Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:46 PM GMT

PDB ID	:	4JDO
Title	:	Secreted chlamydial protein pgp3, coiled-coil deletion
Authors	:	Galaleldeen, A.; Taylor, A.B.; Chen, D.; Holloway, S.P.; Zhong, G.; Hart, P.J.
Deposited on	:	2013-02-25
Resolution	:	2.30 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

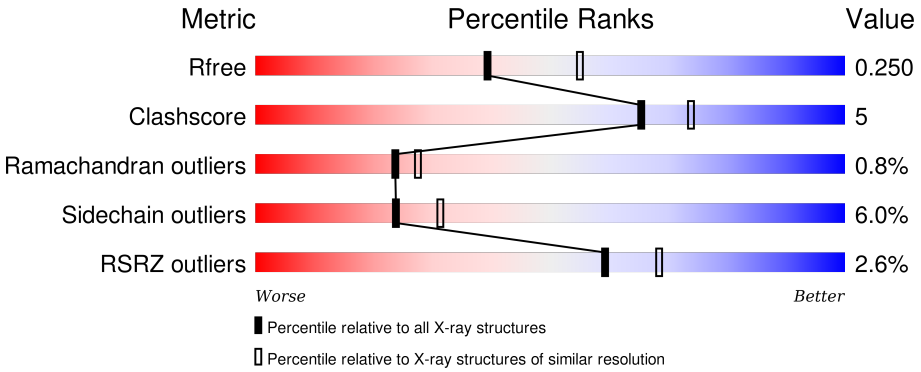
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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 <=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	219	86% 12%
1	B	219	6% 83% 16%
1	C	219	2% 83% 15%
1	D	219	3% 85% 13%
1	E	219	2% 82% 16%

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Mol	Chain	Length	Quality of chain
1	F	219	84% 12%
1	G	219	2% 82% 16%
1	H	219	2% 83% 12%
1	I	219	3% 83% 13%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NA	G	301	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 15034 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 Virulence plasmid protein pGP3-D.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	215	Total	C	N	O	S	Se	0	0	0
			1578	990	261	319	4	4			
1	B	218	Total	C	N	O	S	Se	0	1	0
			1603	1006	264	323	4	6			
1	C	217	Total	C	N	O	S	Se	0	0	0
			1593	999	263	322	4	5			
1	D	217	Total	C	N	O	S	Se	0	0	0
			1593	998	264	323	4	4			
1	E	215	Total	C	N	O	S	Se	0	0	0
			1580	992	261	318	4	5			
1	F	217	Total	C	N	O	S	Se	0	1	0
			1598	1003	263	322	4	6			
1	G	217	Total	C	N	O	S	Se	0	0	0
			1593	999	263	322	4	5			
1	H	216	Total	C	N	O	S	Se	0	0	0
			1586	995	262	320	4	5			
1	I	217	Total	C	N	O	S	Se	0	0	0
			1593	999	263	322	4	5			

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	1	Total	Na	0	0
			1	1		
2	A	1	Total	Na	0	0
			1	1		
2	D	1	Total	Na	0	0
			1	1		

- Molecule 3 is water.

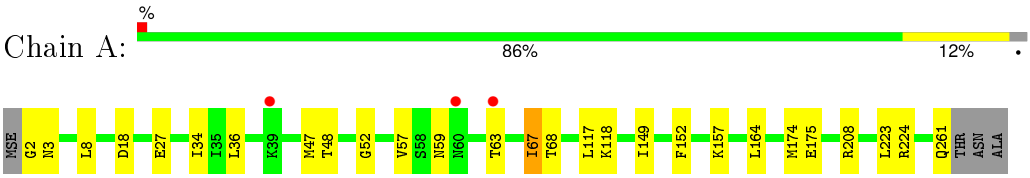
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	71	Total O 71 71	0	0
3	B	65	Total O 65 65	0	0
3	C	77	Total O 77 77	0	0
3	D	85	Total O 85 85	0	0
3	E	71	Total O 71 71	0	0
3	F	87	Total O 87 87	0	0
3	G	78	Total O 78 78	0	0
3	H	84	Total O 84 84	0	0
3	I	96	Total O 96 96	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

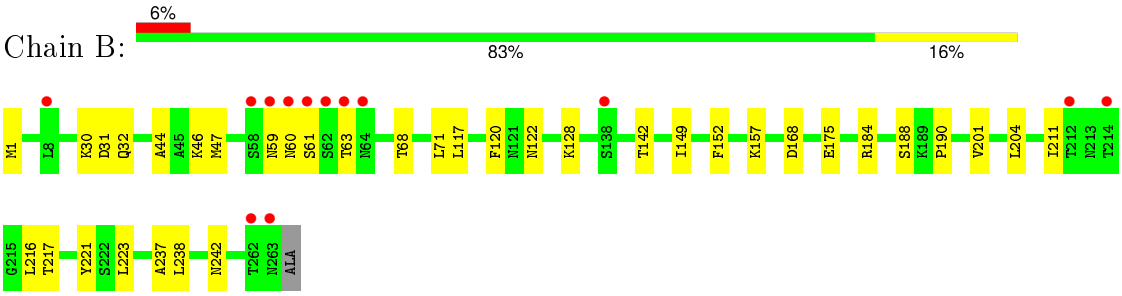
- Molecule 1: Virulence plasmid protein pGP3-D

Chain A:



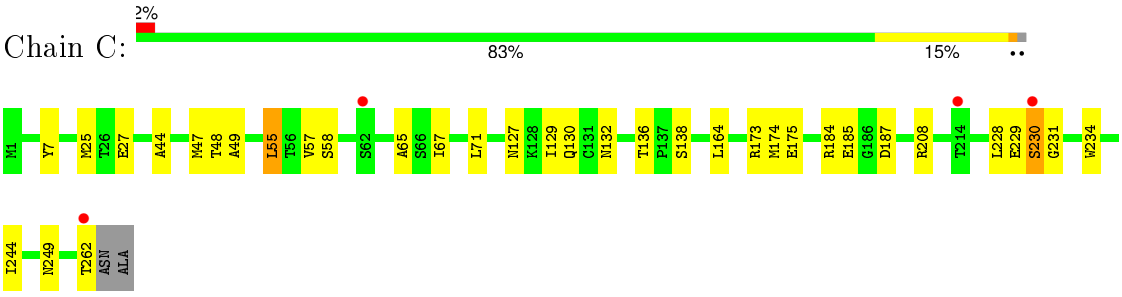
- Molecule 1: Virulence plasmid protein pGP3-D

Chain B:



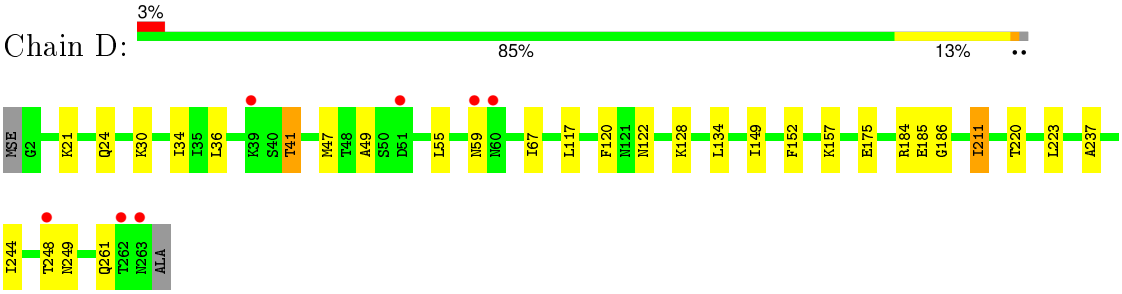
- Molecule 1: Virulence plasmid protein pGP3-D

Chain C:



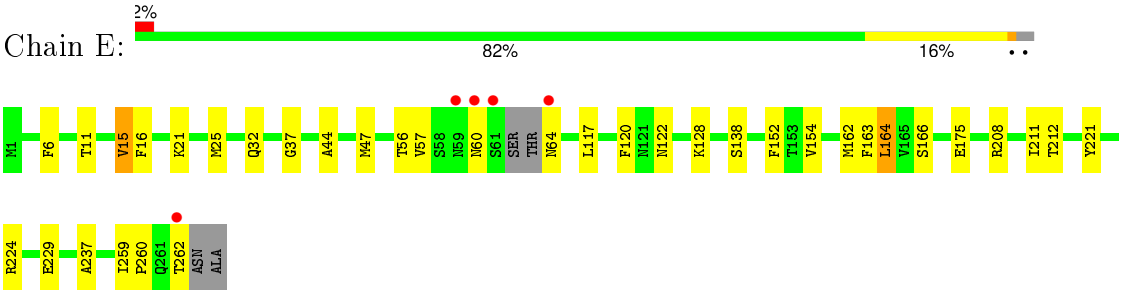
- Molecule 1: Virulence plasmid protein pGP3-D

Chain D:



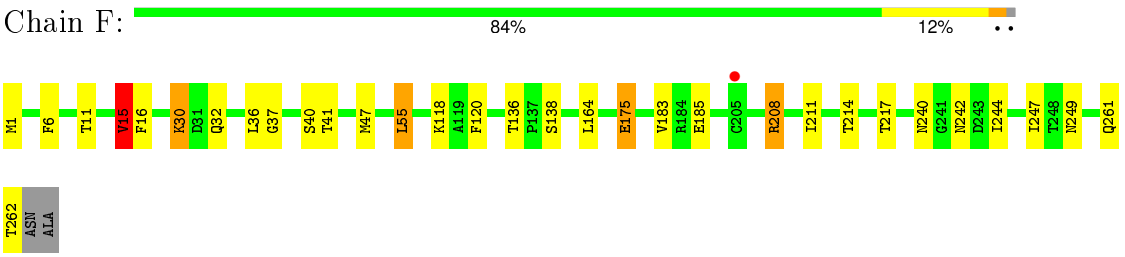
• Molecule 1: Virulence plasmid protein pGP3-D

Chain E:



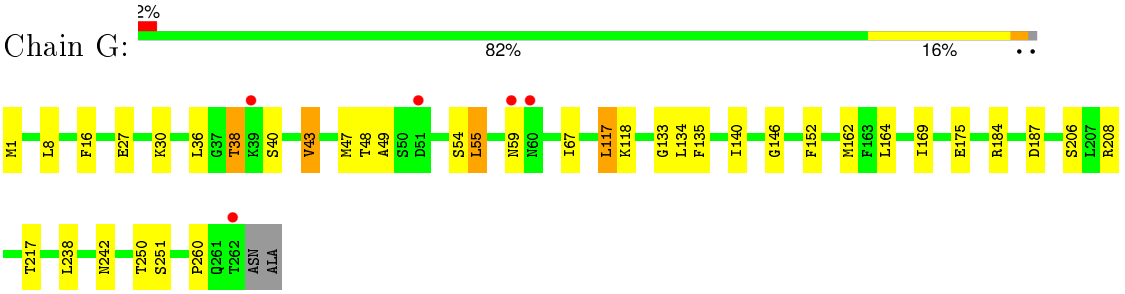
• Molecule 1: Virulence plasmid protein pGP3-D

Chain F:



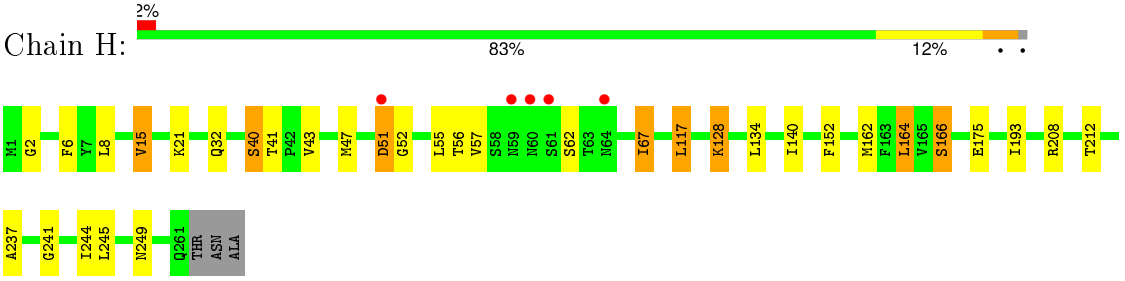
• Molecule 1: Virulence plasmid protein pGP3-D

Chain G:



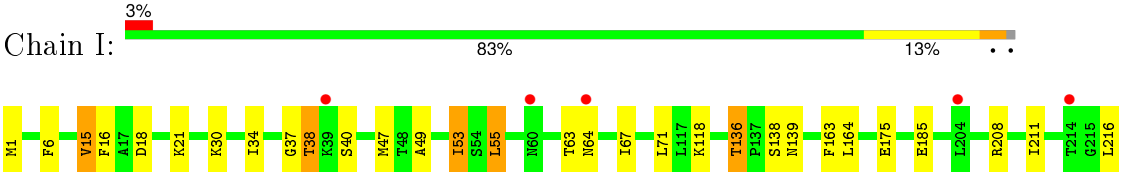
• Molecule 1: Virulence plasmid protein pGP3-D

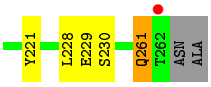
Chain H:



• Molecule 1: Virulence plasmid protein pGP3-D

Chain I:




Y221
L228
E229
S230
Q261
T262
ASN
ALA

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α, β, γ	146.24Å 146.24Å 161.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.46 – 2.30 29.46 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.7 (29.46-2.30) 99.8 (29.46-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$< I/\sigma(I) >$ [1]	2.72 (at 2.31Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8.1_1161)	Depositor
R, R_{free}	0.184 , 0.242 0.192 , 0.250	Depositor DCC
R_{free} test set	4312 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	28.0	Xtriage
Anisotropy	0.189	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 39.6	EDS
Estimated twinning fraction	0.031 for h,-h-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 85989 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	15034	wwPDB-VP
Average B, all atoms (Å^2)	29.0	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 68.00 % 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 4.6973e-06.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, 0.375 respectively for untwinned datasets, and 0.333, 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: NA

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	0.42	0/1597	0.59	0/2166
1	B	0.40	0/1625	0.62	0/2203
1	C	0.41	0/1612	0.58	0/2186
1	D	0.45	0/1612	0.62	0/2187
1	E	0.44	0/1598	0.60	0/2165
1	F	0.42	0/1620	0.64	1/2196 (0.0%)
1	G	0.46	0/1612	0.64	0/2186
1	H	0.45	0/1605	0.64	0/2176
1	I	0.45	0/1612	0.64	0/2186
All	All	0.43	0/14493	0.62	1/19651 (0.0%)

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
1	G	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	15	VAL	CB-CA-C	-5.98	100.03	111.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	1	MSE	Peptide

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	1578	0	1590	14	0
1	B	1603	0	1620	18	0
1	C	1593	0	1609	22	0
1	D	1593	0	1603	16	0
1	E	1580	0	1596	23	0
1	F	1598	0	1619	20	0
1	G	1593	0	1609	22	0
1	H	1586	0	1602	20	0
1	I	1593	0	1609	22	0
2	A	1	0	0	0	0
2	D	1	0	0	0	0
2	G	1	0	0	0	0
3	A	71	0	0	1	0
3	B	65	0	0	2	0
3	C	77	0	0	0	0
3	D	85	0	0	0	0
3	E	71	0	0	2	0
3	F	87	0	0	0	0
3	G	78	0	0	0	0
3	H	84	0	0	0	0
3	I	96	0	0	1	0
All	All	15034	0	14457	145	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 5.

All (145) 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:F:136:THR:HG22	1:F:138:SER:H	1.33	0.94
1:E:162:MSE:HE2	1:E:260:PRO:HB3	1.52	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:128:LYS:HG2	1:E:237:ALA:HB2	1.57	0.85
1:H:128:LYS:HG2	1:H:237:ALA:HB2	1.60	0.82
1:G:118:LYS:HE2	1:I:261:GLN:HA	1.60	0.81
1:B:128:LYS:HG2	1:B:237:ALA:HB2	1.65	0.78
1:I:49:ALA:HB2	1:I:55:LEU:HB2	1.71	0.70
1:E:259:ILE:HG22	1:F:118:LYS:HG3	1.72	0.69
1:G:38:THR:HG22	1:G:40:SER:H	1.57	0.68
1:I:136:THR:HG22	1:I:139:ASN:H	1.60	0.66
1:D:24:GLN:HG3	1:D:41:THR:HG22	1.76	0.66
1:I:136:THR:HG23	1:I:138:SER:H	1.60	0.65
1:G:54:SER:HB2	1:G:117:LEU:HD13	1.79	0.63
1:B:117:LEU:HD13	1:B:157:LYS:HB3	1.80	0.63
1:E:6:PHE:CE2	1:E:15:VAL:HG13	2.33	0.62
1:H:162:MSE:HE2	1:H:212:THR:HG22	1.80	0.62
1:I:47:MSE:HE1	1:I:67:ILE:HD13	1.81	0.62
1:C:57:VAL:HG22	1:C:67:ILE:HD12	1.82	0.62
1:D:49:ALA:HB2	1:D:55:LEU:HB2	1.82	0.62
1:C:173:ARG:HH12	1:C:230:SER:HB3	1.64	0.62
1:D:186:GLY:O	1:I:30:LYS:NZ	2.33	0.61
1:G:206:SER:HB3	1:G:208:ARG:NH1	2.16	0.61
1:H:51:ASP:HB2	1:I:71:LEU:H	1.66	0.61
1:C:136:THR:HG22	1:C:138:SER:H	1.64	0.61
1:H:47:MSE:HE3	1:H:67:ILE:HD12	1.81	0.60
1:E:162:MSE:CE	1:E:260:PRO:HB3	2.30	0.60
1:D:184:ARG:HH21	1:D:211:ILE:HD13	1.68	0.59
1:G:206:SER:HB3	1:G:208:ARG:HH12	1.68	0.59
1:D:67:ILE:HD11	1:F:36:LEU:HD22	1.85	0.58
1:H:52:GLY:HA2	1:H:117:LEU:HD22	1.84	0.58
1:D:34:ILE:HG21	1:D:47:MSE:HE2	1.85	0.58
1:E:162:MSE:HE2	1:E:260:PRO:CB	2.33	0.56
1:C:228:LEU:O	1:C:230:SER:N	2.39	0.55
1:E:162:MSE:HE3	1:F:120:PHE:HD2	1.73	0.54
1:B:201:VAL:HG23	3:B:341:HOH:O	2.07	0.54
1:D:185:GLU:HG3	1:D:220:THR:HB	1.89	0.54
1:A:149:ILE:HD11	1:A:223:LEU:HD23	1.90	0.53
1:E:260:PRO:O	1:F:118:LYS:HG2	2.08	0.53
1:I:49:ALA:HB1	1:I:53:ILE:HG22	1.89	0.53
1:G:38:THR:HG22	1:G:40:SER:N	2.24	0.52
1:G:49:ALA:HB2	1:G:55:LEU:HB2	1.91	0.52
1:E:224:ARG:HD2	3:E:339:HOH:O	2.10	0.52
1:C:184:ARG:HG2	1:C:184:ARG:HH11	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:47:MSE:SE	1:H:47:MSE:HE1	2.61	0.51
1:E:120:PHE:CE2	1:E:122:ASN:HB2	2.45	0.51
1:F:6:PHE:CE2	1:F:15:VAL:HG13	2.46	0.51
1:C:184:ARG:NH1	1:C:185:GLU:O	2.44	0.51
1:E:162:MSE:HE3	1:F:120:PHE:CD2	2.45	0.50
1:A:57:VAL:HG22	1:A:67:ILE:HD13	1.92	0.50
1:E:211:ILE:HD12	1:E:221:TYR:CZ	2.46	0.50
1:C:228:LEU:C	1:C:230:SER:H	2.17	0.49
1:I:6:PHE:CE2	1:I:15:VAL:HG13	2.48	0.48
1:G:43:VAL:HG22	1:H:62:SER:HA	1.95	0.48
1:F:244:ILE:HB	1:F:249:ASN:ND2	2.28	0.48
1:A:224:ARG:HD2	3:A:469:HOH:O	2.12	0.48
1:B:168:ASP:HB3	1:B:204:LEU:HD11	1.95	0.48
1:B:149:ILE:HD11	1:B:223:LEU:HD23	1.95	0.48
1:D:120:PHE:CE2	1:D:122:ASN:HB2	2.48	0.48
1:H:128:LYS:NZ	1:H:241:GLY:O	2.46	0.48
1:A:164:LEU:HD11	1:A:208:ARG:NH2	2.28	0.48
1:A:52:GLY:HA2	1:A:117:LEU:HD12	1.96	0.48
1:B:44:ALA:O	1:C:65:ALA:HB3	2.14	0.47
1:G:30:LYS:HA	1:G:30:LYS:HD3	1.57	0.47
1:I:1:MSE:HE3	1:I:18:ASP:OD1	2.13	0.47
1:I:38:THR:HG22	1:I:40:SER:N	2.29	0.47
1:G:36:LEU:HD11	1:H:32:GLN:HA	1.97	0.47
1:H:140:ILE:HD11	1:H:193:ILE:HD13	1.96	0.47
1:E:164:LEU:HD21	1:E:208:ARG:HH21	1.81	0.47
1:A:48:THR:OG1	1:B:68:THR:HG22	2.16	0.47
1:E:37:GLY:HA3	1:F:30:LYS:O	2.15	0.46
1:C:164:LEU:HD21	1:C:208:ARG:NH2	2.30	0.46
1:B:32:GLN:HB2	1:B:46:LYS:HE2	1.97	0.46
1:H:244:ILE:HB	1:H:249:ASN:ND2	2.30	0.46
1:I:211:ILE:HD12	1:I:221:TYR:CZ	2.51	0.46
1:A:47:MSE:HE1	1:A:67:ILE:HD12	1.98	0.46
1:E:60:ASN:O	1:E:64:ASN:HB3	2.15	0.46
1:A:68:THR:HG22	1:C:48:THR:OG1	2.15	0.46
1:A:174:MSE:HA	1:A:174:MSE:HE2	1.98	0.46
1:D:30:LYS:HA	1:D:30:LYS:HD3	1.62	0.46
1:D:36:LEU:HD11	1:E:32:GLN:HA	1.99	0.45
1:H:32:GLN:HG2	1:H:57:VAL:HG11	1.98	0.45
1:B:59:ASN:C	1:B:61:SER:H	2.20	0.45
1:B:71:LEU:HD21	1:C:71:LEU:HD21	1.98	0.45
1:D:117:LEU:HD13	1:D:157:LYS:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:LEU:HD11	1:B:32:GLN:HA	1.98	0.45
1:D:149:ILE:HD11	1:D:223:LEU:HD23	1.98	0.45
1:F:136:THR:HG22	1:F:138:SER:N	2.16	0.45
1:I:38:THR:HG22	1:I:40:SER:H	1.80	0.45
1:B:211:ILE:HD12	1:B:221:TYR:CZ	2.51	0.45
1:H:6:PHE:CE2	1:H:15:VAL:HG13	2.52	0.45
1:H:47:MSE:HE3	1:H:67:ILE:HG21	1.99	0.45
1:A:34:ILE:HG21	1:A:47:MSE:HE2	1.98	0.45
1:C:130:GLN:HG3	1:C:234:TRP:CE2	2.51	0.45
1:F:118:LYS:HB2	1:F:118:LYS:HE2	1.71	0.44
1:E:208:ARG:HH12	1:F:208:ARG:HH21	1.64	0.44
1:D:21:LYS:O	1:E:16:PHE:HA	2.18	0.44
1:B:184:ARG:HD3	3:B:363:HOH:O	2.18	0.44
1:H:21:LYS:O	1:I:16:PHE:HA	2.17	0.44
1:C:25:MSE:HE2	1:C:27:GLU:O	2.17	0.44
1:E:208:ARG:NH1	3:E:332:HOH:O	2.51	0.44
1:C:127:ASN:HB2	1:C:129:ILE:HD11	1.99	0.44
1:G:67:ILE:HD12	1:I:34:ILE:HD11	2.00	0.44
1:G:169:ILE:HA	1:G:251:SER:HB3	2.00	0.44
1:B:31:ASP:OD2	1:B:32:GLN:HG3	2.18	0.44
1:D:30:LYS:O	1:F:37:GLY:HA3	2.18	0.44
1:A:261:GLN:HG3	1:F:138:SER:HB2	2.00	0.43
1:F:40:SER:OG	1:F:41:THR:N	2.50	0.43
1:A:2:GLY:N	1:A:18:ASP:OD2	2.51	0.43
1:E:25:MSE:HE3	1:E:44:ALA:HB2	2.00	0.43
1:I:136:THR:HG22	1:I:139:ASN:N	2.31	0.43
1:A:68:THR:HA	1:C:48:THR:O	2.19	0.43
1:C:184:ARG:HG2	1:C:184:ARG:NH1	2.34	0.43
1:I:163:PHE:HB2	1:I:211:ILE:HG12	2.01	0.43
1:G:250:THR:HB	3:I:392:HOH:O	2.18	0.43
1:E:163:PHE:HB2	1:E:211:ILE:HG12	2.01	0.43
1:E:21:LYS:O	1:F:16:PHE:HA	2.18	0.43
1:H:40:SER:HB3	1:H:41:THR:H	1.52	0.43
1:G:30:LYS:O	1:I:37:GLY:HA3	2.19	0.42
1:G:140:ILE:HD13	1:H:245:LEU:HD13	2.01	0.42
1:H:164:LEU:HD22	1:H:208:ARG:HH21	1.84	0.42
1:G:162:MSE:HG3	1:G:260:PRO:HG3	2.00	0.42
1:C:244:ILE:HB	1:C:249:ASN:ND2	2.35	0.42
1:G:16:PHE:HA	1:I:21:LYS:O	2.19	0.42
1:H:51:ASP:HB2	1:I:71:LEU:HB2	2.00	0.42
1:I:38:THR:CG2	1:I:40:SER:H	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:55:LEU:HD13	1:F:55:LEU:HA	1.67	0.42
1:B:120:PHE:CE2	1:B:122:ASN:HB2	2.54	0.42
1:C:49:ALA:HB2	1:C:55:LEU:HB2	2.01	0.42
1:G:238:LEU:HD12	1:G:242:ASN:HB2	2.02	0.42
1:C:230:SER:HB3	1:C:231:GLY:H	1.61	0.42
1:I:228:LEU:O	1:I:230:SER:N	2.52	0.42
1:B:47:MSE:HA	1:C:67:ILE:HG23	2.02	0.41
1:G:135:PHE:CE2	1:G:146:GLY:HA3	2.54	0.41
1:B:142:THR:O	1:B:190:PRO:HD3	2.21	0.41
1:F:240:ASN:ND2	1:F:242:ASN:OD1	2.53	0.41
1:E:208:ARG:HH12	1:F:208:ARG:NH2	2.19	0.41
1:G:184:ARG:NH1	1:G:187:ASP:OD2	2.54	0.41
1:C:25:MSE:HE3	1:C:44:ALA:HB2	2.02	0.41
1:D:128:LYS:HD2	1:D:237:ALA:HB2	2.03	0.41
1:D:244:ILE:HB	1:D:249:ASN:ND2	2.35	0.41
1:G:133:GLY:O	1:G:146:GLY:HA2	2.22	0.40
1:B:238:LEU:HD12	1:B:242:ASN:HB2	2.04	0.40
1:C:47:MSE:HE3	1:C:67:ILE:HD13	2.03	0.40
1:H:166:SER:HA	1:H:208:ARG:HD2	2.02	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	213/219 (97%)	202 (95%)	10 (5%)	1 (0%)	34	41
1	B	217/219 (99%)	207 (95%)	8 (4%)	2 (1%)	21	24
1	C	215/219 (98%)	206 (96%)	7 (3%)	2 (1%)	21	24
1	D	215/219 (98%)	200 (93%)	14 (6%)	1 (0%)	34	41
1	E	211/219 (96%)	203 (96%)	7 (3%)	1 (0%)	34	41

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	216/219 (99%)	207 (96%)	8 (4%)	1 (0%)	34	41
1	G	215/219 (98%)	205 (95%)	8 (4%)	2 (1%)	21	24
1	H	214/219 (98%)	205 (96%)	6 (3%)	3 (1%)	14	13
1	I	215/219 (98%)	204 (95%)	9 (4%)	2 (1%)	21	24
All	All	1931/1971 (98%)	1839 (95%)	77 (4%)	15 (1%)	24	27

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	229	GLU
1	H	51	ASP
1	B	175	GLU
1	F	175	GLU
1	A	175	GLU
1	B	60	ASN
1	C	175	GLU
1	E	175	GLU
1	G	59	ASN
1	G	175	GLU
1	H	175	GLU
1	I	175	GLU
1	I	229	GLU
1	D	175	GLU
1	H	2	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	182/180 (101%)	173 (95%)	9 (5%)	31	41
1	B	185/180 (103%)	178 (96%)	7 (4%)	40	54
1	C	184/180 (102%)	176 (96%)	8 (4%)	35	47
1	D	184/180 (102%)	177 (96%)	7 (4%)	40	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	E	182/180 (101%)	168 (92%)	14 (8%)	16 20
1	F	185/180 (103%)	168 (91%)	17 (9%)	11 13
1	G	184/180 (102%)	173 (94%)	11 (6%)	24 31
1	H	183/180 (102%)	170 (93%)	13 (7%)	18 23
1	I	184/180 (102%)	171 (93%)	13 (7%)	18 23
All	All	1653/1620 (102%)	1554 (94%)	99 (6%)	24 31

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	8	LEU
1	A	27	GLU
1	A	59	ASN
1	A	63	THR
1	A	67	ILE
1	A	118	LYS
1	A	152	PHE
1	A	157	LYS
1	B	1	MSE
1	B	30	LYS
1	B	63	THR
1	B	152	PHE
1	B	188	SER
1	B	216	LEU
1	B	217	THR
1	C	7	TYR
1	C	55	LEU
1	C	58	SER
1	C	132	ASN
1	C	174	MSE
1	C	187	ASP
1	C	230	SER
1	C	262	THR
1	D	41	THR
1	D	59	ASN
1	D	134	LEU
1	D	152	PHE
1	D	211	ILE
1	D	248	THR

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Mol	Chain	Res	Type
1	D	261	GLN
1	E	11	THR
1	E	15	VAL
1	E	47	MSE
1	E	56	THR
1	E	57	VAL
1	E	117	LEU
1	E	138	SER
1	E	152	PHE
1	E	154	VAL
1	E	164	LEU
1	E	166	SER
1	E	212	THR
1	E	229	GLU
1	E	262	THR
1	F	1	MSE
1	F	11	THR
1	F	15	VAL
1	F	30	LYS
1	F	32	GLN
1	F	47	MSE
1	F	55	LEU
1	F	164	LEU
1	F	183	VAL
1	F	185	GLU
1	F	208	ARG
1	F	211	ILE
1	F	214	THR
1	F	217	THR
1	F	247	ILE
1	F	261	GLN
1	F	262	THR
1	G	8	LEU
1	G	27	GLU
1	G	38	THR
1	G	43	VAL
1	G	48	THR
1	G	55	LEU
1	G	117	LEU
1	G	134	LEU
1	G	152	PHE
1	G	164	LEU

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Mol	Chain	Res	Type
1	G	217	THR
1	H	8	LEU
1	H	15	VAL
1	H	40	SER
1	H	43	VAL
1	H	55	LEU
1	H	56	THR
1	H	67	ILE
1	H	117	LEU
1	H	128	LYS
1	H	134	LEU
1	H	152	PHE
1	H	164	LEU
1	H	166	SER
1	I	15	VAL
1	I	38	THR
1	I	53	ILE
1	I	55	LEU
1	I	63	THR
1	I	64	ASN
1	I	118	LYS
1	I	136	THR
1	I	164	LEU
1	I	185	GLU
1	I	208	ARG
1	I	216	LEU
1	I	261	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	252	ASN
1	B	261	GLN
1	D	252	ASN
1	E	252	ASN
1	G	24	GLN
1	H	252	ASN

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

Of 3 ligands modelled in this entry, 3 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

There are no such residues in this entry.

5.8 Polymer linkage issues

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	211/219 (96%)	-0.17	3 (1%)	78	83	18, 28, 43, 53	0
1	B	213/219 (97%)	0.04	13 (6%)	25	33	20, 32, 49, 66	0
1	C	212/219 (96%)	0.05	4 (1%)	70	76	21, 31, 46, 53	0
1	D	213/219 (97%)	-0.06	7 (3%)	50	59	17, 26, 37, 58	0
1	E	210/219 (95%)	-0.03	5 (2%)	62	71	18, 29, 42, 63	0
1	F	212/219 (96%)	-0.04	1 (0%)	91	94	17, 28, 40, 44	0
1	G	212/219 (96%)	-0.10	5 (2%)	62	71	16, 26, 43, 53	0
1	H	211/219 (96%)	-0.05	5 (2%)	62	71	15, 25, 42, 57	0
1	I	212/219 (96%)	-0.10	6 (2%)	56	66	15, 25, 38, 48	0
All	All	1906/1971 (96%)	-0.05	49 (2%)	59	68	15, 28, 43, 66	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	60	ASN	6.1
1	D	60	ASN	5.3
1	C	62	SER	5.0
1	E	60	ASN	4.7
1	D	262	THR	4.6
1	B	262	THR	4.3
1	D	59	ASN	4.2
1	H	60	ASN	4.2
1	H	61	SER	4.0
1	C	262	THR	3.9
1	A	39	LYS	3.9
1	B	59	ASN	3.9
1	D	263	ASN	3.9
1	B	62	SER	3.8
1	C	214	THR	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	64	ASN	3.6
1	A	63	THR	3.4
1	I	262	THR	3.4
1	H	51	ASP	3.3
1	E	59	ASN	3.2
1	D	39	LYS	3.2
1	G	39	LYS	3.1
1	B	58	SER	3.1
1	H	64	ASN	3.0
1	G	262	THR	3.0
1	G	51	ASP	3.0
1	B	138	SER	2.8
1	I	214	THR	2.8
1	I	60	ASN	2.7
1	B	61	SER	2.7
1	B	263	ASN	2.6
1	I	204	LEU	2.5
1	B	63	THR	2.5
1	C	230	SER	2.4
1	E	61	SER	2.4
1	G	59	ASN	2.4
1	G	60	ASN	2.4
1	H	59	ASN	2.4
1	B	214	THR	2.3
1	E	262	THR	2.3
1	A	60	ASN	2.3
1	B	8	LEU	2.2
1	B	212	THR	2.2
1	I	64	ASN	2.2
1	D	51	ASP	2.1
1	F	205	CYS	2.1
1	I	39	LYS	2.1
1	D	248	THR	2.1
1	E	64	ASN	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)

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
2	NA	G	301	1/1	0.95	0.21	2.80	29,29,29,29	0
2	NA	A	301	1/1	0.94	0.11	-0.25	31,31,31,31	0
2	NA	D	301	1/1	0.95	0.05	-3.37	32,32,32,32	0

6.5 Other polymers (i)

There are no such residues in this entry.