



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:28 PM GMT

PDB ID : 3ZIW
Title : Clostridium perfringens enterotoxin, D48A mutation and N-terminal 37 residues deleted
Authors : Yelland, T.; Naylor, C.E.; Savva, C.G.; Basak, A.K.
Deposited on : 2013-01-14
Resolution : 1.90 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

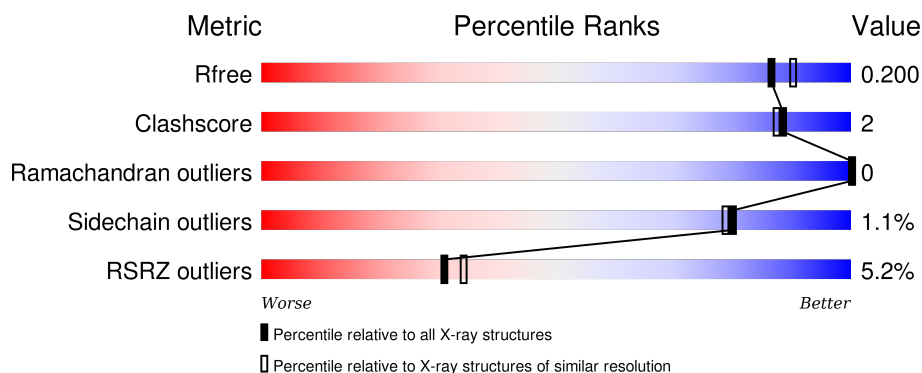
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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.



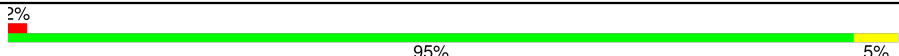
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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 $\leq 5\%$. 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	286	<div> <div>3%</div> <div>96%</div> <div>.</div> </div>
1	B	286	<div> <div>3%</div> <div>95%</div> <div>5%</div> </div>
1	C	286	<div> <div>9%</div> <div>93%</div> <div>6%</div> <div>.</div> </div>
1	D	286	<div> <div>7%</div> <div>95%</div> <div>.</div> </div>
1	E	286	<div> <div>7%</div> <div>94%</div> <div>6%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	286	

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	P6G	A	400	-	-	-	X
2	P6G	A	401	-	-	-	X
2	P6G	B	400	-	-	-	X
2	P6G	C	400	-	-	-	X
2	P6G	C	401	-	-	-	X
2	P6G	F	400	-	-	-	X

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 15261 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 HEAT-LABILE ENTEROTOXIN B CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	286	Total	C	N	O	S	0	6	0
			2248	1426	363	456	3			
1	B	286	Total	C	N	O	S	0	4	0
			2225	1414	357	450	4			
1	C	286	Total	C	N	O	S	0	4	0
			2234	1418	363	450	3			
1	D	286	Total	C	N	O	S	0	7	0
			2233	1418	358	454	3			
1	E	286	Total	C	N	O	S	0	5	0
			2217	1411	357	446	3			
1	F	286	Total	C	N	O	S	0	4	0
			2240	1419	365	453	3			

There are 30 discrepancies between the modelled and reference sequences:

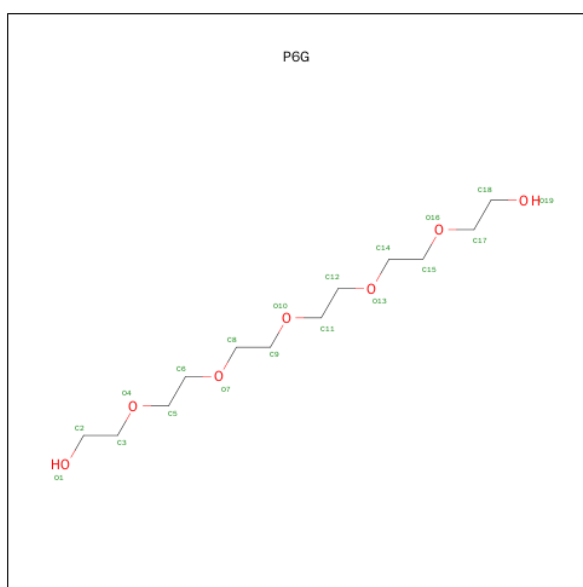
Chain	Residue	Modelled	Actual	Comment	Reference
A	34	GLY	-	EXPRESSION TAG	UNP P01558
A	35	ALA	-	EXPRESSION TAG	UNP P01558
A	36	MET	-	EXPRESSION TAG	UNP P01558
A	37	GLY	-	EXPRESSION TAG	UNP P01558
A	48	ALA	ASP	ENGINEERED MUTATION	UNP P01558
B	34	GLY	-	EXPRESSION TAG	UNP P01558
B	35	ALA	-	EXPRESSION TAG	UNP P01558
B	36	MET	-	EXPRESSION TAG	UNP P01558
B	37	GLY	-	EXPRESSION TAG	UNP P01558
B	48	ALA	ASP	ENGINEERED MUTATION	UNP P01558
C	34	GLY	-	EXPRESSION TAG	UNP P01558
C	35	ALA	-	EXPRESSION TAG	UNP P01558
C	36	MET	-	EXPRESSION TAG	UNP P01558
C	37	GLY	-	EXPRESSION TAG	UNP P01558
C	48	ALA	ASP	ENGINEERED MUTATION	UNP P01558
D	34	GLY	-	EXPRESSION TAG	UNP P01558
D	35	ALA	-	EXPRESSION TAG	UNP P01558

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Chain	Residue	Modelled	Actual	Comment	Reference
D	36	MET	-	EXPRESSION TAG	UNP P01558
D	37	GLY	-	EXPRESSION TAG	UNP P01558
D	48	ALA	ASP	ENGINEERED MUTATION	UNP P01558
E	34	GLY	-	EXPRESSION TAG	UNP P01558
E	35	ALA	-	EXPRESSION TAG	UNP P01558
E	36	MET	-	EXPRESSION TAG	UNP P01558
E	37	GLY	-	EXPRESSION TAG	UNP P01558
E	48	ALA	ASP	ENGINEERED MUTATION	UNP P01558
F	34	GLY	-	EXPRESSION TAG	UNP P01558
F	35	ALA	-	EXPRESSION TAG	UNP P01558
F	36	MET	-	EXPRESSION TAG	UNP P01558
F	37	GLY	-	EXPRESSION TAG	UNP P01558
F	48	ALA	ASP	ENGINEERED MUTATION	UNP P01558

- Molecule 2 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula: $C_{12}H_{26}O_7$).



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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	C	O	0	0
			16	10	6		
2	C	1	Total	C	O	0	0
			8	5	3		
2	D	1	Total	C	O	0	0
			16	10	6		
2	D	1	Total	C	O	0	0
			10	6	4		
2	E	1	Total	C	O	0	0
			14	9	5		
2	E	1	Total	C	O	0	0
			13	8	5		
2	E	1	Total	C	O	0	0
			10	6	4		
2	F	1	Total	C	O	0	0
			19	12	7		
2	F	1	Total	C	O	0	0
			8	5	3		

- Molecule 3 is water.

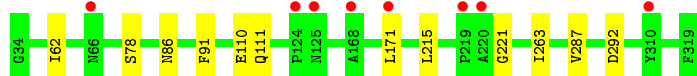
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	307	Total	O	0	0
			307	307		
3	B	306	Total	O	0	0
			306	306		
3	C	249	Total	O	0	0
			249	249		
3	D	259	Total	O	0	0
			259	259		
3	E	251	Total	O	0	0
			251	251		
3	F	307	Total	O	0	0
			307	307		

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.

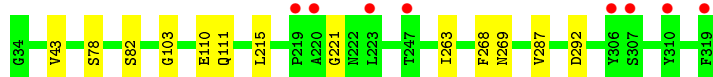
- Molecule 1: HEAT-LABILE ENTEROTOXIN B CHAIN

Chain A: 



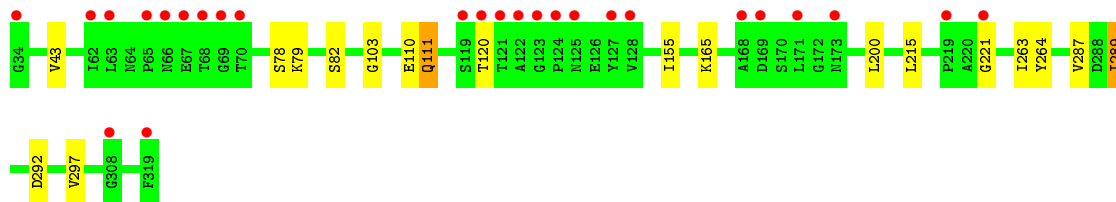
- Molecule 1: HEAT-LABILE ENTEROTOXIN B CHAIN

Chain B: 



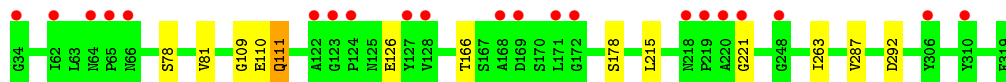
- Molecule 1: HEAT-LABILE ENTEROTOXIN B CHAIN

Chain C: 



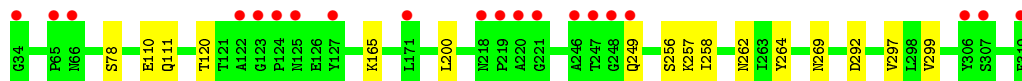
- Molecule 1: HEAT-LABILE ENTEROTOXIN B CHAIN

Chain D: 



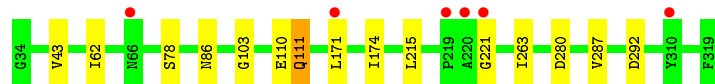
- Molecule 1: HEAT-LABILE ENTEROTOXIN B CHAIN

Chain E: 



● Molecule 1: HEAT-LABILE ENTEROTOXIN B CHAIN

Chain F:  2% 95% 5%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	190.66Å 128.02Å 136.43Å 90.00° 133.81° 90.00°	Depositor
Resolution (Å)	49.23 – 1.90 49.23 – 1.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.23-1.90) 100.0 (49.23-1.90)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.48 (at 1.90Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.175 , 0.196 0.180 , 0.200	Depositor DCC
R_{free} test set	9298 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	36.5	Xtriage
Anisotropy	0.143	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 56.2	EDS
Estimated twinning fraction	0.002 for h+2*l,k,-h-l 0.014 for h,-k,-h-l 0.035 for -h-2*l,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 185456 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	15261	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.27% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: P6G

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	0.50	0/2312	0.67	0/3137
1	B	0.50	0/2281	0.65	0/3101
1	C	0.48	0/2289	0.65	0/3108
1	D	0.50	0/2298	0.66	0/3125
1	E	0.48	0/2275	0.66	0/3095
1	F	0.52	0/2296	0.65	0/3117
All	All	0.50	0/13751	0.66	0/18683

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2248	0	2192	11	0
1	B	2225	0	2159	11	0
1	C	2234	0	2182	20	0
1	D	2233	0	2169	12	0
1	E	2217	0	2161	13	0
1	F	2240	0	2190	15	0
2	A	43	0	55	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	28	0	34	1	0
2	C	24	0	30	1	0
2	D	26	0	34	1	0
2	E	37	0	46	0	0
2	F	27	0	35	1	0
3	A	307	0	0	2	0
3	B	306	0	0	0	0
3	C	249	0	0	0	0
3	D	259	0	0	0	0
3	E	251	0	0	0	0
3	F	307	0	0	1	0
All	All	15261	0	13287	67	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 2.

All (67) 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:E:110:GLU:HG3	1:F:110[A]:GLU:HG2	1.39	1.03
1:A:110[A]:GLU:HG3	1:B:110:GLU:HG2	1.44	0.97
1:B:82:SER:HA	2:B:400:P6G:H172	1.64	0.79
1:A:110[A]:GLU:HG2	1:C:110[A]:GLU:HG3	1.67	0.77
1:B:110:GLU:HG3	1:C:110[A]:GLU:HG2	1.67	0.76
1:D:110[A]:GLU:HG3	1:F:110[A]:GLU:HG3	1.69	0.75
1:A:110[A]:GLU:CG	1:B:110:GLU:HG2	2.18	0.72
1:D:110[A]:GLU:HG2	1:E:110:GLU:HG2	1.73	0.71
1:E:110:GLU:HG3	1:F:110[A]:GLU:CG	2.20	0.70
3:A:2134:HOH:O	1:C:110[B]:GLU:HG3	1.91	0.70
1:C:110[B]:GLU:CD	1:C:110[B]:GLU:H	1.95	0.68
1:E:264:TYR:HE1	1:E:299[B]:VAL:CG1	2.11	0.64
1:D:263:ILE:HD11	1:D:287:VAL:HG21	1.80	0.63
1:F:78:SER:HA	1:F:111[B]:GLN:HG3	1.81	0.63
1:C:120:THR:HG21	1:C:165:LYS:HD3	1.81	0.62
1:D:109:GLY:HA2	1:F:110[B]:GLU:OE1	2.03	0.59
1:F:280:ASP:HA	2:F:401:P6G:H62	1.85	0.59
1:A:110[B]:GLU:HG2	3:A:2135:HOH:O	2.03	0.57
1:B:263:ILE:HD11	1:B:287:VAL:HG21	1.85	0.57
1:B:110:GLU:HG3	1:C:110[A]:GLU:CG	2.37	0.55
1:D:110[B]:GLU:OE2	1:F:110[B]:GLU:HG2	2.07	0.54
1:E:120:THR:HG21	1:E:165:LYS:HD3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:263:ILE:HD11	1:F:287:VAL:HG21	1.90	0.54
1:E:264:TYR:HE1	1:E:299[B]:VAL:HG11	1.73	0.54
1:F:62:ILE:HG21	1:F:171:LEU:CD2	2.39	0.52
1:B:263:ILE:CD1	1:B:287:VAL:HG21	2.40	0.52
1:C:263:ILE:HD11	1:C:287:VAL:HG21	1.92	0.51
1:A:78:SER:HA	1:A:111[A]:GLN:HG3	1.93	0.51
1:E:200:LEU:HD21	1:E:297[B]:VAL:HG11	1.93	0.51
1:D:110[A]:GLU:HG2	1:E:110:GLU:CG	2.41	0.51
1:E:262:ASN:HB2	1:E:299[B]:VAL:CG1	2.41	0.51
1:A:263:ILE:HD11	1:A:287:VAL:HG21	1.93	0.50
1:F:263:ILE:CD1	1:F:287:VAL:HG21	2.42	0.49
1:D:78:SER:HA	1:D:111[A]:GLN:HG3	1.94	0.49
1:C:78:SER:HA	1:C:111[A]:GLN:HG3	1.95	0.48
1:E:264:TYR:HE1	1:E:299[B]:VAL:HG12	1.79	0.47
1:D:81:VAL:O	2:D:400:P6G:H21	2.14	0.47
1:E:257:LYS:HG3	1:E:258:ILE:HG23	1.97	0.47
1:D:215:LEU:O	1:D:221:GLY:HA2	2.16	0.46
1:C:264:TYR:HB2	1:C:297[B]:VAL:HG12	1.96	0.46
1:C:82:SER:HB2	2:C:400:P6G:H61	1.97	0.46
1:F:215:LEU:O	1:F:221:GLY:HA2	2.16	0.46
1:B:78:SER:HA	1:B:111:GLN:HG3	1.97	0.46
1:D:110[A]:GLU:HG3	1:F:110[A]:GLU:CG	2.44	0.45
1:D:263:ILE:CD1	1:D:287:VAL:HG21	2.47	0.45
1:C:200:LEU:HD21	1:C:297[B]:VAL:HG11	1.98	0.45
1:C:43:VAL:HG21	1:C:103:GLY:HA3	1.99	0.44
1:C:287:VAL:HG23	1:C:289:ILE:HD12	2.00	0.44
1:B:215:LEU:O	1:B:221:GLY:HA2	2.18	0.44
1:C:79:LYS:HE3	1:C:110[A]:GLU:OE2	2.18	0.43
1:A:215:LEU:O	1:A:221:GLY:HA2	2.18	0.43
1:F:86:ASN:ND2	3:F:2082:HOH:O	2.51	0.43
1:C:263:ILE:CD1	1:C:287:VAL:HG21	2.49	0.43
1:C:215:LEU:O	1:C:221:GLY:HA2	2.18	0.43
1:E:262:ASN:HB2	1:E:299[B]:VAL:HG13	2.00	0.43
1:C:79:LYS:HD2	1:C:155:ILE:HD11	2.01	0.42
1:A:62:ILE:HD12	1:B:268:PHE:CZ	2.54	0.42
1:A:110[A]:GLU:HG2	1:C:110[A]:GLU:CG	2.44	0.42
1:A:86[B]:ASN:ND2	1:A:91:PHE:HB3	2.35	0.41
1:E:78:SER:HA	1:E:111:GLN:HG3	2.02	0.41
1:F:43:VAL:HG21	1:F:103:GLY:HA3	2.02	0.41
1:F:171:LEU:HA	1:F:174:ILE:HD12	2.01	0.41
1:A:263:ILE:CD1	1:A:287:VAL:HG21	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:166[A]:THR:HG21	1:D:178:SER:OG	2.20	0.41
1:B:43:VAL:HG21	1:B:103:GLY:HA3	2.02	0.40
1:C:264:TYR:HB2	1:C:297[B]:VAL:CG1	2.51	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	289/286 (101%)	284 (98%)	5 (2%)	0	100	100
1	B	288/286 (101%)	282 (98%)	6 (2%)	0	100	100
1	C	288/286 (101%)	284 (99%)	4 (1%)	0	100	100
1	D	291/286 (102%)	288 (99%)	3 (1%)	0	100	100
1	E	289/286 (101%)	285 (99%)	4 (1%)	0	100	100
1	F	288/286 (101%)	284 (99%)	4 (1%)	0	100	100
All	All	1733/1716 (101%)	1707 (98%)	26 (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	250/246 (102%)	248 (99%)	2 (1%)	86	86
1	B	245/246 (100%)	243 (99%)	2 (1%)	86	86
1	C	248/246 (101%)	244 (98%)	4 (2%)	70	66
1	D	248/246 (101%)	244 (98%)	4 (2%)	70	66
1	E	246/246 (100%)	242 (98%)	4 (2%)	70	66
1	F	250/246 (102%)	247 (99%)	3 (1%)	78	76
All	All	1487/1476 (101%)	1468 (99%)	19 (1%)	80	73

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	171	LEU
1	A	292	ASP
1	B	269	ASN
1	B	292	ASP
1	C	111[A]	GLN
1	C	111[B]	GLN
1	C	289	ILE
1	C	292	ASP
1	D	111[A]	GLN
1	D	111[B]	GLN
1	D	126	GLU
1	D	292	ASP
1	E	249	GLN
1	E	256	SER
1	E	269	ASN
1	E	292	ASP
1	F	111[A]	GLN
1	F	111[B]	GLN
1	F	292	ASP

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

Mol	Chain	Res	Type
1	A	241	HIS

5.3.3 RNA ⓘ

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

14 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	P6G	A	400	-	18,18,18	0.53	0	17,17,17	0.45	0
2	P6G	A	401	-	13,13,18	0.51	0	12,12,17	0.18	0
2	P6G	A	402	-	9,9,18	0.47	0	8,8,17	0.32	0
2	P6G	B	400	-	16,16,18	0.58	0	15,15,17	0.79	0
2	P6G	B	401	-	10,10,18	0.49	0	9,9,17	0.26	0
2	P6G	C	400	-	15,15,18	0.50	0	14,14,17	0.27	0
2	P6G	C	401	-	7,7,18	0.48	0	6,6,17	0.18	0
2	P6G	D	400	-	15,15,18	0.46	0	14,14,17	0.39	0
2	P6G	D	401	-	9,9,18	0.48	0	8,8,17	0.26	0
2	P6G	E	400	-	13,13,18	0.54	0	12,12,17	0.16	0
2	P6G	E	401	-	12,12,18	0.49	0	11,11,17	0.22	0
2	P6G	E	403	-	9,9,18	0.46	0	8,8,17	0.26	0
2	P6G	F	400	-	18,18,18	0.40	0	17,17,17	0.76	0
2	P6G	F	401	-	7,7,18	0.46	0	6,6,17	0.22	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	P6G	A	400	-	-	0/16/16/16	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	P6G	A	401	-	-	0/11/11/16	0/0/0/0
2	P6G	A	402	-	-	0/7/7/16	0/0/0/0
2	P6G	B	400	-	-	0/14/14/16	0/0/0/0
2	P6G	B	401	-	-	0/8/8/16	0/0/0/0
2	P6G	C	400	-	-	0/13/13/16	0/0/0/0
2	P6G	C	401	-	-	0/5/5/16	0/0/0/0
2	P6G	D	400	-	-	0/13/13/16	0/0/0/0
2	P6G	D	401	-	-	0/7/7/16	0/0/0/0
2	P6G	E	400	-	-	0/11/11/16	0/0/0/0
2	P6G	E	401	-	-	0/10/10/16	0/0/0/0
2	P6G	E	403	-	-	0/7/7/16	0/0/0/0
2	P6G	F	400	-	-	0/16/16/16	0/0/0/0
2	P6G	F	401	-	-	0/5/5/16	0/0/0/0

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.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	400	P6G	1	0
2	C	400	P6G	1	0
2	D	400	P6G	1	0
2	F	401	P6G	1	0

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, 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	286/286 (100%)	-0.06	8 (2%)	56	60	29, 47, 68, 81	0
1	B	286/286 (100%)	-0.04	8 (2%)	56	60	29, 45, 69, 94	0
1	C	286/286 (100%)	0.23	26 (9%)	11	13	31, 47, 87, 108	0
1	D	286/286 (100%)	0.08	21 (7%)	18	20	30, 47, 80, 97	0
1	E	286/286 (100%)	0.15	20 (6%)	19	21	28, 47, 77, 97	0
1	F	286/286 (100%)	-0.03	6 (2%)	67	70	27, 41, 65, 87	0
All	All	1716/1716 (100%)	0.05	89 (5%)	31	34	27, 46, 75, 108	0

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	171	LEU	6.3
1	D	168	ALA	5.6
1	C	127	TYR	5.4
1	B	219	PRO	4.8
1	C	122	ALA	4.6
1	C	69	GLY	4.6
1	C	124	PRO	4.4
1	C	219	PRO	4.3
1	E	319	PHE	4.2
1	C	123	GLY	4.2
1	E	220	ALA	3.9
1	C	66	ASN	3.9
1	E	249	GLN	3.9
1	C	125	ASN	3.8
1	C	62	ILE	3.8
1	D	122	ALA	3.8
1	E	171	LEU	3.7
1	E	221	GLY	3.7
1	C	68	THR	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	308	GLY	3.5
1	D	220	ALA	3.4
1	E	66	ASN	3.4
1	E	127	TYR	3.4
1	C	63	LEU	3.4
1	D	65	PRO	3.3
1	D	219	PRO	3.3
1	C	171	LEU	3.2
1	E	248	GLY	3.2
1	F	219	PRO	3.2
1	F	171	LEU	3.1
1	C	319	PHE	3.1
1	D	123	GLY	3.1
1	C	70	THR	3.1
1	C	128	VAL	3.1
1	E	307	SER	3.0
1	D	124	PRO	3.0
1	E	218	ASN	3.0
1	C	169	ASP	2.9
1	A	124	PRO	2.9
1	A	219	PRO	2.9
1	D	221	GLY	2.9
1	C	65	PRO	2.8
1	E	247	THR	2.8
1	C	221	GLY	2.8
1	D	128	VAL	2.7
1	D	310	TYR	2.7
1	E	123	GLY	2.7
1	B	319	PHE	2.7
1	E	65	PRO	2.7
1	A	168	ALA	2.7
1	C	168	ALA	2.6
1	E	122	ALA	2.6
1	D	66	ASN	2.6
1	F	310	TYR	2.6
1	B	307	SER	2.6
1	D	34	GLY	2.6
1	E	34	GLY	2.6
1	D	62	ILE	2.5
1	A	310	TYR	2.5
1	D	172	GLY	2.4
1	D	218	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	219	PRO	2.4
1	D	248	GLY	2.4
1	B	220	ALA	2.4
1	C	173	ASN	2.3
1	E	125	ASN	2.3
1	A	66	ASN	2.3
1	E	306	TYR	2.3
1	F	220	ALA	2.3
1	D	127	TYR	2.3
1	D	169	ASP	2.3
1	D	64	ASN	2.3
1	C	67	GLU	2.2
1	E	246	ALA	2.2
1	B	223	LEU	2.2
1	E	124	PRO	2.2
1	A	125	ASN	2.2
1	C	34	GLY	2.2
1	C	120	THR	2.2
1	B	306	TYR	2.2
1	C	119	SER	2.1
1	D	171	LEU	2.1
1	B	247	THR	2.1
1	C	121	THR	2.1
1	F	221	GLY	2.1
1	F	66	ASN	2.1
1	A	220	ALA	2.0
1	D	306	TYR	2.0
1	B	310	TYR	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, 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	LLDF	B-factors(Å ²)	Q<0.9
2	P6G	F	400	19/19	0.88	0.50	19.77	30,36,43,49	19
2	P6G	B	400	17/19	0.79	0.22	6.37	53,59,79,83	0
2	P6G	C	401	8/19	0.80	0.15	5.61	65,66,70,70	0
2	P6G	A	400	19/19	0.90	0.15	3.18	50,62,70,74	0
2	P6G	A	401	14/19	0.85	0.16	2.65	70,75,77,78	0
2	P6G	C	400	16/19	0.85	0.12	2.37	62,66,69,70	0
2	P6G	F	401	8/19	0.91	0.11	1.12	65,66,71,71	0
2	P6G	D	401	10/19	0.75	0.16	1.11	70,73,74,75	0
2	P6G	E	403	10/19	0.90	0.14	0.73	53,56,66,69	0
2	P6G	B	401	11/19	0.82	0.12	0.52	62,65,68,68	0
2	P6G	E	400	14/19	0.92	0.11	0.50	58,59,65,65	0
2	P6G	E	401	13/19	0.89	0.11	0.41	65,69,73,75	0
2	P6G	D	400	16/19	0.94	0.09	0.17	51,54,67,70	0
2	P6G	A	402	10/19	0.91	0.10	-0.89	71,71,79,80	0

6.5 Other polymers [i](#)

There are no such residues in this entry.