Full wwPDB X-ray Structure Validation Report (i)

Oct 1, 2023 – 04:03 AM EDT

PDB ID	:	3WXX
Title	:	Crystal Structure of a T3SS complex from Aeromonas hydrophila
Authors	:	Nguyen, V.S.; Jobichen, C.; Sivaraman, J.; Henry, Y.K.M.
Deposited on	:	2014-08-12
Resolution	:	2.70 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 (i)) were used in the production of this report:

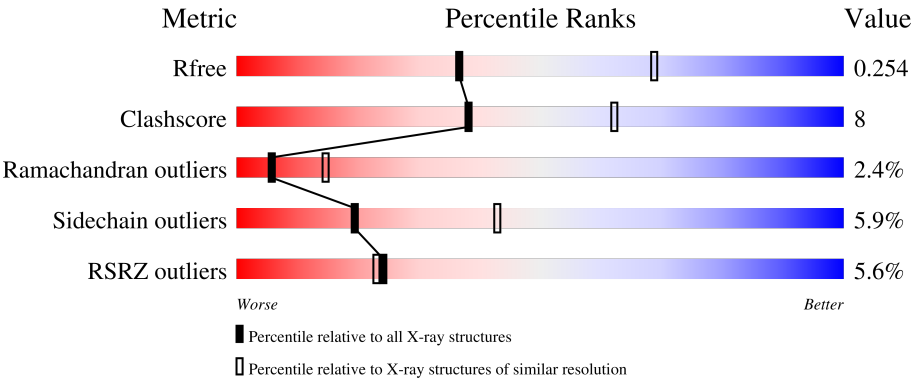
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	151	93% 5%
1	C	151	2% 87% 10%
1	E	151	93% 5%
1	G	151	3% 89% 8%
2	B	219	7% 64% 16% 16%

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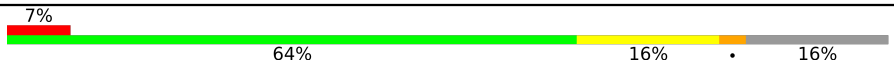
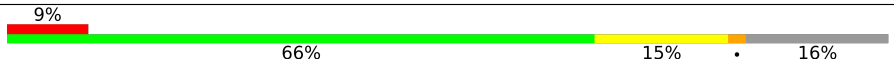
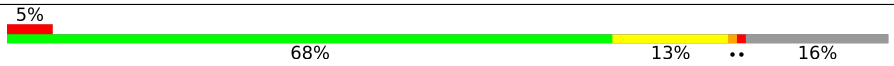
Mol	Chain	Length	Quality of chain
2	D	219	
2	F	219	
2	H	219	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 9737 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 AcrH.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	150	Total	C	N	O	S	Se	0	1	0
			1161	739	193	220	3	6			
1	C	150	Total	C	N	O	S	Se	0	1	0
			1161	739	193	220	3	6			
1	E	151	Total	C	N	O	S	Se	0	1	0
			1158	738	194	217	3	6			
1	G	151	Total	C	N	O	S	Se	0	1	0
			1166	742	194	221	3	6			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	107	HIS	ARG	ENGINEERED MUTATION	UNP Q6TLM1
C	107	HIS	ARG	ENGINEERED MUTATION	UNP Q6TLM1
E	107	HIS	ARG	ENGINEERED MUTATION	UNP Q6TLM1
G	107	HIS	ARG	ENGINEERED MUTATION	UNP Q6TLM1

- Molecule 2 is a protein called AopB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	183	Total	C	N	O	Se	0	0	0
			1253	793	215	236	9			
2	D	183	Total	C	N	O	Se	0	0	0
			1259	799	215	236	9			
2	F	183	Total	C	N	O	Se	0	0	0
			1259	799	215	236	9			
2	H	183	Total	C	N	O	Se	0	0	0
			1263	801	215	238	9			

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	1	Total Mg 1 1	0	0

- Molecule 4 is water.

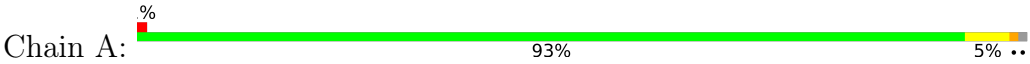
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	9	Total O 9 9	0	0
4	B	5	Total O 5 5	0	0
4	C	8	Total O 8 8	0	0
4	D	6	Total O 6 6	0	0
4	E	11	Total O 11 11	0	0
4	F	5	Total O 5 5	0	0
4	G	8	Total O 8 8	0	0
4	H	4	Total O 4 4	0	0

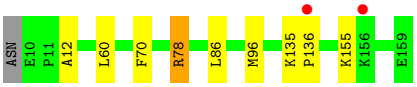
3 Residue-property plots (i)

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: AcrH

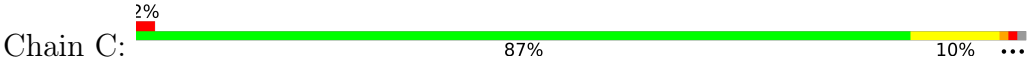
Chain A:

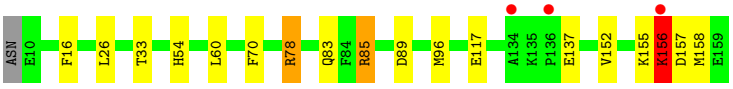




• Molecule 1: AcrH

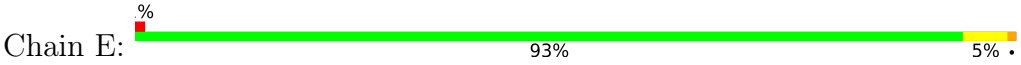
Chain C:

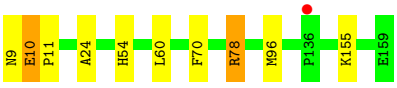




• Molecule 1: AcrH

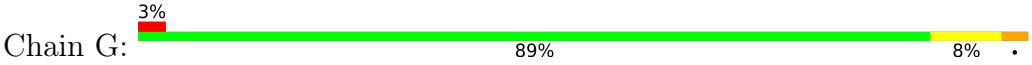
Chain E:

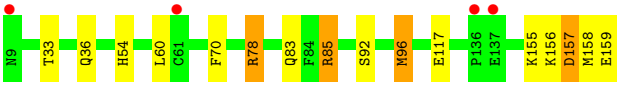




• Molecule 1: AcrH

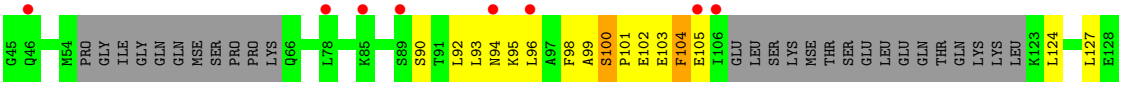
Chain G:

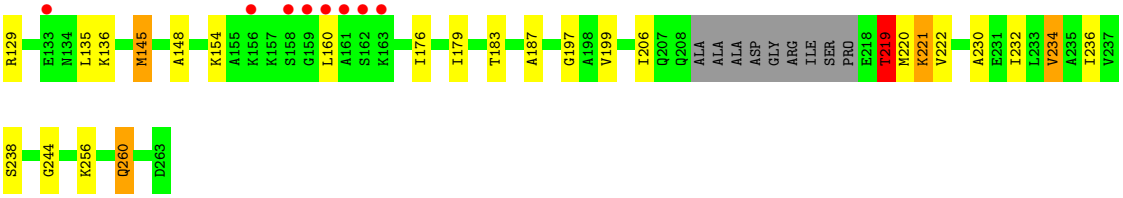




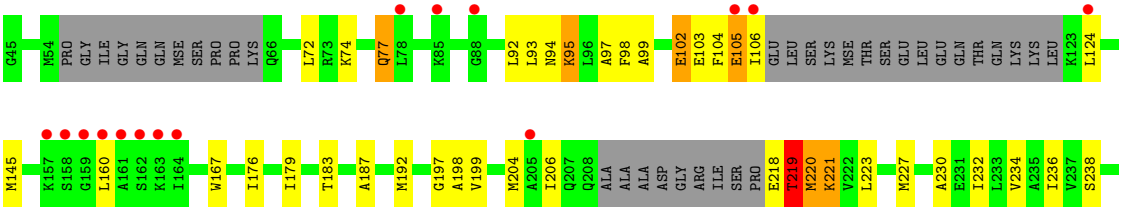
• Molecule 2: AopB

Chain B:

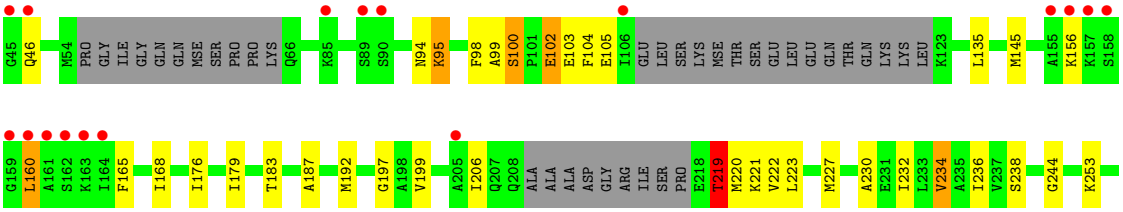




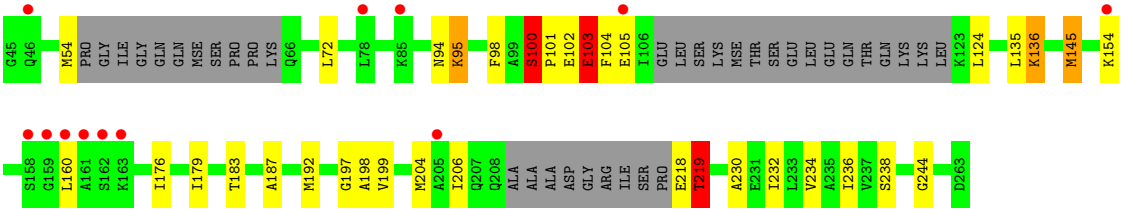
• Molecule 2: AopB



• Molecule 2: AopB



• Molecule 2: AopB



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	124.66Å 151.94Å 106.25Å 90.00° 104.95° 90.00°	Depositor
Resolution (Å)	15.00 – 2.70 36.40 – 2.49	Depositor EDS
% Data completeness (in resolution range)	93.2 (15.00-2.70) 85.3 (36.40-2.49)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	9.36 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.213 , 0.252 0.218 , 0.254	Depositor DCC
R_{free} test set	3136 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	50.7	Xtriage
Anisotropy	0.469	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 51.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	9737	wwPDB-VP
Average B, all atoms (Å^2)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 39.32 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.2287e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.64	0/1181	0.74	1/1583 (0.1%)
1	C	0.65	0/1181	0.79	3/1583 (0.2%)
1	E	0.67	0/1178	0.75	1/1580 (0.1%)
1	G	0.66	0/1186	0.79	1/1590 (0.1%)
2	B	0.60	0/1250	0.86	2/1669 (0.1%)
2	D	0.60	0/1257	0.86	3/1678 (0.2%)
2	F	0.64	0/1257	0.84	2/1678 (0.1%)
2	H	0.62	0/1261	0.82	2/1683 (0.1%)
All	All	0.64	0/9751	0.81	15/13044 (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	F	0	1

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	160	LEU	CA-CB-CG	7.41	132.35	115.30
1	A	78	ARG	CG-CD-NE	7.12	126.76	111.80
1	C	156	LYS	CA-CB-CG	6.91	128.60	113.40
2	B	129	ARG	CA-CB-CG	6.27	127.20	113.40
2	D	192	MSE	CG-SE-CE	-6.17	85.32	98.90
1	G	78	ARG	NE-CZ-NH1	5.99	123.30	120.30
2	D	93	LEU	N-CA-C	5.58	126.07	111.00
2	F	192	MSE	CG-SE-CE	-5.54	86.72	98.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	78	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	C	78	ARG	NE-CZ-NH1	5.38	122.99	120.30
2	H	145	MSE	CG-SE-CE	-5.24	87.36	98.90
2	D	160	LEU	CA-CB-CG	5.23	127.33	115.30
1	C	89	ASP	CB-CG-OD2	-5.20	113.62	118.30
2	H	192	MSE	CG-SE-CE	-5.18	87.50	98.90
2	B	145	MSE	CG-SE-CE	-5.13	87.61	98.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	F	221	LYS	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	1161	0	1124	8	0
1	C	1161	0	1124	12	0
1	E	1158	0	1118	11	0
1	G	1166	0	1126	19	0
2	B	1253	0	1279	28	0
2	D	1259	0	1286	31	0
2	F	1259	0	1286	28	0
2	H	1263	0	1290	27	0
3	G	1	0	0	0	0
4	A	9	0	0	0	0
4	B	5	0	0	0	0
4	C	8	0	0	0	0
4	D	6	0	0	1	0
4	E	11	0	0	1	0
4	F	5	0	0	0	0
4	G	8	0	0	2	0
4	H	4	0	0	0	0
All	All	9737	0	9633	147	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 (147) 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:G:157:ASP:O	1:G:158:MSE:HG2	1.64	0.96
2:H:103:GLU:CB	2:H:104:PHE:HA	2.00	0.91
2:H:103:GLU:HB2	2:H:104:PHE:HA	1.56	0.87
2:F:145:MSE:HE2	2:F:179:ILE:HG23	1.59	0.85
1:G:158:MSE:HB3	1:G:159:GLU:HA	1.58	0.84
2:H:145:MSE:HE2	2:H:179:ILE:HG23	1.60	0.83
2:D:145:MSE:HE2	2:D:179:ILE:HG23	1.61	0.83
1:E:10:GLU:CB	1:E:11:PRO:HD2	2.08	0.83
2:B:145:MSE:HE2	2:B:179:ILE:HG23	1.61	0.82
1:E:9:ASN:O	1:E:10:GLU:CB	2.30	0.79
2:H:94:ASN:CB	2:H:95:LYS:HB2	2.13	0.78
2:F:145:MSE:HE3	2:F:187:ALA:HB2	1.66	0.77
2:D:103:GLU:N	2:D:104:PHE:HA	1.99	0.77
2:D:145:MSE:HE3	2:D:187:ALA:HB2	1.67	0.77
2:H:145:MSE:HE3	2:H:187:ALA:HB2	1.67	0.77
2:B:145:MSE:HE3	2:B:187:ALA:HB2	1.69	0.75
2:B:219:THR:OG1	2:B:220:MSE:N	2.19	0.75
1:G:158:MSE:CB	1:G:159:GLU:HA	2.15	0.74
1:C:85:ARG:NH2	1:C:117:GLU:OE2	2.21	0.73
1:G:54:HIS:NE2	1:G:78:ARG:HD2	2.03	0.72
2:B:230:ALA:O	2:B:234:VAL:HG13	1.89	0.72
1:E:10:GLU:CB	1:E:11:PRO:CD	2.66	0.71
1:G:85:ARG:NH2	1:G:117:GLU:OE2	2.24	0.71
1:C:54:HIS:NE2	1:C:78:ARG:HD2	2.05	0.71
2:F:230:ALA:O	2:F:234:VAL:HG13	1.89	0.70
1:E:54:HIS:NE2	1:E:78:ARG:HD2	2.06	0.70
2:B:220:MSE:O	2:B:221:LYS:HB2	1.91	0.70
2:F:102:GLU:HB2	2:F:104:PHE:HB3	1.74	0.69
2:D:94:ASN:CB	2:D:95:LYS:HB2	2.22	0.68
2:D:94:ASN:N	2:D:95:LYS:O	2.25	0.68
2:B:90:SER:O	2:B:92:LEU:CB	2.42	0.68
1:E:96[B]:MSE:HE3	2:F:168:ILE:HD11	1.76	0.67
1:G:158:MSE:HB2	1:G:159:GLU:HG2	1.78	0.66
1:G:156:LYS:O	1:G:158:MSE:N	2.30	0.65
2:F:103:GLU:N	2:F:104:PHE:HA	2.11	0.65
1:E:96[B]:MSE:SE	2:F:176:ILE:HD11	2.47	0.64
2:B:103:GLU:H	2:B:104:PHE:HA	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:95:LYS:HD3	2:F:95:LYS:H	1.63	0.63
2:B:260:GLN:OE1	2:B:260:GLN:N	2.32	0.62
2:F:219:THR:OG1	2:F:220:MSE:N	2.21	0.62
2:B:100:SER:OG	2:B:101:PRO:HA	1.99	0.62
2:F:145:MSE:HE2	2:F:179:ILE:CG2	2.30	0.62
1:C:156:LYS:O	1:C:158:MSE:N	2.32	0.62
2:H:94:ASN:N	2:H:95:LYS:O	2.28	0.61
2:H:145:MSE:HE2	2:H:179:ILE:CG2	2.31	0.60
2:B:145:MSE:HE2	2:B:179:ILE:CG2	2.32	0.60
1:G:85:ARG:NH2	4:G:302:HOH:O	2.35	0.59
2:D:145:MSE:HE2	2:D:179:ILE:CG2	2.32	0.59
2:H:230:ALA:O	2:H:234:VAL:HG23	2.04	0.58
2:D:232:ILE:O	2:D:236:ILE:HD12	2.04	0.58
2:B:93:LEU:HA	2:B:94:ASN:CB	2.33	0.58
2:D:230:ALA:O	2:D:234:VAL:HG23	2.04	0.57
1:A:78:ARG:NH1	1:A:86:LEU:HB3	2.19	0.57
2:F:100:SER:HA	2:F:102:GLU:OE1	2.04	0.57
1:G:96[B]:MSE:SE	2:H:176:ILE:HG13	2.55	0.56
2:H:100:SER:OG	2:H:101:PRO:HA	2.04	0.56
2:H:101:PRO:HB2	2:H:103:GLU:HG3	1.87	0.56
2:D:198:ALA:HB3	2:D:234:VAL:HG11	1.87	0.56
1:C:96[A]:MSE:HE2	2:D:176:ILE:HD11	1.88	0.56
2:H:232:ILE:O	2:H:236:ILE:HD12	2.05	0.56
1:G:85:ARG:NE	4:G:302:HOH:O	2.04	0.55
2:F:232:ILE:O	2:F:236:ILE:HD12	2.06	0.55
2:H:198:ALA:HB3	2:H:234:VAL:HG11	1.88	0.55
2:B:92:LEU:HA	2:B:94:ASN:CB	2.38	0.54
2:H:145:MSE:HE1	2:H:183:THR:O	2.08	0.54
1:E:24:ALA:HB3	4:E:203:HOH:O	2.08	0.54
2:F:145:MSE:HE1	2:F:183:THR:O	2.08	0.54
2:D:145:MSE:HE1	2:D:183:THR:O	2.08	0.53
2:B:232:ILE:O	2:B:236:ILE:HD12	2.07	0.53
2:D:145:MSE:CE	2:D:187:ALA:HB2	2.38	0.53
2:D:102:GLU:HG2	2:D:245:ALA:HB1	1.89	0.53
1:E:96[B]:MSE:HE1	2:F:165:PHE:CE1	2.43	0.53
1:G:157:ASP:O	1:G:158:MSE:CG	2.48	0.52
1:C:96[A]:MSE:SE	2:D:176:ILE:HG13	2.59	0.52
1:G:157:ASP:C	1:G:158:MSE:HG2	2.28	0.52
2:F:94:ASN:HA	2:F:95:LYS:C	2.30	0.52
1:G:158:MSE:CB	1:G:159:GLU:CA	2.86	0.52
2:B:145:MSE:HE1	2:B:183:THR:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:152:VAL:O	1:C:156:LYS:HB2	2.10	0.52
1:E:96[A]:MSE:SE	2:F:176:ILE:HG13	2.60	0.51
2:B:145:MSE:CE	2:B:187:ALA:HB2	2.38	0.51
1:C:96[A]:MSE:HE2	2:D:176:ILE:CD1	2.40	0.51
2:B:100:SER:HA	2:B:101:PRO:C	2.31	0.51
1:E:60:LEU:HB3	1:E:70:PHE:CD2	2.45	0.51
2:F:145:MSE:CE	2:F:187:ALA:HB2	2.38	0.51
1:A:96[B]:MSE:SE	2:B:176:ILE:HG13	2.62	0.50
1:C:33:THR:HG22	2:D:72:LEU:HD22	1.93	0.50
2:D:103:GLU:N	2:D:104:PHE:CA	2.74	0.50
2:F:102:GLU:N	2:F:102:GLU:CD	2.66	0.50
1:G:157:ASP:C	1:G:158:MSE:CG	2.80	0.49
2:F:102:GLU:HG2	2:F:103:GLU:O	2.13	0.49
2:H:145:MSE:CE	2:H:187:ALA:HB2	2.38	0.49
1:G:60:LEU:HB3	1:G:70:PHE:CD2	2.48	0.48
2:H:100:SER:HA	2:H:101:PRO:C	2.32	0.48
1:A:12:ALA:HB1	2:B:127:LEU:HD23	1.96	0.47
2:H:145:MSE:CE	2:H:179:ILE:HG12	2.44	0.47
1:A:60:LEU:HB3	1:A:70:PHE:CD2	2.49	0.47
2:H:218:GLU:O	2:H:219:THR:O	2.32	0.47
2:F:145:MSE:CE	2:F:179:ILE:HG12	2.45	0.47
2:B:199:VAL:HG22	2:B:199:VAL:O	2.15	0.47
2:D:218:GLU:O	2:D:219:THR:O	2.32	0.47
2:D:145:MSE:CE	2:D:179:ILE:HG12	2.45	0.47
1:G:92:SER:O	1:G:96[B]:MSE:HG3	2.15	0.46
2:B:145:MSE:CE	2:B:179:ILE:HG12	2.46	0.46
2:B:102:GLU:N	2:B:103:GLU:HA	2.31	0.46
2:F:199:VAL:HG22	2:F:199:VAL:O	2.15	0.46
2:B:92:LEU:HA	2:B:93:LEU:HA	1.78	0.46
2:D:199:VAL:O	2:D:199:VAL:HG22	2.17	0.45
1:G:83:GLN:HG3	2:H:204:MSE:HE2	1.97	0.45
2:H:199:VAL:O	2:H:199:VAL:HG22	2.15	0.45
2:F:100:SER:CA	2:F:102:GLU:OE1	2.63	0.45
2:H:145:MSE:HE1	2:H:183:THR:C	2.38	0.45
1:C:60:LEU:HB3	1:C:70:PHE:CD2	2.52	0.45
2:B:220:MSE:O	2:B:221:LYS:CB	2.64	0.44
2:B:232:ILE:HG22	2:B:236:ILE:CD1	2.48	0.44
1:E:96[B]:MSE:HE3	2:F:168:ILE:CD1	2.47	0.44
2:D:220:MSE:O	2:D:221:LYS:HB3	2.16	0.44
2:H:100:SER:CB	2:H:101:PRO:HA	2.48	0.43
1:C:156:LYS:O	1:C:158:MSE:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:99:ALA:O	2:F:100:SER:OG	2.23	0.43
2:H:103:GLU:CB	2:H:104:PHE:CA	2.83	0.43
1:A:78:ARG:HH11	1:A:86:LEU:HB3	1.84	0.43
2:D:99:ALA:O	2:D:102:GLU:OE1	2.36	0.43
2:H:232:ILE:HG22	2:H:236:ILE:CD1	2.48	0.43
1:A:96[A]:MSE:HE3	2:B:148:ALA:HB1	2.00	0.43
2:D:105:GLU:HA	2:D:106:ILE:C	2.39	0.43
2:F:232:ILE:HG22	2:F:236:ILE:CD1	2.48	0.42
2:D:167:TRP:O	4:D:303:HOH:O	2.21	0.42
2:F:145:MSE:HE1	2:F:183:THR:C	2.40	0.42
1:G:158:MSE:HB2	1:G:159:GLU:CG	2.48	0.42
1:A:135:LYS:HA	1:A:136:PRO:HD3	1.94	0.42
1:A:96[A]:MSE:CE	2:B:148:ALA:HB1	2.49	0.42
1:C:83:GLN:HG3	2:D:204:MSE:HE2	2.02	0.42
2:D:74:LYS:HA	2:D:77:GLN:OE1	2.21	0.41
2:D:145:MSE:HE1	2:D:183:THR:C	2.41	0.41
2:D:92:LEU:HA	2:D:94:ASN:N	2.36	0.41
2:F:46:GLN:O	2:F:46:GLN:HG2	2.20	0.41
1:C:16:PHE:CE2	1:C:26:LEU:HD13	2.56	0.41
2:D:223:LEU:O	2:D:227:MSE:HG2	2.20	0.41
2:B:99:ALA:O	2:B:100:SER:CB	2.69	0.40
2:F:223:LEU:O	2:F:227:MSE:HG2	2.21	0.40
1:G:33:THR:HG22	2:H:72:LEU:HD22	2.02	0.40
2:H:103:GLU:HB3	2:H:104:PHE:HA	1.97	0.40
2:B:93:LEU:CB	2:B:96:LEU:CB	2.99	0.40
2:D:97:ALA:C	2:D:98:PHE:CG	2.94	0.40
2:D:232:ILE:HG22	2:D:236:ILE:CD1	2.51	0.40
2:H:136:LYS:HD3	2:H:136:LYS:H	1.86	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	149/151 (99%)	144 (97%)	5 (3%)	0	100 100
1	C	149/151 (99%)	145 (97%)	3 (2%)	1 (1%)	22 46
1	E	150/151 (99%)	145 (97%)	4 (3%)	1 (1%)	22 46
1	G	150/151 (99%)	144 (96%)	5 (3%)	1 (1%)	22 46
2	B	175/219 (80%)	145 (83%)	23 (13%)	7 (4%)	3 6
2	D	175/219 (80%)	145 (83%)	25 (14%)	5 (3%)	4 10
2	F	175/219 (80%)	147 (84%)	21 (12%)	7 (4%)	3 6
2	H	175/219 (80%)	142 (81%)	24 (14%)	9 (5%)	2 3
All	All	1298/1480 (88%)	1157 (89%)	110 (8%)	31 (2%)	6 15

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	105	GLU
2	B	219	THR
2	B	221	LYS
1	C	157	ASP
2	D	105	GLU
2	D	219	THR
1	E	10	GLU
2	F	105	GLU
2	F	219	THR
1	G	157	ASP
2	H	98	PHE
2	H	103	GLU
2	H	105	GLU
2	H	219	THR
2	B	244	GLY
2	D	197	GLY
2	D	244	GLY
2	F	197	GLY
2	F	244	GLY
2	H	102	GLU
2	H	197	GLY
2	H	244	GLY
2	B	197	GLY
2	F	98	PHE
2	F	100	SER
2	B	98	PHE
2	D	206	ILE

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Mol	Chain	Res	Type
2	F	206	ILE
2	B	206	ILE
2	H	206	ILE
2	H	100	SER

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	116/112 (104%)	115 (99%)	1 (1%)	78 92
1	C	116/112 (104%)	112 (97%)	4 (3%)	37 66
1	E	114/112 (102%)	113 (99%)	1 (1%)	78 92
1	G	116/112 (104%)	111 (96%)	5 (4%)	29 57
2	B	115/152 (76%)	101 (88%)	14 (12%)	5 11
2	D	116/152 (76%)	108 (93%)	8 (7%)	15 35
2	F	116/152 (76%)	105 (90%)	11 (10%)	8 20
2	H	117/152 (77%)	106 (91%)	11 (9%)	8 20
All	All	926/1056 (88%)	871 (94%)	55 (6%)	19 43

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	155	LYS
2	B	95	LYS
2	B	100	SER
2	B	104	PHE
2	B	124	LEU
2	B	135	LEU
2	B	136	LYS
2	B	154	LYS
2	B	160	LEU
2	B	219	THR
2	B	222	VAL

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Mol	Chain	Res	Type
2	B	234	VAL
2	B	238	SER
2	B	256	LYS
2	B	260	GLN
1	C	85	ARG
1	C	137	GLU
1	C	155	LYS
1	C	156	LYS
2	D	77	GLN
2	D	95	LYS
2	D	102	GLU
2	D	124	LEU
2	D	219	THR
2	D	220	MSE
2	D	221	LYS
2	D	238	SER
1	E	155	LYS
2	F	95	LYS
2	F	102	GLU
2	F	135	LEU
2	F	156	LYS
2	F	160	LEU
2	F	219	THR
2	F	222	VAL
2	F	234	VAL
2	F	238	SER
2	F	253	LYS
2	F	256	LYS
1	G	36	GLN
1	G	85	ARG
1	G	96[A]	MSE
1	G	96[B]	MSE
1	G	155	LYS
2	H	54	MSE
2	H	95	LYS
2	H	100	SER
2	H	103	GLU
2	H	124	LEU
2	H	135	LEU
2	H	136	LYS
2	H	154	LYS
2	H	160	LEU

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Mol	Chain	Res	Type
2	H	219	THR
2	H	238	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	52	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 1 ligands modelled in this entry, 1 is 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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	145/151 (96%)	-0.14	2 (1%) 75 77	30, 53, 88, 110	0
1	C	145/151 (96%)	-0.10	3 (2%) 63 65	33, 52, 87, 130	0
1	E	146/151 (96%)	-0.07	1 (0%) 87 89	32, 56, 94, 113	0
1	G	146/151 (96%)	-0.17	4 (2%) 54 55	37, 54, 90, 125	0
2	B	174/219 (79%)	0.30	16 (9%) 9 7	37, 76, 143, 194	0
2	D	174/219 (79%)	0.26	15 (8%) 10 8	36, 78, 128, 159	0
2	F	174/219 (79%)	0.33	19 (10%) 5 4	32, 75, 134, 156	0
2	H	174/219 (79%)	0.24	12 (6%) 16 15	32, 70, 136, 158	0
All	All	1278/1480 (86%)	0.10	72 (5%) 24 23	30, 62, 127, 194	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	159	GLY	9.2
2	F	163	LYS	5.4
2	D	161	ALA	5.4
2	B	160	LEU	5.3
2	D	159	GLY	5.3
2	B	159	GLY	5.0
2	B	161	ALA	4.9
2	H	159	GLY	4.9
2	D	160	LEU	4.8
2	H	46	GLN	4.6
2	B	105	GLU	4.6
2	F	162	SER	4.6
2	F	158	SER	4.5
2	B	163	LYS	4.4
2	F	161	ALA	4.2
2	D	158	SER	4.2

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Mol	Chain	Res	Type	RSRZ
2	B	162	SER	4.1
2	B	46	GLN	4.0
2	D	162	SER	4.0
2	H	163	LYS	3.9
2	F	157	LYS	3.9
2	F	156	LYS	3.8
2	H	160	LEU	3.8
2	B	94	ASN	3.8
2	H	161	ALA	3.7
1	C	156	LYS	3.6
2	F	46	GLN	3.6
1	C	136	PRO	3.4
2	B	85	LYS	3.4
2	H	162	SER	3.4
1	A	136	PRO	3.4
1	C	134	ALA	3.3
2	F	90	SER	3.2
2	F	85	LYS	3.2
2	F	160	LEU	3.1
2	H	154	LYS	3.0
2	H	158	SER	3.0
2	H	205	ALA	3.0
2	B	106	ILE	3.0
2	F	263	ASP	2.9
1	G	136	PRO	2.9
2	D	164	ILE	2.7
2	B	158	SER	2.7
2	F	89	SER	2.7
2	D	106	ILE	2.7
2	F	106	ILE	2.7
2	F	205	ALA	2.7
1	G	137	GLU	2.6
2	B	89	SER	2.6
2	H	105	GLU	2.5
2	B	156	LYS	2.5
2	H	85	LYS	2.5
1	E	136	PRO	2.4
2	D	85	LYS	2.4
1	A	156	LYS	2.4
2	D	105	GLU	2.4
2	H	78	LEU	2.3
2	F	45	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
2	D	205	ALA	2.3
2	F	155	ALA	2.3
2	F	164	ILE	2.3
1	G	61	CYS	2.3
2	F	259	THR	2.3
2	B	96	LEU	2.2
2	D	124	LEU	2.2
2	D	163	LYS	2.2
2	B	78	LEU	2.2
2	D	157	LYS	2.2
1	G	9	ASN	2.1
2	D	88	GLY	2.1
2	B	133	GLU	2.1
2	D	78	LEU	2.1

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, 95^{th} 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
3	MG	G	201	1/1	0.91	0.43	55,55,55,55	0

6.5 Other polymers (i)

There are no such residues in this entry.