



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 6, 2024 – 07:25 pm GMT

PDB ID : 6GJT
Title : Chlamydia protein Pgp3 studied at high resolution in a new crystal form
Authors : Helliwell, J.R.
Deposited on : 2018-05-17
Resolution : 1.98 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 ⓘ 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 ⓘ](#)) 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

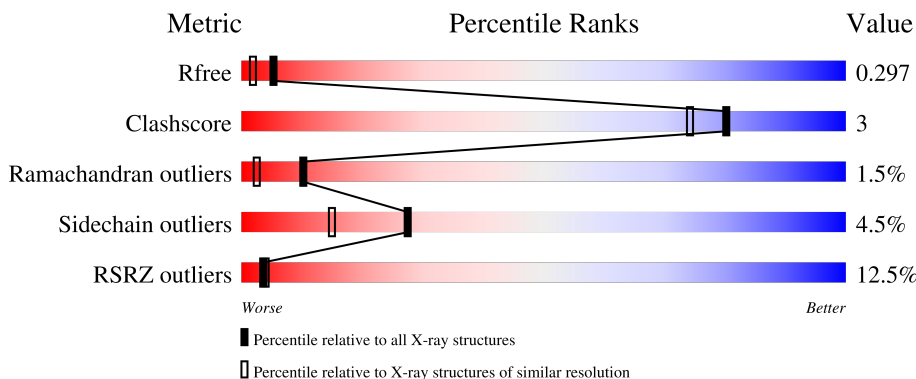
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.98 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.



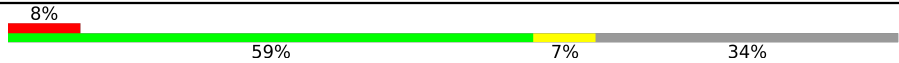
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	11647 (2.00-1.96)
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)
RSRZ outliers	127900	11410 (2.00-1.96)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	264	<div style="display: flex; align-items: center;"> <div style="width: 10%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 61%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 32%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">10% 61% 5% 2% 2% 32%</p>
1	B	264	<div style="display: flex; align-items: center;"> <div style="width: 8%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 59%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 25%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">8% 59% 8% 33%</p>
1	C	264	<div style="display: flex; align-items: center;"> <div style="width: 8%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 57%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 36%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">8% 57% 6% 1% 1% 36%</p>
1	D	264	<div style="display: flex; align-items: center;"> <div style="width: 7%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 59%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 33%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">7% 59% 6% 1% 1% 33%</p>
1	E	264	<div style="display: flex; align-items: center;"> <div style="width: 9%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 61%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 31%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">9% 61% 7% 1% 1% 31%</p>

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Mol	Chain	Length	Quality of chain
1	F	264	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into four segments: a red segment at the beginning labeled '8%', a large green segment labeled '59%', a yellow segment labeled '7%', and a grey segment at the end labeled '34%'.</p>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 8249 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
			Total	C	N	O	S			
1	A	179	1354	857	227	265	5	0	1	0
1	B	178	1355	858	228	264	5	0	2	0
1	C	169	1279	810	215	249	5	0	1	0
1	D	177	1368	862	233	268	5	0	4	0
1	E	181	1380	872	231	271	6	0	2	0
1	F	175	1324	839	221	259	5	0	1	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	90	GLN	GLY	conflict	UNP P0CE18
B	90	GLN	GLY	conflict	UNP P0CE18
C	90	GLN	GLY	conflict	UNP P0CE18
D	90	GLN	GLY	conflict	UNP P0CE18
E	90	GLN	GLY	conflict	UNP P0CE18
F	90	GLN	GLY	conflict	UNP P0CE18

- Molecule 2 is BROMIDE ION (three-letter code: BR) (formula: Br).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total 3	Br 3	0	0
2	B	6	Total 6	Br 6	0	0
2	C	5	Total 5	Br 5	0	0

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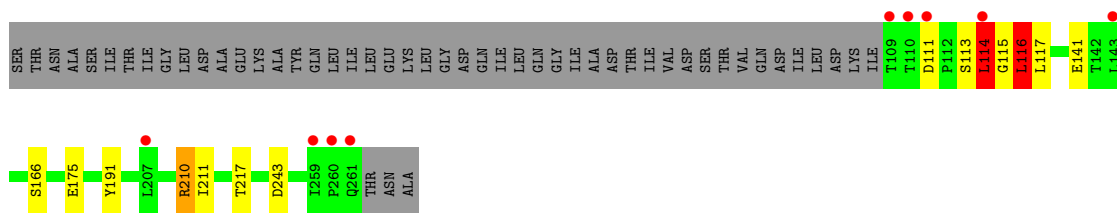
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	3	Total 3	Br 3	0	0
2	E	7	Total 7	Br 7	0	0
2	F	4	Total 4	Br 4	0	0

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

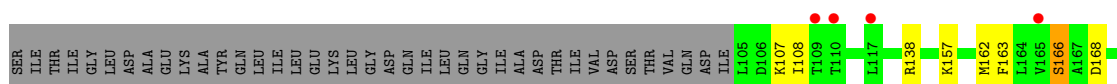
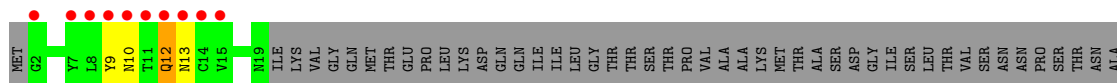
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total 3	K 3	0	0
3	D	2	Total 2	K 2	0	0
3	F	1	Total 1	K 1	0	0

- Molecule 4 is water.

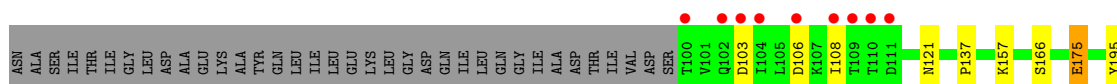
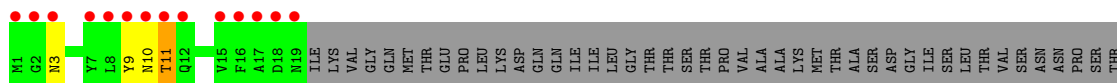
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	26	Total 26	O 26	0	0
4	B	28	Total 28	O 28	0	0
4	C	23	Total 23	O 23	0	0
4	D	31	Total 31	O 31	0	0
4	E	29	Total 29	O 29	0	0
4	F	18	Total 18	O 18	0	0



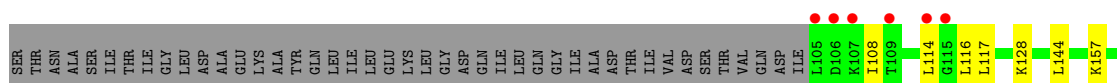
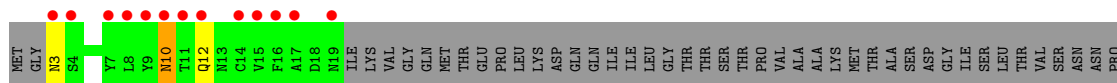
• Molecule 1: Virulence plasmid protein pGP3-D



• Molecule 1: Virulence plasmid protein pGP3-D



• Molecule 1: Virulence plasmid protein pGP3-D



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	85.41Å 108.25Å 207.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.62 – 1.98 41.82 – 1.98	Depositor EDS
% Data completeness (in resolution range)	97.8 (42.62-1.98) 97.8 (41.82-1.98)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.95 (at 1.98Å)	Xtrriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.273 , 0.292 0.277 , 0.297	Depositor DCC
R_{free} test set	6594 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	26.9	Xtrriage
Anisotropy	0.256	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 46.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	8249	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 39.80 % 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 3.0059e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: BR, K

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	0.92	0/1376	0.96	4/1871 (0.2%)
1	B	0.97	1/1377 (0.1%)	0.95	5/1872 (0.3%)
1	C	0.90	0/1301	0.97	5/1769 (0.3%)
1	D	0.95	0/1390	0.92	2/1888 (0.1%)
1	E	0.99	1/1402 (0.1%)	0.90	1/1905 (0.1%)
1	F	0.91	0/1346	0.90	3/1831 (0.2%)
All	All	0.94	2/8192 (0.0%)	0.93	20/11136 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	195	TYR	N-CA	5.38	1.57	1.46
1	B	197	TYR	CB-CG	5.18	1.59	1.51

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	224	ARG	NE-CZ-NH1	7.12	123.86	120.30
1	C	210	ARG	NE-CZ-NH2	-6.95	116.82	120.30
1	F	114	LEU	N-CA-C	6.88	129.59	111.00
1	E	239	SER	CB-CA-C	-6.83	97.13	110.10
1	B	210	ARG	NE-CZ-NH2	-6.81	116.89	120.30
1	B	8	LEU	CA-CB-CG	6.65	130.59	115.30
1	A	117	LEU	N-CA-C	6.61	128.85	111.00
1	A	138	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	B	222	SER	N-CA-CB	-6.04	101.44	110.50
1	F	243	ASP	CB-CG-OD2	5.92	123.63	118.30
1	D	224[A]	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	D	224[B]	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	C	243	ASP	CB-CG-OD1	-5.74	113.13	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	164	LEU	CA-CB-CG	5.66	128.32	115.30
1	B	173	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	C	114	LEU	CA-C-N	5.50	127.20	116.20
1	C	18	ASP	CB-CA-C	5.28	120.96	110.40
1	C	243	ASP	CB-CG-OD2	5.27	123.04	118.30
1	A	210	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	F	114	LEU	CA-C-N	5.10	126.40	116.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1354	0	1359	8	0
1	B	1355	0	1361	10	0
1	C	1279	0	1280	5	0
1	D	1368	0	1365	15	0
1	E	1380	0	1384	8	0
1	F	1324	0	1325	8	0
2	A	3	0	0	1	0
2	B	6	0	0	1	0
2	C	5	0	0	0	0
2	D	3	0	0	0	0
2	E	7	0	0	2	0
2	F	4	0	0	1	0
3	A	3	0	0	0	0
3	D	2	0	0	0	0
3	F	1	0	0	0	0
4	A	26	0	0	0	0
4	B	28	0	0	0	0
4	C	23	0	0	0	0
4	D	31	0	0	0	0
4	E	29	0	0	0	0
4	F	18	0	0	0	0
All	All	8249	0	8074	44	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 3.

All (44) 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:106:ASP:O	1:B:110:THR:HG22	1.76	0.83
1:F:117:LEU:HB3	1:F:157:LYS:HE2	1.66	0.77
1:C:6:PHE:CE2	1:C:15:VAL:HG22	2.26	0.71
1:F:128:LYS:HE2	1:F:241:GLY:O	1.92	0.69
1:E:103:ASP:O	1:E:106:ASP:OD1	2.13	0.67
1:D:9:TYR:O	1:D:12:GLN:OE1	2.13	0.65
1:B:137:PRO:HD2	2:B:306:BR:BR	2.52	0.65
1:A:104:ILE:CD1	1:B:101:VAL:HG22	2.29	0.63
1:D:261[B]:GLN:OE1	1:E:121:ASN:OD1	2.18	0.62
1:D:208[B]:ARG:HE	1:E:208[B]:ARG:NH2	1.98	0.61
1:D:163:PHE:HB2	1:D:211:ILE:CG1	2.31	0.60
1:D:163:PHE:HB2	1:D:211:ILE:HG12	1.83	0.60
1:C:115:GLY:C	1:C:116:LEU:O	2.39	0.58
1:C:6:PHE:CE2	1:C:15:VAL:CG2	2.89	0.56
1:D:261[A]:GLN:O	1:D:262:THR:HG23	2.06	0.55
1:A:104:ILE:HD11	1:B:101:VAL:HG22	1.90	0.53
1:A:137:PRO:HD2	2:A:303:BR:BR	2.64	0.53
1:D:261[B]:GLN:O	1:D:262:THR:HG23	2.08	0.53
1:E:175[B]:GLU:HG3	1:E:199:SER:O	2.10	0.52
1:A:104:ILE:HD12	1:B:101:VAL:HG22	1.92	0.52
1:A:108:ILE:HD12	1:A:116:LEU:HD22	1.91	0.52
1:B:3:ASN:OD1	1:B:16:PHE:HZ	1.93	0.51
1:B:3:ASN:OD1	1:B:16:PHE:CZ	2.64	0.51
1:F:108:ILE:O	1:F:117:LEU:HD11	2.11	0.50
1:A:109:THR:O	1:A:109:THR:HG22	2.11	0.50
1:D:166:SER:OG	1:D:208[B]:ARG:NH1	2.45	0.50
1:E:137:PRO:HD2	2:E:307:BR:BR	2.68	0.48
1:E:9:TYR:O	1:E:11:THR:N	2.46	0.48
1:B:105:LEU:HA	1:B:108:ILE:HG12	1.96	0.47
1:F:128:LYS:O	1:F:128:LYS:HG2	2.14	0.47
1:D:168:ASP:OD1	1:D:208[B]:ARG:NH2	2.44	0.47
1:A:164:LEU:HD22	1:A:208:ARG:HH12	1.80	0.47
1:D:157:LYS:HD2	1:F:261[A]:GLN:CD	2.36	0.46
1:D:13:ASN:HD22	1:F:3:ASN:HA	1.81	0.45
1:B:168:ASP:OD1	1:B:208[B]:ARG:NH1	2.41	0.44
1:F:222:SER:HB3	2:F:301:BR:BR	2.74	0.43
1:C:111:ASP:HB3	1:C:114:LEU:HD22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:GLY:HA2	1:B:13:ASN:OD1	2.20	0.42
1:D:108:ILE:HG21	1:F:116:LEU:HD21	2.01	0.41
1:C:191:TYR:CE1	1:C:211:ILE:HD12	2.55	0.41
1:D:261[A]:GLN:OE1	1:E:157:LYS:NZ	2.48	0.41
1:E:215:GLY:HA2	2:E:304:BR:BR	2.76	0.41
1:D:162:MET:HA	1:D:211:ILE:O	2.22	0.40
1:D:211:ILE:HD12	1:D:221:TYR:CZ	2.56	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	176/264 (67%)	170 (97%)	3 (2%)	3 (2%)	9	2
1	B	176/264 (67%)	171 (97%)	3 (2%)	2 (1%)	14	5
1	C	166/264 (63%)	157 (95%)	5 (3%)	4 (2%)	6	1
1	D	177/264 (67%)	167 (94%)	7 (4%)	3 (2%)	9	2
1	E	179/264 (68%)	170 (95%)	6 (3%)	3 (2%)	9	2
1	F	172/264 (65%)	163 (95%)	7 (4%)	2 (1%)	13	4
All	All	1046/1584 (66%)	998 (95%)	31 (3%)	17 (2%)	10	2

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	117	LEU
1	A	10	ASN
1	A	117	LEU
1	C	116	LEU
1	D	10	ASN

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Mol	Chain	Res	Type
1	E	10	ASN
1	F	10	ASN
1	A	175	GLU
1	B	175	GLU
1	C	175	GLU
1	D	175	GLU
1	E	175[A]	GLU
1	E	175[B]	GLU
1	F	175	GLU
1	B	10	ASN
1	D	262	THR
1	C	114	LEU

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	154/224 (69%)	145 (94%)	9 (6%)	20	9
1	B	154/224 (69%)	149 (97%)	5 (3%)	39	28
1	C	145/224 (65%)	137 (94%)	8 (6%)	21	10
1	D	155/224 (69%)	150 (97%)	5 (3%)	39	28
1	E	157/224 (70%)	150 (96%)	7 (4%)	27	15
1	F	151/224 (67%)	144 (95%)	7 (5%)	27	14
All	All	916/1344 (68%)	875 (96%)	41 (4%)	27	15

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	11	THR
1	A	12	GLN
1	A	100	THR
1	A	103	ASP
1	A	117	LEU

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Mol	Chain	Res	Type
1	A	164	LEU
1	A	166	SER
1	A	210	ARG
1	B	11	THR
1	B	102	GLN
1	B	166	SER
1	B	210	ARG
1	B	217	THR
1	C	10	ASN
1	C	113	SER
1	C	114	LEU
1	C	116	LEU
1	C	141	GLU
1	C	166	SER
1	C	210	ARG
1	C	217	THR
1	D	12	GLN
1	D	107	LYS
1	D	138	ARG
1	D	166	SER
1	D	210	ARG
1	E	3	ASN
1	E	11	THR
1	E	108	ILE
1	E	166	SER
1	E	210	ARG
1	E	217	THR
1	E	248	THR
1	F	10	ASN
1	F	12	GLN
1	F	144	LEU
1	F	166	SER
1	F	210	ARG
1	F	217	THR
1	F	262	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	10	ASN
1	D	13	ASN
1	E	121	ASN

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 34 ligands modelled in this entry, 34 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	179/264 (67%)	1.09	26 (14%) 2 2	16, 31, 83, 92	0
1	B	178/264 (67%)	0.71	21 (11%) 4 5	13, 29, 71, 96	0
1	C	169/264 (64%)	0.75	20 (11%) 4 5	17, 30, 76, 111	0
1	D	177/264 (67%)	0.76	18 (10%) 6 7	18, 28, 77, 101	0
1	E	181/264 (68%)	0.74	25 (13%) 2 3	16, 29, 72, 102	0
1	F	175/264 (66%)	0.87	22 (12%) 3 4	18, 31, 75, 103	0
All	All	1059/1584 (66%)	0.82	132 (12%) 3 4	13, 30, 77, 111	0

All (132) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2	GLY	19.1
1	A	8	LEU	14.2
1	A	9	TYR	12.4
1	F	3	ASN	8.3
1	B	101	VAL	8.1
1	B	100	THR	8.0
1	A	101	VAL	7.9
1	D	262	THR	7.3
1	A	11	THR	7.1
1	E	9	TYR	7.1
1	D	11	THR	6.9
1	E	16	PHE	6.9
1	D	10	ASN	6.4
1	A	7	TYR	6.3
1	C	114	LEU	6.2
1	D	9	TYR	6.1
1	E	100	THR	6.1
1	A	102	GLN	6.0
1	E	109	THR	5.9

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Mol	Chain	Res	Type	RSRZ
1	A	103	ASP	5.8
1	C	8	LEU	5.7
1	F	15	VAL	5.7
1	F	11	THR	5.6
1	E	17	ALA	5.6
1	D	7	TYR	5.6
1	B	110	THR	5.6
1	E	110	THR	5.5
1	C	11	THR	5.4
1	F	19	ASN	5.3
1	F	12	GLN	5.3
1	A	10	ASN	5.3
1	D	14	CYS	5.3
1	E	10	ASN	5.2
1	C	18	ASP	5.0
1	F	107	LYS	4.9
1	A	100	THR	4.9
1	E	103	ASP	4.8
1	A	106	ASP	4.8
1	A	104	ILE	4.7
1	C	110	THR	4.7
1	F	106	ASP	4.6
1	C	12	GLN	4.6
1	F	10	ASN	4.5
1	C	10	ASN	4.5
1	C	9	TYR	4.5
1	C	14	CYS	4.4
1	F	9	TYR	4.4
1	B	104	ILE	4.4
1	D	117	LEU	4.2
1	F	261[A]	GLN	4.1
1	E	1	MET	4.1
1	B	106	ASP	4.1
1	D	15	VAL	4.0
1	C	7	TYR	4.0
1	F	16	PHE	4.0
1	A	113	SER	4.0
1	B	103	ASP	4.0
1	A	159	SER	3.9
1	F	262	THR	3.9
1	E	15	VAL	3.8
1	D	109	THR	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	109	THR	3.7
1	E	2	GLY	3.7
1	C	109	THR	3.7
1	A	107	LYS	3.7
1	D	12	GLN	3.6
1	E	106	ASP	3.6
1	A	114	LEU	3.6
1	F	105	LEU	3.6
1	A	12	GLN	3.6
1	F	14	CYS	3.6
1	F	17	ALA	3.6
1	E	104	ILE	3.6
1	A	14	CYS	3.5
1	D	8	LEU	3.5
1	B	114	LEU	3.4
1	C	111	ASP	3.4
1	A	108	ILE	3.3
1	D	2	GLY	3.2
1	E	261	GLN	3.2
1	E	12	GLN	3.1
1	E	111	ASP	3.1
1	B	109	THR	3.0
1	E	11	THR	3.0
1	F	109	THR	3.0
1	A	116	LEU	3.0
1	E	18	ASP	3.0
1	B	261	GLN	2.9
1	E	3	ASN	2.9
1	C	261	GLN	2.8
1	B	208[A]	ARG	2.8
1	F	115	GLY	2.8
1	D	263	ASN	2.8
1	D	208[A]	ARG	2.8
1	E	208[A]	ARG	2.8
1	C	143	LEU	2.7
1	F	114	LEU	2.7
1	E	19	ASN	2.7
1	E	108	ILE	2.7
1	E	7	TYR	2.7
1	B	218	PRO	2.6
1	F	7	TYR	2.6
1	B	105	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	13	ASN	2.6
1	F	4	SER	2.6
1	C	260	PRO	2.6
1	A	105	LEU	2.5
1	C	19	ASN	2.5
1	A	117	LEU	2.5
1	D	165	VAL	2.5
1	B	9	TYR	2.4
1	D	261[A]	GLN	2.4
1	B	111	ASP	2.4
1	C	5	GLY	2.4
1	B	102	GLN	2.4
1	E	8	LEU	2.4
1	F	8	LEU	2.4
1	B	3	ASN	2.4
1	A	167	ALA	2.3
1	A	216	LEU	2.3
1	C	259	ILE	2.3
1	D	110	THR	2.3
1	B	108	ILE	2.3
1	F	214	THR	2.1
1	B	15	VAL	2.1
1	D	13	ASN	2.1
1	B	186	GLY	2.1
1	E	102	GLN	2.1
1	A	138	ARG	2.1
1	B	10	ASN	2.1
1	C	6	PHE	2.0
1	C	207	LEU	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
2	BR	E	304	1/1	0.90	0.22	87,87,87,87	0
2	BR	C	305	1/1	0.92	0.23	80,80,80,80	0
2	BR	B	303	1/1	0.92	0.21	72,72,72,72	0
2	BR	F	303	1/1	0.92	0.16	72,72,72,72	0
3	K	D	304	1/1	0.92	0.07	47,47,47,47	0
2	BR	F	302	1/1	0.93	0.24	76,76,76,76	0
2	BR	D	302	1/1	0.94	0.15	66,66,66,66	0
2	BR	D	303	1/1	0.94	0.27	69,69,69,69	0
2	BR	B	302	1/1	0.95	0.12	57,57,57,57	0
2	BR	B	306	1/1	0.96	0.21	77,77,77,77	0
2	BR	A	303	1/1	0.96	0.27	90,90,90,90	0
2	BR	E	303	1/1	0.97	0.29	73,73,73,73	0
2	BR	A	302	1/1	0.97	0.19	65,65,65,65	0
2	BR	E	307	1/1	0.97	0.18	71,71,71,71	0
2	BR	C	303	1/1	0.97	0.19	59,59,59,59	0
2	BR	C	304	1/1	0.97	0.15	71,71,71,71	0
2	BR	F	304	1/1	0.97	0.18	76,76,76,76	0
2	BR	E	302	1/1	0.97	0.15	50,50,50,50	0
2	BR	E	305	1/1	0.98	0.15	64,64,64,64	0
2	BR	E	306	1/1	0.98	0.21	80,80,80,80	0
2	BR	C	301	1/1	0.98	0.21	64,64,64,64	0
2	BR	F	301	1/1	0.98	0.15	66,66,66,66	0
2	BR	C	302	1/1	0.98	0.20	63,63,63,63	0
2	BR	B	304	1/1	0.98	0.19	69,69,69,69	0
2	BR	B	305	1/1	0.98	0.18	64,64,64,64	0
3	K	A	304	1/1	0.98	0.10	45,45,45,45	0
3	K	A	305	1/1	0.98	0.05	49,49,49,49	0
3	K	A	306	1/1	0.98	0.20	55,55,55,55	0
2	BR	A	301	1/1	0.98	0.06	32,32,32,32	0
3	K	D	305	1/1	0.98	0.10	44,44,44,44	0
3	K	F	305	1/1	0.98	0.07	52,52,52,52	0
2	BR	D	301	1/1	0.99	0.04	28,28,28,28	0
2	BR	E	301	1/1	0.99	0.09	49,49,49,49	0
2	BR	B	301	1/1	0.99	0.07	41,41,41,41	0

6.5 Other polymers [i](#)

There are no such residues in this entry.