



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:02 AM GMT

PDB ID : 2P5T  
Title : Molecular and structural characterization of the PezAT chromosomal toxin-antitoxin system of the human pathogen *Streptococcus pneumoniae*  
Authors : Loll, B.; Meinhart, A.  
Deposited on : 2007-03-16  
Resolution : 3.20 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](mailto: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

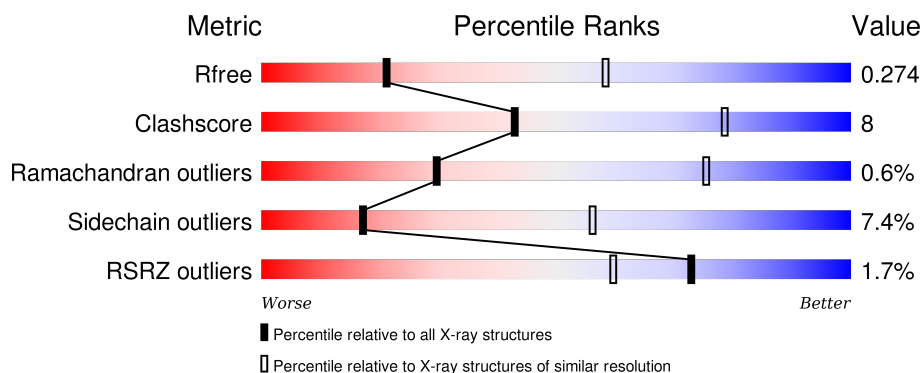
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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  $\geq 3$ , 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	X	33	<div> <div></div> <div>100%</div> </div>
2	A	158	<div> <div></div> <div>44%13%•42%</div> </div>
2	C	158	<div> <div></div> <div>42%16%•41%</div> </div>
2	E	158	<div> <div>%</div> <div>43%15%•40%</div> </div>
2	G	158	<div> <div>%</div> <div>43%14%•41%</div> </div>

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	B	253	<div><div><div></div><div>4%</div></div><div><div></div><div>75%</div><div>20%</div><div></div><div></div></div><div><div></div><div></div><div></div><div></div><div></div></div></div>
3	D	253	<div><div><div></div><div>%</div></div><div><div></div><div>74%</div><div>20%</div><div></div><div></div></div><div><div></div><div></div><div></div><div></div><div></div></div></div>
3	F	253	<div><div><div></div><div>2%</div></div><div><div></div><div>77%</div><div>16%</div><div></div><div>5%</div></div><div><div></div><div></div><div></div><div></div><div></div></div></div>
3	H	253	<div><div><div></div><div>%</div></div><div><div></div><div>70%</div><div>23%</div><div></div><div></div></div><div><div></div><div></div><div></div><div></div><div></div></div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11093 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 fragment of PezA helix-turn-helix motif.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	X	33	Total	C	N	O	0	0	0
			132	66	33	33			

- Molecule 2 is a protein called Putative transcriptional regulator PezA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	92	Total	C	N	O	S	0	0	0
			759	478	122	156	3			
2	C	93	Total	C	N	O	S	0	0	0
			767	483	123	157	4			
2	E	95	Total	C	N	O	S	0	0	0
			784	493	126	161	4			
2	G	93	Total	C	N	O	S	0	0	0
			767	483	123	157	4			

- Molecule 3 is a protein called PezT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	244	Total	C	N	O	S	0	0	0
			1979	1253	342	381	3			
3	D	247	Total	C	N	O	S	0	0	0
			2002	1268	345	385	4			
3	F	240	Total	C	N	O	S	0	0	0
			1944	1232	332	377	3			
3	H	242	Total	C	N	O	S	0	0	0
			1959	1242	334	379	4			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	109	GLY	ARG	CONFLICT	UNP Q97QZ1
B	228	PHE	LEU	CONFLICT	UNP Q97QZ1

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
D	109	GLY	ARG	CONFLICT	UNP Q97QZ1
D	228	PHE	LEU	CONFLICT	UNP Q97QZ1
F	109	GLY	ARG	CONFLICT	UNP Q97QZ1
F	228	PHE	LEU	CONFLICT	UNP Q97QZ1
H	109	GLY	ARG	CONFLICT	UNP Q97QZ1
H	228	PHE	LEU	CONFLICT	UNP Q97QZ1

### 3 Residue-property plots

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.

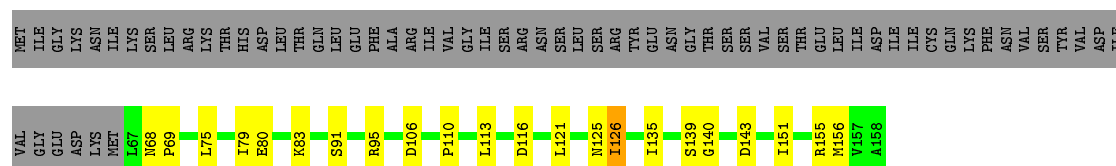
- Molecule 1: fragment of PezA helix-turn-helix motif

Chain X:  100%

There are no outlier residues recorded for this chain.

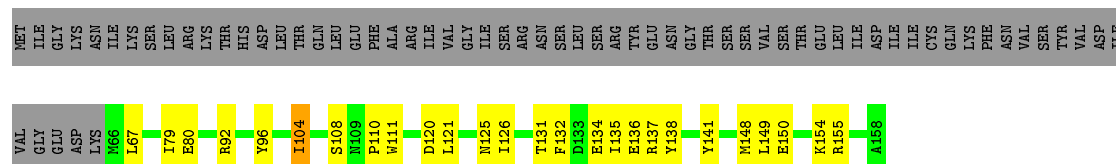
- Molecule 2: Putative transcriptional regulator PezA

Chain A:  44% 13% • 42%




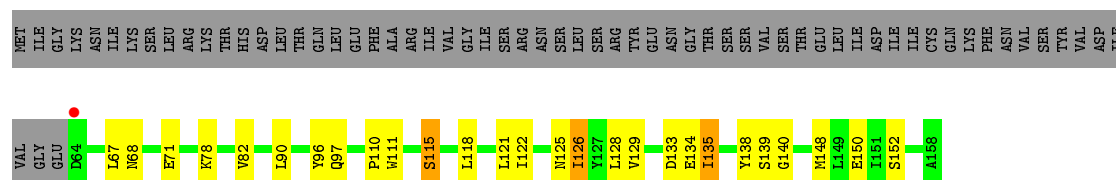
- Molecule 2: Putative transcriptional regulator PezA

Chain C:  42% 16% • 41%




- Molecule 2: Putative transcriptional regulator PezA

Chain E:  43% 15% • 40%



- Molecule 2: Putative transcriptional regulator PezA

Chain G:  43% 14% • 41%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	80.52Å 102.86Å 254.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.67 – 3.20 47.68 – 3.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.67-3.20) 98.5 (47.68-3.20)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.00 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.214 , 0.277 0.211 , 0.274	Depositor DCC
$R_{free}$ test set	1726 reflections (5.16%)	DCC
Wilson B-factor (Å <sup>2</sup> )	90.3	Xtriage
Anisotropy	0.014	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 84.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 35187 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	11093	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.97% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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](#)

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
2	A	0.38	0/770	0.54	0/1039
2	C	0.39	0/778	0.55	0/1049
2	E	0.44	0/795	0.56	0/1071
2	G	0.41	0/778	0.55	0/1049
3	B	0.38	0/2010	0.52	0/2703
3	D	0.39	0/2034	0.55	0/2736
3	F	0.38	0/1972	0.54	0/2650
3	H	0.43	0/1988	0.57	0/2672
All	All	0.40	0/11125	0.55	0/14969

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	X	132	0	2	0	0
2	A	759	0	740	20	0
2	C	767	0	749	22	0
2	E	784	0	766	18	0
2	G	767	0	749	24	0
3	B	1979	0	1997	31	0
3	D	2002	0	2023	37	0
3	F	1944	0	1968	18	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	1959	0	1987	42	0
All	All	11093	0	10981	180	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 (180) 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)
2:G:104:ILE:HD11	3:H:17:ARG:HB2	1.51	0.89
3:D:147:PRO:HB2	3:H:148:GLU:HG2	1.58	0.85
2:G:79:ILE:HD13	3:H:50:ARG:HD2	1.61	0.80
3:H:40:GLN:HB2	3:H:43:ALA:HB2	1.65	0.79
2:C:131:THR:HG23	2:C:134:GLU:HB2	1.66	0.77
3:B:204:GLN:HE21	3:B:227:LEU:HD21	1.48	0.76
2:G:116:ASP:HB3	3:H:24:ARG:NH1	2.02	0.75
3:H:204:GLN:HA	3:H:204:GLN:HE21	1.53	0.73
3:B:45:LYS:HG3	3:B:143:ILE:HG21	1.69	0.72
3:B:204:GLN:NE2	3:B:227:LEU:HD21	2.08	0.68
3:H:240:LEU:O	3:H:244:GLU:HB2	1.94	0.67
3:D:118:LEU:HD11	3:D:140:LEU:HD11	1.78	0.66
2:A:121:LEU:HD23	2:A:125:ASN:HD22	1.61	0.66
3:H:26:LYS:NZ	3:H:58:GLY:O	2.29	0.65
3:F:24:ARG:HH11	3:F:24:ARG:HG3	1.62	0.65
2:C:120:ASP:OD1	3:D:24:ARG:HD3	1.97	0.65
2:E:129:VAL:HG11	2:E:135:ILE:HG12	1.79	0.64
2:G:104:ILE:HD12	3:H:13:HIS:CE1	2.32	0.64
3:D:69:ARG:HE	3:D:90:THR:HG23	1.61	0.63
3:F:185:VAL:HG11	3:F:225:GLN:HG3	1.80	0.63
3:D:95:GLY:O	3:D:99:GLU:HG2	1.98	0.63
3:F:117:THR:HB	3:F:180:ILE:HD11	1.79	0.63
3:D:72:HIS:HD2	3:D:74:HIS:H	1.45	0.62
3:B:204:GLN:HE21	3:B:227:LEU:CD2	2.12	0.62
2:A:140:GLY:CA	2:C:137:ARG:HG2	2.30	0.62
3:D:62:ILE:HD12	3:D:113:LEU:HD23	1.81	0.61
3:B:160:GLU:HG3	3:B:250:LEU:HD21	1.82	0.61
2:G:73:TYR:CE1	3:H:205:ARG:HG2	2.36	0.60
3:H:159:GLU:HB3	3:H:250:LEU:HD23	1.82	0.60
2:C:131:THR:CG2	2:C:134:GLU:HB2	2.30	0.60
3:B:45:LYS:HG3	3:B:143:ILE:CG2	2.32	0.59
3:B:81:GLU:HG3	3:B:82:TYR:H	1.66	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:250:LEU:HD12	3:H:253:LYS:HD2	1.83	0.59
2:C:121:LEU:HA	2:C:125:ASN:HB2	1.85	0.58
3:B:33:ILE:H	3:B:111:ASN:HD22	1.51	0.58
3:B:69:ARG:HH21	3:B:87:VAL:HG13	1.68	0.57
2:A:75:LEU:O	2:A:79:ILE:HG12	2.03	0.57
3:B:4:GLN:HG3	3:B:89:TYR:HD1	1.69	0.57
2:A:79:ILE:HD13	2:A:135:ILE:HD11	1.87	0.56
2:G:104:ILE:CD1	3:H:17:ARG:HB2	2.28	0.56
3:B:165:ASN:HB3	3:B:168:GLN:HG3	1.88	0.56
3:D:219:SER:HB2	3:D:222:ASP:H	1.71	0.56
2:G:79:ILE:CD1	3:H:50:ARG:HD2	2.35	0.55
3:D:131:LEU:O	3:D:136:TYR:HB2	2.06	0.55
3:D:211:TYR:CD2	3:D:223:VAL:HG21	2.41	0.55
2:E:68:ASN:HB2	2:E:71:GLU:HB2	1.88	0.55
3:B:62:ILE:HG12	3:B:113:LEU:HD23	1.89	0.55
3:B:212:ASP:H	3:B:216:ASN:HD22	1.54	0.55
3:H:14:ALA:O	3:H:18:ASN:ND2	2.40	0.55
3:D:51:ILE:HD13	3:D:203:TYR:CD1	2.43	0.54
2:A:116:ASP:HB3	3:B:24:ARG:NH2	2.22	0.54
3:B:53:GLN:HE21	3:B:58:GLY:HA2	1.72	0.54
2:A:80:GLU:HG3	3:B:46:THR:HG21	1.90	0.54
3:D:175:GLU:HG2	3:D:176:HIS:HD2	1.72	0.54
3:H:35:ILE:HB	3:H:113:LEU:HD12	1.90	0.54
2:E:111:TRP:CE2	2:G:110:PRO:HG3	2.43	0.54
3:H:50:ARG:NH2	3:H:207:ARG:HH11	2.05	0.54
2:E:121:LEU:HD11	2:E:138:TYR:CE1	2.43	0.54
2:A:143:ASP:CB	2:C:137:ARG:NH1	2.71	0.53
2:G:121:LEU:HD12	2:G:126:ILE:HG12	1.89	0.53
3:D:87:VAL:HA	3:D:90:THR:HG22	1.89	0.53
2:A:151:ILE:O	2:A:155:ARG:HG3	2.08	0.53
3:D:69:ARG:HE	3:D:90:THR:CG2	2.22	0.53
2:A:140:GLY:HA3	2:C:137:ARG:HG2	1.89	0.53
3:F:27:LYS:H	3:F:59:ASN:ND2	2.07	0.52
2:C:79:ILE:HG23	2:C:126:ILE:HG12	1.91	0.52
2:A:68:ASN:HB2	2:A:69:PRO:HD2	1.92	0.52
2:G:151:ILE:O	2:G:155:ARG:HG2	2.09	0.52
3:D:114:ILE:HG22	3:D:115:GLU:O	2.10	0.52
3:B:199:ARG:HD2	3:B:214:LYS:HD3	1.92	0.52
2:A:143:ASP:HB3	2:C:137:ARG:NH1	2.25	0.52
2:G:141:TYR:CE2	2:G:145:ILE:HD11	2.45	0.51
3:H:32:PRO:HB2	3:H:136:TYR:CE1	2.46	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:67:LEU:HD22	2:E:71:GLU:HB3	1.91	0.51
2:E:121:LEU:O	2:E:126:ILE:HG12	2.10	0.51
3:H:119:ARG:CG	3:H:183:HIS:HD2	2.24	0.51
3:H:50:ARG:O	3:H:54:LYS:HG3	2.11	0.51
3:H:121:VAL:O	3:H:125:LYS:HB2	2.10	0.51
2:C:150:GLU:O	2:C:154:LYS:HG3	2.11	0.51
2:E:121:LEU:HD21	2:E:138:TYR:CD1	2.46	0.50
3:H:62:ILE:HG12	3:H:113:LEU:HD23	1.92	0.50
3:D:204:GLN:CD	3:D:210:VAL:HG21	2.32	0.50
3:F:59:ASN:CG	3:F:59:ASN:O	2.49	0.50
2:G:73:TYR:CD1	3:H:205:ARG:HG2	2.47	0.50
2:C:80:GLU:OE1	3:D:157:ARG:NH2	2.44	0.50
3:D:70:SER:HA	3:D:75:TYR:CD1	2.45	0.50
3:B:40:GLN:NE2	3:B:178:ASP:O	2.34	0.49
3:D:229:PHE:HB3	3:H:232:TRP:HB2	1.94	0.49
3:B:32:PRO:HB2	3:B:136:TYR:CE1	2.48	0.49
2:E:148:MET:HE1	2:G:114:MET:HG3	1.94	0.49
3:D:69:ARG:NH2	3:D:91:LYS:HB3	2.28	0.49
2:C:104:ILE:HG12	3:D:17:ARG:HB3	1.95	0.49
2:A:110:PRO:HG3	2:C:111:TRP:CE2	2.48	0.49
2:A:121:LEU:O	2:A:126:ILE:HG12	2.13	0.48
2:A:113:LEU:HB3	2:C:148:MET:HG2	1.95	0.48
2:E:97:GLN:OE1	2:E:115:SER:OG	2.31	0.48
2:G:86:GLY:HA3	2:G:122:ILE:CD1	2.44	0.48
3:D:66:ASP:HA	3:D:69:ARG:HG3	1.96	0.48
2:E:78:LYS:HB3	2:E:135:ILE:HG21	1.95	0.47
3:F:160:GLU:O	3:F:164:ILE:HG12	2.14	0.47
3:H:50:ARG:NH2	3:H:207:ARG:NH1	2.63	0.47
3:H:51:ILE:HD11	3:H:207:ARG:HA	1.96	0.47
3:H:139:GLN:HG2	3:H:199:ARG:HB3	1.97	0.47
3:H:125:LYS:HG3	3:H:196:ILE:HD13	1.97	0.46
3:F:122:ASP:OD1	3:F:122:ASP:N	2.47	0.46
3:D:72:HIS:HD2	3:D:74:HIS:N	2.12	0.46
2:G:133:ASP:N	2:G:133:ASP:OD1	2.45	0.46
2:A:91:SER:OG	3:B:70:SER:HB2	2.15	0.46
3:H:119:ARG:HG2	3:H:183:HIS:HD2	1.81	0.46
3:D:151:TYR:HD1	3:D:174:LYS:HE2	1.81	0.46
2:A:110:PRO:HG2	2:C:110:PRO:HB2	1.98	0.46
3:B:69:ARG:NH2	3:B:87:VAL:HG13	2.29	0.46
2:E:122:ILE:O	2:E:126:ILE:HD11	2.16	0.46
3:B:206:ASP:OD1	3:B:208:SER:OG	2.31	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:157:ARG:HG3	3:B:161:LEU:HD12	1.98	0.46
3:H:152:LEU:O	3:H:156:ILE:HG12	2.16	0.45
2:E:96:TYR:CE1	2:E:152:SER:HB3	2.51	0.45
3:F:24:ARG:NH1	3:F:24:ARG:HG3	2.28	0.45
2:E:82:VAL:HG21	2:E:135:ILE:HD12	1.99	0.45
2:C:138:TYR:O	2:C:141:TYR:HB3	2.17	0.45
3:D:35:ILE:HB	3:D:113:LEU:HD13	1.99	0.45
3:H:7:THR:HG22	3:H:9:SER:H	1.82	0.45
3:D:69:ARG:NH2	3:D:87:VAL:HG13	2.32	0.45
3:H:246:ARG:HH12	3:H:253:LYS:HE2	1.82	0.44
2:G:98:ASP:OD1	3:H:17:ARG:NH2	2.44	0.44
3:H:159:GLU:HB3	3:H:250:LEU:CD2	2.46	0.44
2:G:135:ILE:HD13	2:G:135:ILE:HA	1.85	0.44
2:A:110:PRO:HG3	2:C:111:TRP:NE1	2.32	0.44
3:F:233:SER:OG	3:F:236:GLU:HG3	2.16	0.44
3:B:131:LEU:O	3:B:136:TYR:HB2	2.18	0.44
3:D:26:LYS:HE2	3:D:58:GLY:O	2.18	0.44
2:C:132:PHE:O	2:C:135:ILE:HB	2.17	0.44
3:F:212:ASP:HB3	3:F:215:GLU:HB2	1.99	0.44
3:F:144:ALA:HB1	3:F:228:PHE:CE1	2.52	0.44
3:D:142:LEU:HB2	3:D:202:ILE:HG12	1.99	0.44
3:B:211:TYR:CD2	3:B:223:VAL:HG21	2.53	0.43
3:D:175:GLU:HG2	3:D:176:HIS:N	2.32	0.43
2:E:140:GLY:HA3	2:G:137:ARG:O	2.19	0.43
3:D:219:SER:O	3:D:223:VAL:HG23	2.18	0.43
3:F:8:ASP:O	3:F:12:LYS:HG2	2.19	0.43
2:E:125:ASN:HA	2:E:128:LEU:HD12	2.00	0.43
3:D:72:HIS:CD2	3:D:74:HIS:H	2.31	0.42
3:D:37:LEU:HB2	3:D:115:GLU:HA	1.99	0.42
2:A:91:SER:HB3	2:A:95:ARG:NH2	2.34	0.42
2:G:111:TRP:HZ2	2:G:152:SER:HG	1.63	0.42
2:G:141:TYR:CZ	2:G:145:ILE:HD11	2.55	0.42
3:F:60:ILE:HG13	3:F:111:ASN:HB3	2.01	0.42
2:C:92:ARG:HD3	2:C:149:LEU:HD13	2.01	0.42
3:B:33:ILE:H	3:B:111:ASN:ND2	2.16	0.42
2:A:83:LYS:NZ	3:B:46:THR:HG22	2.34	0.42
3:D:202:ILE:HB	3:D:211:TYR:HB3	2.01	0.42
3:H:51:ILE:HG13	3:H:207:ARG:HD2	2.02	0.42
3:D:53:GLN:NE2	3:D:60:ILE:HG22	2.35	0.42
3:H:221:ALA:HA	3:H:224:LEU:HD12	2.02	0.41
3:H:106:SER:HA	3:H:136:TYR:OH	2.20	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:78:LYS:HB3	2:G:135:ILE:HG21	2.02	0.41
3:H:84:LYS:HE2	3:H:84:LYS:H	1.85	0.41
3:H:94:ALA:O	3:H:98:VAL:HG23	2.20	0.41
3:F:46:THR:HA	3:F:49:HIS:CD2	2.56	0.41
3:F:46:THR:HA	3:F:49:HIS:HD2	1.85	0.41
3:H:37:LEU:HD21	3:H:113:LEU:HD11	2.02	0.41
2:E:110:PRO:HB2	2:G:110:PRO:HG2	2.01	0.41
3:F:118:LEU:HD22	3:F:124:PRO:HG3	2.03	0.41
3:D:140:LEU:HB3	3:D:200:ILE:HG23	2.02	0.41
3:D:210:VAL:O	3:D:210:VAL:HG12	2.21	0.41
2:G:86:GLY:HA3	2:G:122:ILE:HD13	2.03	0.41
3:D:165:ASN:HB3	3:D:168:GLN:HB2	2.02	0.41
3:H:182:ASN:OD1	3:H:182:ASN:N	2.54	0.41
3:B:198:GLU:HG2	3:B:198:GLU:H	1.67	0.41
2:C:96:TYR:OH	2:C:155:ARG:NH2	2.38	0.41
2:E:90:LEU:HD13	2:E:118:LEU:HG	2.03	0.41
3:B:248:ASN:O	3:B:251:LEU:HB3	2.21	0.40
3:B:79:GLN:C	3:B:81:GLU:H	2.24	0.40
2:G:127:TYR:CE2	3:H:62:ILE:HD13	2.56	0.40
3:F:245:LYS:O	3:F:249:GLU:HB2	2.22	0.40
2:E:129:VAL:HG22	2:E:134:GLU:HB3	2.04	0.40
2:A:143:ASP:HB3	2:C:137:ARG:HH12	1.83	0.40
2:C:136:GLU:O	2:C:137:ARG:C	2.60	0.40
3:B:20:ARG:O	3:B:24:ARG:HG2	2.21	0.40
3:F:19:LEU:O	3:F:23:THR:HB	2.20	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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
2	A	90/158 (57%)	84 (93%)	5 (6%)	1 (1%)	<b>17</b> 62

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	91/158 (58%)	87 (96%)	3 (3%)	1 (1%)	17	62
2	E	93/158 (59%)	88 (95%)	5 (5%)	0	100	100
2	G	91/158 (58%)	87 (96%)	4 (4%)	0	100	100
3	B	240/253 (95%)	218 (91%)	21 (9%)	1 (0%)	39	80
3	D	243/253 (96%)	226 (93%)	15 (6%)	2 (1%)	24	69
3	F	236/253 (93%)	221 (94%)	13 (6%)	2 (1%)	24	69
3	H	238/253 (94%)	224 (94%)	13 (6%)	1 (0%)	39	80
All	All	1322/1644 (80%)	1235 (93%)	79 (6%)	8 (1%)	30	75

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	B	164	ILE
3	F	24	ARG
2	A	106	ASP
2	C	104	ILE
3	D	177	HIS
3	F	83	GLY
3	D	166	PRO
3	H	83	GLY

### 5.3.2 Protein sidechains ⓘ

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	
2	A	86/147 (58%)	83 (96%)	3 (4%)	43	80
2	C	87/147 (59%)	85 (98%)	2 (2%)	58	87
2	E	89/147 (60%)	83 (93%)	6 (7%)	20	60
2	G	87/147 (59%)	81 (93%)	6 (7%)	19	59
3	B	219/226 (97%)	203 (93%)	16 (7%)	17	57
3	D	222/226 (98%)	204 (92%)	18 (8%)	15	51

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	F	215/226 (95%)	198 (92%)	17 (8%)	15	53
3	H	217/226 (96%)	194 (89%)	23 (11%)	8	34
All	All	1222/1492 (82%)	1131 (93%)	91 (7%)	17	56

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	126	ILE
2	A	139	SER
2	A	156	MET
3	B	3	ILE
3	B	21	SER
3	B	23	THR
3	B	45	LYS
3	B	70	SER
3	B	84	LYS
3	B	118	LEU
3	B	120	THR
3	B	121	VAL
3	B	145	THR
3	B	153	SER
3	B	161	LEU
3	B	180	ILE
3	B	227	LEU
3	B	238	GLU
3	B	250	LEU
2	C	67	LEU
2	C	108	SER
3	D	7	THR
3	D	26	LYS
3	D	46	THR
3	D	64	ASP
3	D	79	GLN
3	D	88	GLU
3	D	90	THR
3	D	91	LYS
3	D	99	GLU
3	D	100	SER
3	D	108	LEU
3	D	118	LEU
3	D	119	ARG

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
3	D	121	VAL
3	D	157	ARG
3	D	175	GLU
3	D	218	THR
3	D	219	SER
2	E	115	SER
2	E	126	ILE
2	E	133	ASP
2	E	135	ILE
2	E	139	SER
2	E	150	GLU
3	F	3	ILE
3	F	7	THR
3	F	23	THR
3	F	28	SER
3	F	41	SER
3	F	70	SER
3	F	79	GLN
3	F	113	LEU
3	F	120	THR
3	F	121	VAL
3	F	122	ASP
3	F	150	SER
3	F	162	TYR
3	F	163	ILE
3	F	179	PHE
3	F	222	ASP
3	F	253	LYS
2	G	68	ASN
2	G	83	LYS
2	G	103	SER
2	G	104	ILE
2	G	126	ILE
2	G	133	ASP
3	H	21	SER
3	H	41	SER
3	H	50	ARG
3	H	70	SER
3	H	79	GLN
3	H	84	LYS
3	H	118	LEU
3	H	120	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
3	H	122	ASP
3	H	129	GLN
3	H	145	THR
3	H	154	THR
3	H	158	TYR
3	H	159	GLU
3	H	178	ASP
3	H	182	ASN
3	H	196	ILE
3	H	204	GLN
3	H	205	ARG
3	H	216	ASN
3	H	217	THR
3	H	241	GLN
3	H	251	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	125	ASN
3	B	53	GLN
3	B	111	ASN
3	B	204	GLN
3	B	216	ASN
3	D	18	ASN
3	D	53	GLN
3	D	71	GLN
3	D	72	HIS
3	D	129	GLN
3	D	176	HIS
3	D	182	ASN
2	E	125	ASN
3	F	59	ASN
3	F	204	GLN
2	G	123	HIS
3	H	49	HIS
3	H	129	GLN
3	H	183	HIS
3	H	204	GLN
3	H	241	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	X	0/33	-	-	-	-
2	A	92/158 (58%)	-0.04	0 100 100	78, 88, 97, 104	0
2	C	93/158 (58%)	-0.11	0 100 100	79, 90, 105, 112	0
2	E	95/158 (60%)	-0.12	1 (1%) 82 72	79, 89, 107, 114	0
2	G	93/158 (58%)	-0.08	2 (2%) 65 50	79, 89, 108, 111	0
3	B	244/253 (96%)	0.08	10 (4%) 41 27	78, 91, 106, 115	0
3	D	247/253 (97%)	-0.13	3 (1%) 81 69	79, 89, 105, 114	0
3	F	240/253 (94%)	-0.06	4 (1%) 73 60	74, 89, 114, 123	0
3	H	242/253 (95%)	-0.04	3 (1%) 81 69	75, 90, 112, 130	0
All	All	1346/1677 (80%)	-0.05	23 (1%) 73 60	74, 90, 107, 130	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	157	VAL	5.8
2	E	64	ASP	5.4
3	H	164	ILE	4.2
3	B	253	LYS	4.1
2	G	158	ALA	4.1
3	H	178	ASP	4.0
3	F	178	ASP	3.8
3	F	253	LYS	3.5
3	B	85	ASP	3.1
3	F	162	TYR	3.0
3	B	191	LEU	2.8
3	B	196	ILE	2.8
3	H	253	LYS	2.7
3	B	167	ASN	2.5
3	D	1	MET	2.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
3	B	69	ARG	2.4
3	D	117	THR	2.4
3	B	72	HIS	2.3
3	D	167	ASN	2.2
3	F	85	ASP	2.2
3	B	93	PHE	2.1
3	B	214	LYS	2.1
3	B	252	GLU	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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.