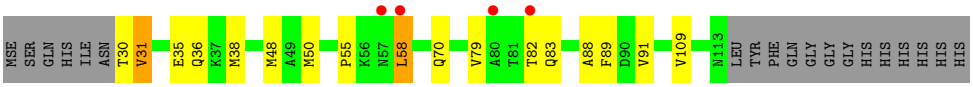
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	73	Total O 73 73	0	0
5	B	101	Total O 101 101	0	0
5	C	55	Total O 55 55	0	0
5	D	112	Total O 112 112	0	0
5	E	55	Total O 55 55	0	0
5	F	94	Total O 94 94	0	0
5	G	46	Total O 46 46	0	0
5	H	75	Total O 75 75	0	0

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.

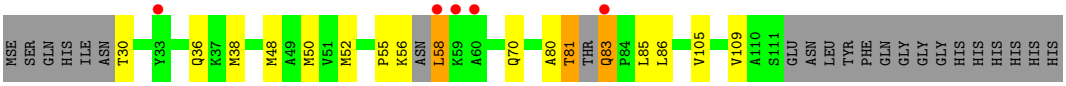
- Molecule 1: Pseudopilin EpsI

Chain A:



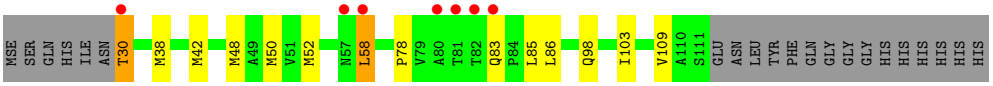
- Molecule 1: Pseudopilin EpsI

Chain C:



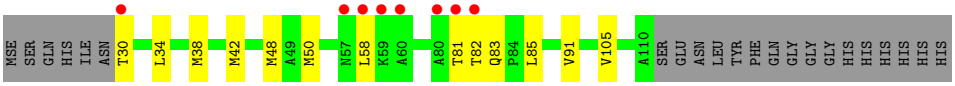
- Molecule 1: Pseudopilin EpsI

Chain E:



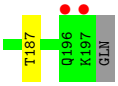
- Molecule 1: Pseudopilin EpsI

Chain G:



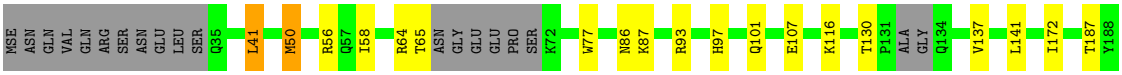
- Molecule 2: EpsJ

Chain B:



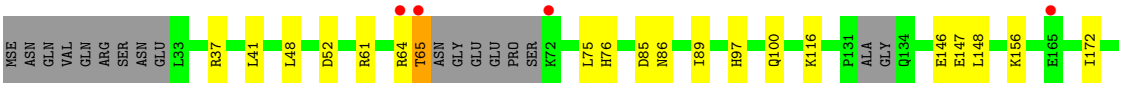
• Molecule 2: EpsJ

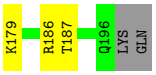
Chain D:



• Molecule 2: EpsJ

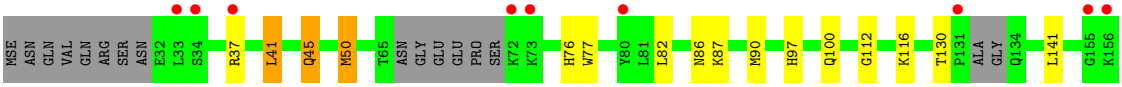
Chain F:





• Molecule 2: EpsJ

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	63.29Å 79.14Å 82.08Å 65.00° 69.19° 69.49°	Depositor
Resolution (Å)	40.39 – 2.21 40.41 – 2.21	Depositor EDS
% Data completeness (in resolution range)	96.3 (40.39-2.21) 96.3 (40.41-2.21)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.68 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.3.0037	Depositor
R, R_{free}	0.185 , 0.245 0.188 , 0.246	Depositor DCC
R_{free} test set	3205 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	36.3	Xtriage
Anisotropy	0.069	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 51.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.013 for -h,-l,-k	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8286	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.58% 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)

Bond lengths and bond angles in the following residue types are not validated in this section: NA, CL

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	0.74	0/647	0.69	0/873
1	C	0.76	0/616	0.72	0/828
1	E	0.75	0/637	0.67	0/859
1	G	0.70	0/627	0.70	0/847
2	B	0.71	0/1352	0.83	1/1825 (0.1%)
2	D	0.69	0/1313	0.83	2/1773 (0.1%)
2	F	0.71	0/1314	0.76	0/1775
2	H	0.64	0/1315	0.80	4/1778 (0.2%)
All	All	0.70	0/7821	0.77	7/10558 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	D	0	1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	93	ARG	NE-CZ-NH1	6.70	123.65	120.30
2	H	186[A]	ARG	NE-CZ-NH1	5.76	123.18	120.30
2	H	186[B]	ARG	NE-CZ-NH1	5.76	123.18	120.30
2	D	93	ARG	NE-CZ-NH1	5.59	123.09	120.30
2	D	56	ARG	NE-CZ-NH1	5.42	123.01	120.30
2	H	186[A]	ARG	NE-CZ-NH2	-5.17	117.71	120.30
2	H	186[B]	ARG	NE-CZ-NH2	-5.17	117.71	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	64	ARG	Peptide

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	637	0	641	20	0
1	C	608	0	611	23	0
1	E	627	0	637	18	0
1	G	617	0	621	21	0
2	B	1321	0	1297	24	0
2	D	1285	0	1265	20	0
2	F	1289	0	1262	20	0
2	H	1287	0	1254	18	0
3	B	1	0	0	0	0
3	F	1	0	0	0	0
4	F	1	0	0	0	0
4	H	1	0	0	0	0
5	A	73	0	0	3	0
5	B	101	0	0	1	0
5	C	55	0	0	2	0
5	D	112	0	0	1	0
5	E	55	0	0	3	0
5	F	94	0	0	2	0
5	G	46	0	0	0	0
5	H	75	0	0	2	0
All	All	8286	0	7588	119	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 8.

All (119) 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:A:30:THR:N	5:A:183:HOH:O	2.14	0.80
1:C:50:MSE:HE3	2:D:187:THR:HG21	1.64	0.79
1:E:30:THR:N	5:E:177:HOH:O	2.18	0.76
1:A:50:MSE:HA	1:A:50:MSE:HE2	1.70	0.73
1:A:83:GLN:HE22	1:E:86:LEU:HD12	1.54	0.73
1:C:38:MSE:HE1	2:D:41:LEU:HD13	1.70	0.72
1:C:83:GLN:HE22	1:C:85:LEU:HD12	1.53	0.71
1:E:50:MSE:HE3	2:F:187:THR:HG21	1.73	0.70
2:B:97:HIS:HE1	2:D:97:HIS:CE1	2.11	0.69
2:B:97:HIS:CE1	2:D:97:HIS:CE1	2.80	0.69
2:H:97:HIS:NE2	5:H:227:HOH:O	2.20	0.69
2:F:48:LEU:HD22	2:F:186[A]:ARG:NH1	2.08	0.68
1:C:83:GLN:NE2	1:C:85:LEU:HD12	2.11	0.66
1:G:50:MSE:HA	1:G:50:MSE:HE2	1.78	0.66
1:A:55:PRO:HB2	1:A:109:VAL:HG11	1.77	0.65
1:A:31:VAL:HG21	2:B:37:ARG:HB3	1.79	0.64
1:A:58:LEU:HD21	1:A:89:PHE:CD1	2.34	0.62
2:F:186[A]:ARG:CZ	5:F:215:HOH:O	2.49	0.61
1:G:38:MSE:HE1	2:H:41:LEU:CD2	2.32	0.59
2:B:130:THR:HG23	5:B:252:HOH:O	2.04	0.58
1:G:38:MSE:CE	2:H:41:LEU:CD2	2.82	0.58
2:B:99:PRO:HG3	2:D:189:LEU:HD12	1.86	0.58
1:A:48[A]:MSE:HE3	5:A:127:HOH:O	2.04	0.58
1:C:38:MSE:HE1	2:D:41:LEU:CD1	2.33	0.58
2:B:64:ARG:O	2:B:65:THR:HB	2.03	0.58
1:G:38:MSE:HE1	2:H:41:LEU:HD22	1.86	0.57
1:G:38:MSE:HE2	2:H:45:GLN:OE1	2.04	0.57
1:C:80:ALA:O	1:G:82:THR:HG21	2.04	0.57
1:A:48[B]:MSE:HG2	1:A:91:VAL:HG21	1.85	0.57
2:H:82:LEU:HD11	2:H:112:GLY:HA3	1.87	0.56
1:E:38:MSE:CE	2:F:41:LEU:HD22	2.36	0.56
1:E:103:ILE:HD12	5:E:129:HOH:O	2.05	0.55
2:B:145:VAL:HG22	2:B:178:LEU:HD22	1.88	0.55
1:C:48[B]:MSE:SE	1:C:105:VAL:HG11	2.56	0.55
1:A:38:MSE:CE	2:B:41:LEU:HD22	2.36	0.54
1:G:83:GLN:NE2	1:G:85:LEU:HD12	2.23	0.54
2:D:50:MSE:HG2	2:D:141:LEU:HD21	1.90	0.54
1:E:58:LEU:HD12	1:E:78:PRO:HG3	1.90	0.54
1:G:38:MSE:HE1	2:H:41:LEU:CD1	2.38	0.54
2:B:110:LYS:NZ	2:B:130:THR:HG22	2.23	0.53
1:E:83:GLN:NE2	1:E:85:LEU:HB2	2.24	0.53
1:A:36:GLN:HE22	1:A:70:GLN:HE22	1.56	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:GLU:HG3	2:B:41:LEU:HD11	1.90	0.52
1:A:48[B]:MSE:HE1	5:D:263:HOH:O	2.10	0.52
1:C:50:MSE:CE	2:D:187:THR:HG21	2.36	0.52
1:E:50:MSE:HA	1:E:50:MSE:HE2	1.91	0.51
2:F:76:HIS:O	2:F:89:ILE:HD12	2.10	0.51
1:C:38:MSE:CE	2:D:41:LEU:HD13	2.40	0.51
2:B:97:HIS:CE1	2:D:97:HIS:NE2	2.79	0.50
1:E:42:MSE:HE3	2:F:186[B]:ARG:HG2	1.94	0.50
2:B:83:ASP:O	2:B:116:LYS:CE	2.60	0.50
1:G:38:MSE:CE	2:H:41:LEU:HD21	2.42	0.49
2:B:130:THR:HG23	2:B:130:THR:O	2.12	0.49
1:C:55:PRO:O	1:C:58:LEU:HB2	2.13	0.49
1:E:38:MSE:HE1	2:F:41:LEU:HD22	1.95	0.49
1:G:38:MSE:HE1	2:H:41:LEU:HD13	1.95	0.49
2:F:75:LEU:HD11	2:F:172:ILE:HD11	1.95	0.49
1:E:50:MSE:HE3	2:F:187:THR:CG2	2.42	0.48
2:F:97:HIS:CE1	2:H:97:HIS:CE1	3.02	0.48
2:B:83:ASP:O	2:B:116:LYS:HE3	2.13	0.48
2:D:58:ILE:CD1	2:D:172:ILE:HD12	2.43	0.48
1:C:50:MSE:HA	1:C:50:MSE:HE2	1.95	0.48
2:B:97:HIS:CE1	2:D:97:HIS:HE1	2.31	0.48
1:A:83:GLN:HE22	1:E:86:LEU:CD1	2.24	0.48
1:G:83:GLN:HE22	1:G:85:LEU:HD12	1.78	0.48
1:C:81:THR:HG23	5:C:269:HOH:O	2.14	0.47
1:G:83:GLN:HE21	1:G:85:LEU:HG	1.79	0.47
2:B:97:HIS:HE1	2:D:97:HIS:NE2	2.12	0.47
2:B:100:GLN:HE21	2:B:105[B]:ARG:NH2	2.12	0.47
1:C:38:MSE:HE1	2:D:41:LEU:HD22	1.95	0.47
1:C:38:MSE:CE	2:D:41:LEU:HD22	2.44	0.47
1:E:98:GLN:NE2	5:E:181:HOH:O	2.42	0.47
2:H:76:HIS:CD2	2:H:90:MSE:HE2	2.49	0.47
2:F:146:GLU:OE2	2:F:179:LYS:HA	2.14	0.47
1:A:50:MSE:HA	1:A:50:MSE:CE	2.43	0.46
2:F:64:ARG:O	2:F:65:THR:HB	2.16	0.46
1:G:38:MSE:CE	2:H:41:LEU:HD22	2.45	0.46
1:C:56:LYS:O	1:C:58:LEU:N	2.49	0.45
1:A:82:THR:HG22	1:A:82:THR:O	2.15	0.45
1:C:38:MSE:CE	2:D:41:LEU:CD1	2.94	0.45
1:G:38:MSE:HE3	2:H:41:LEU:HD21	1.97	0.45
2:H:50:MSE:HG2	2:H:141:LEU:HD21	1.98	0.45
1:E:52:MSE:SE	1:E:109:VAL:HG22	2.67	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:186[A]:ARG:NH1	5:F:215:HOH:O	2.49	0.44
2:B:73:LYS:HB2	2:B:76:HIS:CE1	2.53	0.44
2:F:85:ASP:OD1	2:F:116:LYS:NZ	2.49	0.44
1:C:50:MSE:HE3	2:D:187:THR:CG2	2.41	0.44
1:E:50:MSE:CE	2:F:187:THR:HG21	2.45	0.44
1:A:83:GLN:OE1	1:E:83:GLN:OE1	2.35	0.44
1:C:86:LEU:HD12	1:G:83:GLN:OE1	2.18	0.44
1:G:50:MSE:HE3	2:H:187:THR:HG21	1.98	0.44
1:A:79:VAL:HB	1:A:88:ALA:HB3	1.98	0.44
1:C:48[A]:MSE:HE3	5:C:223:HOH:O	2.17	0.44
1:C:48[B]:MSE:SE	1:C:105:VAL:CG1	3.16	0.44
2:F:147:GLU:HG3	2:F:148:LEU:N	2.32	0.43
1:C:36:GLN:HE22	1:C:70:GLN:HE22	1.67	0.43
2:B:116:LYS:O	2:B:119:ARG:HB2	2.18	0.43
1:G:42:MSE:HE3	2:H:186[A]:ARG:HG2	2.00	0.43
1:C:81:THR:O	1:C:83:GLN:N	2.52	0.42
1:A:50:MSE:HE3	2:B:187:THR:HG21	2.00	0.42
1:G:30:THR:O	1:G:34:LEU:HG	2.19	0.42
2:F:97:HIS:CE1	5:H:260:HOH:O	2.72	0.42
2:D:101:GLN:H	2:D:101:GLN:CD	2.16	0.42
1:G:48[B]:MSE:SE	1:G:105:VAL:CG1	3.18	0.42
2:B:100:GLN:HE21	2:B:105[B]:ARG:HH22	1.67	0.42
1:A:83:GLN:NE2	1:E:86:LEU:HD12	2.30	0.41
2:F:41:LEU:HD23	2:F:41:LEU:HA	1.95	0.41
2:D:77:TRP:CH2	2:D:87:LYS:HB3	2.56	0.41
2:H:77:TRP:CZ3	2:H:87:LYS:HB3	2.56	0.41
2:B:110:LYS:HZ3	2:B:130:THR:HG22	1.85	0.41
1:G:48[B]:MSE:CG	1:G:91:VAL:HG21	2.51	0.41
2:B:130:THR:O	2:B:130:THR:CG2	2.69	0.41
1:E:42:MSE:HE3	2:F:186[A]:ARG:HG2	2.01	0.41
2:H:77:TRP:CH2	2:H:87:LYS:HB3	2.55	0.41
1:A:48[B]:MSE:SE	5:A:136:HOH:O	2.89	0.40
1:G:50:MSE:HA	1:G:50:MSE:CE	2.50	0.40
2:B:45:GLN:NE2	2:D:137:VAL:HG22	2.37	0.40
2:F:52:ASP:OD2	2:F:186[A]:ARG:NH2	2.51	0.40
1:C:52:MSE:SE	1:C:109:VAL:HG22	2.72	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	83/103 (81%)	81 (98%)	2 (2%)	0	100	100
1	C	75/103 (73%)	75 (100%)	0	0	100	100
1	E	81/103 (79%)	79 (98%)	2 (2%)	0	100	100
1	G	80/103 (78%)	78 (98%)	2 (2%)	0	100	100
2	B	156/175 (89%)	153 (98%)	3 (2%)	0	100	100
2	D	150/175 (86%)	148 (99%)	2 (1%)	0	100	100
2	F	151/175 (86%)	149 (99%)	2 (1%)	0	100	100
2	H	152/175 (87%)	150 (99%)	2 (1%)	0	100	100
All	All	928/1112 (84%)	913 (98%)	15 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	67/78 (86%)	65 (97%)	2 (3%)	41	51
1	C	64/78 (82%)	60 (94%)	4 (6%)	18	19
1	E	67/78 (86%)	63 (94%)	4 (6%)	19	21
1	G	65/78 (83%)	63 (97%)	2 (3%)	40	50
2	B	137/152 (90%)	134 (98%)	3 (2%)	52	64
2	D	135/152 (89%)	128 (95%)	7 (5%)	23	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	134/152 (88%)	128 (96%)	6 (4%)	27	33
2	H	133/152 (88%)	123 (92%)	10 (8%)	13	13
All	All	802/920 (87%)	764 (95%)	38 (5%)	26	31

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	VAL
1	A	58	LEU
2	B	65	THR
2	B	156	LYS
2	B	165	GLU
1	C	30	THR
1	C	58	LEU
1	C	81	THR
1	C	83	GLN
2	D	41	LEU
2	D	50	MSE
2	D	65	THR
2	D	86	ASN
2	D	107	GLU
2	D	116	LYS
2	D	130	THR
1	E	30	THR
1	E	48[A]	MSE
1	E	48[B]	MSE
1	E	58	LEU
2	F	37	ARG
2	F	61	ARG
2	F	65	THR
2	F	86	ASN
2	F	100	GLN
2	F	156	LYS
1	G	58	LEU
1	G	81	THR
2	H	37	ARG
2	H	41	LEU
2	H	45	GLN
2	H	50	MSE
2	H	86	ASN
2	H	100	GLN

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Mol	Chain	Res	Type
2	H	116	LYS
2	H	130	THR
2	H	175	GLU
2	H	194	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	GLN
1	A	83	GLN
2	B	45	GLN
2	B	57	GLN
2	B	86	ASN
2	B	97	HIS
2	B	100	GLN
1	C	36	GLN
1	C	83	GLN
1	E	36	GLN
1	E	70	GLN
1	G	70	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)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	79/103 (76%)	0.06	4 (5%)	28	26	12, 22, 28, 33	0
1	C	75/103 (72%)	-0.01	5 (6%)	17	16	12, 22, 28, 32	0
1	E	77/103 (74%)	0.12	7 (9%)	9	7	11, 22, 27, 30	0
1	G	76/103 (73%)	0.05	8 (10%)	6	5	12, 21, 27, 30	0
2	B	156/175 (89%)	-0.27	5 (3%)	47	45	8, 17, 24, 38	0
2	D	152/175 (86%)	-0.32	2 (1%)	77	75	11, 20, 27, 34	0
2	F	153/175 (87%)	-0.12	4 (2%)	56	54	13, 20, 26, 31	0
2	H	154/175 (88%)	-0.02	10 (6%)	18	17	13, 23, 29, 34	0
All	All	922/1112 (82%)	-0.10	45 (4%)	29	28	8, 21, 28, 38	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	82	THR	8.1
1	E	82	THR	5.8
1	A	82	THR	4.5
1	G	57	ASN	4.3
1	C	59	LYS	4.2
1	A	58	LEU	3.6
2	D	196	GLN	3.6
1	G	59	LYS	3.5
1	C	58	LEU	3.4
1	G	58	LEU	3.4
1	A	57	ASN	3.3
1	E	57	ASN	3.2
2	H	33	LEU	3.2
2	F	64	ARG	3.2
2	F	165	GLU	3.1
1	E	83	GLN	3.1

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Mol	Chain	Res	Type	RSRZ
2	B	196	GLN	3.0
1	G	81	THR	3.0
1	E	58	LEU	3.0
2	B	33	LEU	2.8
1	G	80	ALA	2.7
1	E	80	ALA	2.7
2	H	80	TYR	2.6
2	B	71	SER	2.6
2	B	197	LYS	2.6
1	C	33	TYR	2.5
1	A	80	ALA	2.4
2	H	155	GLY	2.4
2	D	197	LYS	2.4
2	H	34	SER	2.4
2	H	131	PRO	2.4
1	G	60	ALA	2.4
1	E	81	THR	2.4
1	C	60	ALA	2.3
2	B	134	GLN	2.3
1	C	83	GLN	2.3
2	F	65	THR	2.3
1	E	30	THR	2.2
2	H	37	ARG	2.2
2	H	163	SER	2.2
2	H	156	LYS	2.2
2	F	72	LYS	2.1
2	H	72	LYS	2.1
2	H	73	LYS	2.1
1	G	30	THR	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)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NA	F	4	1/1	0.96	0.20	37,37,37,37	0
3	CL	F	2	1/1	0.98	0.09	32,32,32,32	0
3	CL	B	1	1/1	0.99	0.05	33,33,33,33	0
4	NA	H	3	1/1	1.00	0.09	29,29,29,29	0

6.5 Other polymers (i)

There are no such residues in this entry.