



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 29, 2025 – 05:13 AM EDT

PDB ID : 3D03 / pdb\_00003d03  
Title : 1.9A structure of Glycerophosphodiesterase (GpdQ) from *Enterobacter aerogenes*  
Authors : Hadler, K.S.; Tanifum, E.; Yip, S.H.-C.; Miti, N.; Guddat, L.W.; Jackson, C.J.; Gahan, L.R.; Carr, P.D.; Nguyen, K.; Ollis, D.L.; Hengge, A.C.; Larrabee, J.A.; Schenk, G.  
Deposited on : 2008-04-30  
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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0rc1
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

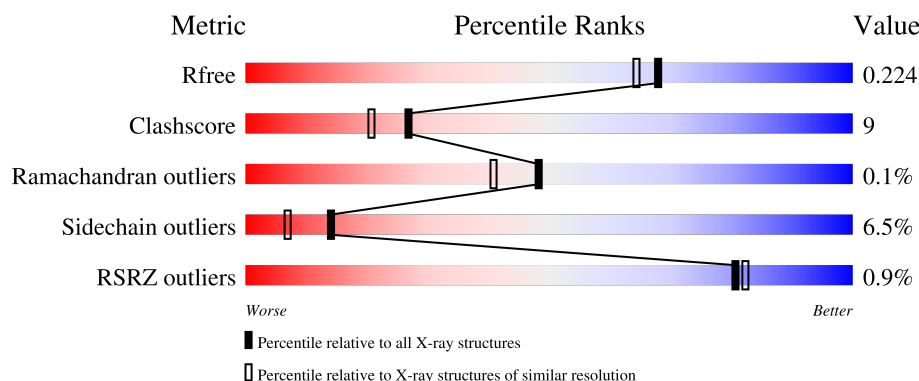
# 1 Overall quality at a glance

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))
$R_{free}$	164625	7293 (1.90-1.90)
Clashscore	180529	8090 (1.90-1.90)
Ramachandran outliers	177936	8022 (1.90-1.90)
Sidechain outliers	177891	8022 (1.90-1.90)
RSRZ outliers	164620	7292 (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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	274	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>84%</span> <span>13%</span> <span>.</span> </div> </div>
1	B	274	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>84%</span> <span>14%</span> <span>..</span> </div> </div>
1	C	274	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>83%</span> <span>14%</span> <span>..</span> </div> </div>
1	D	274	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>80%</span> <span>16%</span> <span>..</span> </div> </div>
1	E	274	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>84%</span> <span>11%</span> <span>..</span> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	274	 A horizontal bar chart showing the quality of the chain. The bar is divided into two segments: a green segment representing 85% and a yellow segment representing 13%. A small black dot is located at the end of the bar.

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13904 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 Phosphohydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	274	Total	C	N	O	S	0	0	0
			2163	1364	378	407	14			
1	B	271	Total	C	N	O	S	0	0	0
			2133	1348	372	399	14			
1	C	271	Total	C	N	O	S	0	0	0
			2133	1348	372	399	14			
1	D	271	Total	C	N	O	S	0	0	0
			2133	1348	372	399	14			
1	E	271	Total	C	N	O	S	0	0	0
			2133	1348	372	399	14			
1	F	274	Total	C	N	O	S	0	0	0
			2163	1364	378	407	14			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	224	ALA	GLU	SEE REMARK 999	UNP Q6XBH1
A	227	ASP	ARG	SEE REMARK 999	UNP Q6XBH1
B	224	ALA	GLU	SEE REMARK 999	UNP Q6XBH1
B	227	ASP	ARG	SEE REMARK 999	UNP Q6XBH1
C	224	ALA	GLU	SEE REMARK 999	UNP Q6XBH1
C	227	ASP	ARG	SEE REMARK 999	UNP Q6XBH1
D	224	ALA	GLU	SEE REMARK 999	UNP Q6XBH1
D	227	ASP	ARG	SEE REMARK 999	UNP Q6XBH1
E	224	ALA	GLU	SEE REMARK 999	UNP Q6XBH1
E	227	ASP	ARG	SEE REMARK 999	UNP Q6XBH1
F	224	ALA	GLU	SEE REMARK 999	UNP Q6XBH1
F	227	ASP	ARG	SEE REMARK 999	UNP Q6XBH1

- Molecule 2 is COBALT (II) ION (CCD ID: CO) (formula: Co).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Co 2 2	0	0
2	B	2	Total Co 2 2	0	0
2	C	2	Total Co 2 2	0	0
2	D	2	Total Co 2 2	0	0
2	E	2	Total Co 2 2	0	0
2	F	2	Total Co 2 2	0	0

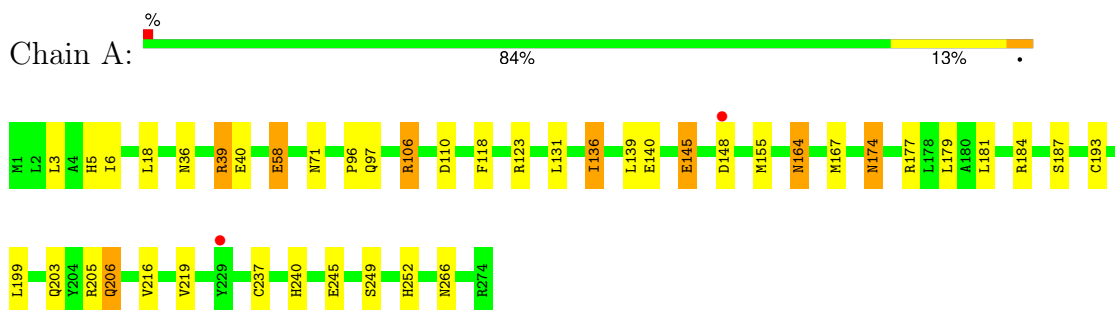
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	179	Total O 179 179	0	0
3	B	178	Total O 178 178	0	0
3	C	178	Total O 178 178	0	0
3	D	181	Total O 181 181	0	0
3	E	139	Total O 139 139	0	0
3	F	179	Total O 179 179	0	0

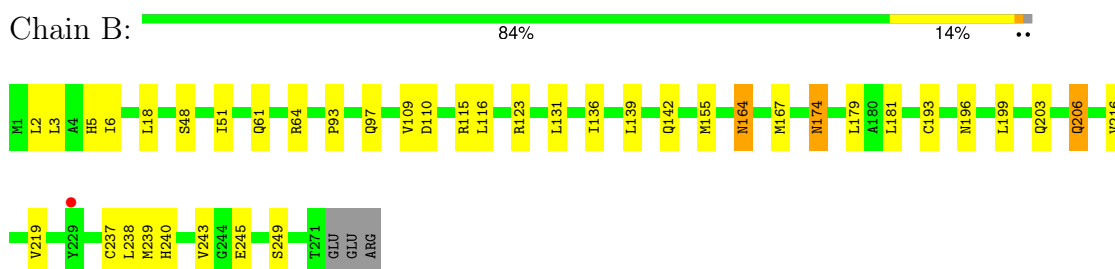
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

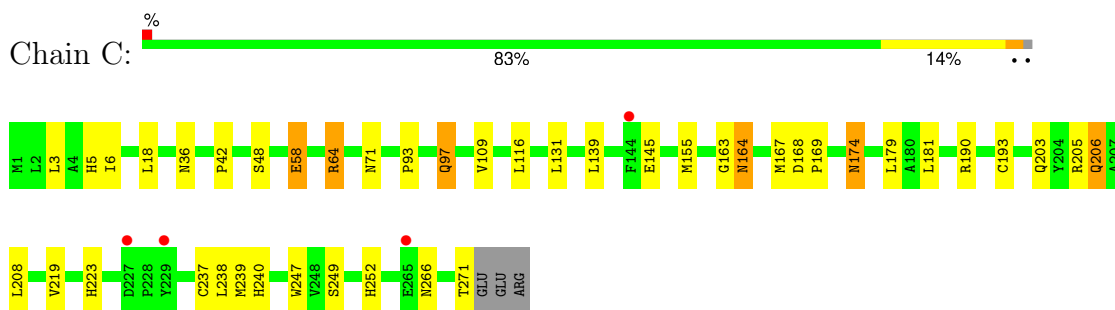
- Molecule 1: Phosphohydrolase



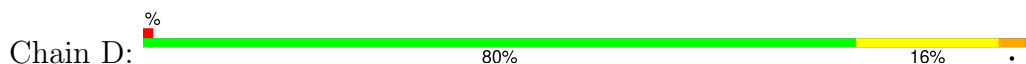
- Molecule 1: Phosphohydrolase

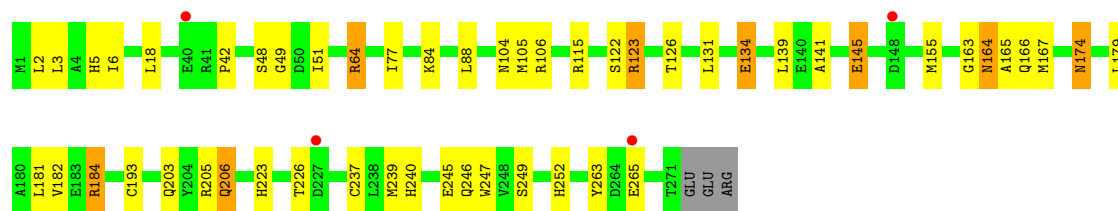


- Molecule 1: Phosphohydrolase

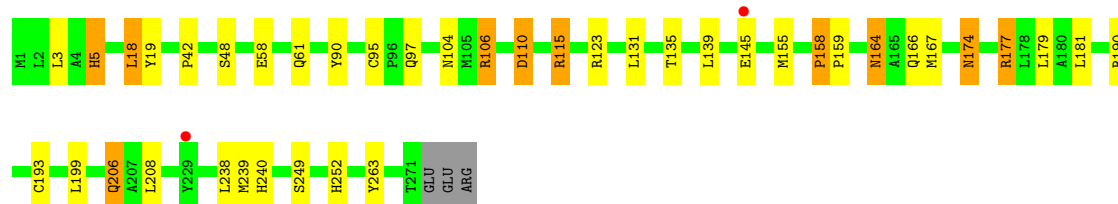
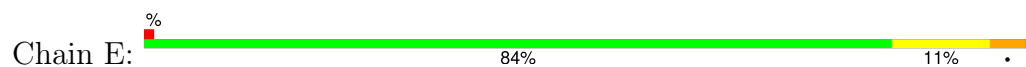


- Molecule 1: Phosphohydrolase

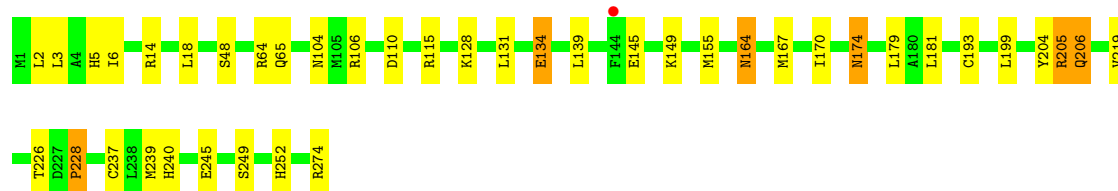
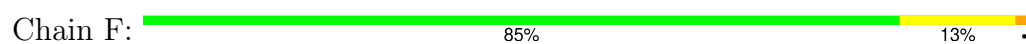




● Molecule 1: Phosphohydrolase



● Molecule 1: Phosphohydrolase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	94.97Å 133.84Å 168.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.27 – 1.90 43.27 – 1.90	Depositor EDS
% Data completeness (in resolution range)	96.7 (43.27-1.90) 96.6 (43.27-1.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.72 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.184 , 0.223 0.187 , 0.224	Depositor DCC
$R_{free}$ test set	8219 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	16.5	Xtriage
Anisotropy	0.188	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 30.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	13904	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	8.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.34% 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, 0.333 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:  
CO

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	0.96	0/2222	0.97	1/3029 (0.0%)
1	B	0.94	1/2192 (0.0%)	0.91	0/2991
1	C	0.94	0/2192	0.92	1/2991 (0.0%)
1	D	0.95	0/2192	0.96	0/2991
1	E	0.83	0/2192	0.92	2/2991 (0.1%)
1	F	0.90	1/2222 (0.0%)	0.92	0/3029
All	All	0.92	2/13212 (0.0%)	0.93	4/18022 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	243	VAL	CA-CB	5.18	1.59	1.53
1	F	228	PRO	CA-C	5.03	1.57	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	158	PRO	CA-C-N	6.29	126.42	119.87
1	E	158	PRO	C-N-CA	6.29	126.42	119.87
1	C	205	ARG	CB-CA-C	-5.20	110.57	116.54
1	A	148	ASP	N-CA-C	5.07	117.54	111.71

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	2163	0	2071	50	0
1	B	2133	0	2046	35	0
1	C	2133	0	2046	37	0
1	D	2133	0	2046	45	0
1	E	2133	0	2046	44	0
1	F	2163	0	2071	41	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
3	A	179	0	0	4	0
3	B	178	0	0	1	0
3	C	178	0	0	6	0
3	D	181	0	0	5	0
3	E	139	0	0	2	0
3	F	179	0	0	6	0
All	All	13904	0	12326	229	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 9.

All (229) 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:A:199:LEU:CD2	1:B:199:LEU:CD2	2.26	1.14
1:A:39:ARG:HD3	1:A:39:ARG:N	1.56	1.12
1:A:199:LEU:HD21	1:B:199:LEU:CD2	1.87	1.01
1:B:97:GLN:HG3	3:B:2124:HOH:O	1.60	1.01
1:E:106:ARG:HH11	1:E:106:ARG:HG3	0.87	1.01
1:A:39:ARG:HD3	1:A:39:ARG:H	1.17	0.98
1:E:106:ARG:HH11	1:E:106:ARG:CG	1.77	0.96
1:E:177:ARG:HG2	1:E:177:ARG:HH11	1.31	0.96
1:C:266:ASN:HB2	3:C:2129:HOH:O	1.65	0.95
1:F:131:LEU:H	1:F:174:ASN:HD21	1.10	0.95
1:E:106:ARG:HG3	1:E:106:ARG:NH1	1.69	0.94
1:E:95:CYS:SG	1:E:97:GLN:NE2	2.40	0.94
1:B:131:LEU:H	1:B:174:ASN:HD21	1.14	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:LEU:CD2	1:B:199:LEU:HD21	1.98	0.93
1:A:199:LEU:HD21	1:B:199:LEU:HD21	1.51	0.93
1:E:199:LEU:CD2	1:F:199:LEU:HD21	1.99	0.92
1:E:199:LEU:HD23	1:F:199:LEU:CD2	2.00	0.91
1:E:199:LEU:CD2	1:F:199:LEU:CD2	2.49	0.91
1:F:104:ASN:HD22	1:F:106:ARG:HH22	1.06	0.91
1:A:39:ARG:H	1:A:39:ARG:CD	1.86	0.88
1:E:199:LEU:HD23	1:F:199:LEU:HD21	1.53	0.87
1:F:5:HIS:HD2	1:F:240:HIS:HE1	1.21	0.86
1:C:131:LEU:H	1:C:174:ASN:HD21	1.17	0.86
1:E:5:HIS:HD2	1:E:240:HIS:HE1	1.25	0.85
1:A:199:LEU:CD2	1:B:199:LEU:HD23	2.08	0.84
1:E:131:LEU:H	1:E:174:ASN:HD21	1.23	0.83
1:A:131:LEU:H	1:A:174:ASN:HD21	1.26	0.83
1:A:199:LEU:HD23	1:B:199:LEU:CD2	2.08	0.83
1:A:199:LEU:HD21	1:B:199:LEU:HD23	1.59	0.82
1:D:174:ASN:HD22	1:D:174:ASN:H	1.28	0.82
1:D:5:HIS:HD2	1:D:240:HIS:HE1	1.27	0.81
1:A:39:ARG:N	1:A:39:ARG:CD	2.42	0.81
1:C:36:ASN:HD21	1:C:71:ASN:H	1.29	0.80
1:E:5:HIS:CD2	1:E:240:HIS:HE1	1.99	0.80
1:D:131:LEU:H	1:D:174:ASN:HD21	1.29	0.80
1:B:5:HIS:HD2	1:B:240:HIS:HE1	1.28	0.79
1:F:5:HIS:CD2	1:F:240:HIS:HE1	2.01	0.79
1:A:266:ASN:HB2	3:A:2102:HOH:O	1.85	0.76
1:F:167:MET:HE2	1:F:219:VAL:HG11	1.67	0.76
1:B:115:ARG:HH12	1:B:142:GLN:HE21	1.31	0.76
1:B:5:HIS:CD2	1:B:240:HIS:HE1	2.04	0.75
1:D:5:HIS:CD2	1:D:240:HIS:HE1	2.06	0.74
1:C:5:HIS:HD2	1:C:240:HIS:HE1	1.38	0.72
1:D:104:ASN:ND2	3:D:2097:HOH:O	2.23	0.70
1:D:64:ARG:HG3	1:D:64:ARG:HH11	1.57	0.70
1:F:104:ASN:HD22	1:F:106:ARG:NH2	1.86	0.70
1:E:61:GLN:HG2	3:E:2127:HOH:O	1.91	0.69
1:A:36:ASN:HD21	1:A:71:ASN:H	1.39	0.69
1:E:166:GLN:HG2	1:E:167:MET:CE	2.22	0.69
1:A:140:GLU:CD	1:A:184:ARG:HH22	2.00	0.68
1:E:199:LEU:HD21	1:F:199:LEU:HD21	1.74	0.68
1:A:174:ASN:HD22	1:A:174:ASN:H	1.39	0.68
1:F:104:ASN:HD21	1:F:134:GLU:HG3	1.57	0.68
1:D:84:LYS:HE2	3:D:2137:HOH:O	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:184:ARG:HH11	1:D:184:ARG:HB3	1.58	0.68
1:A:167:MET:HE2	1:A:219:VAL:HG11	1.76	0.67
1:C:252:HIS:HE1	3:C:2019:HOH:O	1.76	0.67
1:A:5:HIS:CD2	1:A:240:HIS:HE1	2.14	0.66
1:C:167:MET:HE3	1:C:219:VAL:HG11	1.76	0.66
1:C:36:ASN:ND2	1:C:71:ASN:H	1.95	0.65
1:F:115:ARG:NE	3:F:2084:HOH:O	2.30	0.64
1:A:145:GLU:HB3	3:A:2078:HOH:O	1.96	0.64
1:F:115:ARG:CD	3:F:2084:HOH:O	2.46	0.64
1:A:5:HIS:HD2	1:A:240:HIS:HE1	1.44	0.64
1:C:5:HIS:CD2	1:C:240:HIS:HE1	2.13	0.63
1:C:174:ASN:H	1:C:174:ASN:HD22	1.46	0.63
1:E:166:GLN:HG2	1:E:167:MET:HE2	1.80	0.63
1:C:240:HIS:HD2	1:C:249:SER:OG	1.82	0.62
1:B:164:ASN:C	1:B:164:ASN:HD22	2.06	0.62
1:E:177:ARG:HH11	1:E:177:ARG:CG	2.09	0.62
1:C:64:ARG:CD	3:C:2015:HOH:O	2.48	0.62
1:F:115:ARG:CZ	3:F:2084:HOH:O	2.48	0.61
1:D:164:ASN:C	1:D:164:ASN:HD22	2.07	0.61
1:B:115:ARG:HH22	1:B:142:GLN:HE22	1.48	0.61
1:A:131:LEU:HB3	1:A:136:ILE:HD11	1.83	0.61
1:A:39:ARG:H	1:A:39:ARG:HH11	1.47	0.60
1:F:5:HIS:HD2	1:F:240:HIS:CE1	2.12	0.60
1:E:199:LEU:HD21	1:F:199:LEU:CD2	2.30	0.60
1:C:167:MET:CE	1:C:219:VAL:HG11	2.31	0.60
1:F:128:LYS:HG2	1:F:170:ILE:HA	1.83	0.60
1:E:58:GLU:OE1	1:E:61:GLN:NE2	2.35	0.59
1:A:58:GLU:CD	1:A:58:GLU:H	2.09	0.59
1:D:115:ARG:HH12	1:D:145:GLU:HG3	1.68	0.59
1:E:5:HIS:HD2	1:E:240:HIS:CE1	2.13	0.58
1:A:164:ASN:C	1:A:164:ASN:HD22	2.12	0.58
1:F:174:ASN:HD22	1:F:174:ASN:H	1.48	0.58
1:D:163:GLY:O	1:D:223:HIS:HD2	1.86	0.58
1:F:14:ARG:NH2	1:F:65:GLN:OE1	2.37	0.58
1:C:64:ARG:HG3	1:C:64:ARG:HH11	1.69	0.58
1:D:174:ASN:H	1:D:174:ASN:ND2	1.97	0.58
1:F:2:LEU:HD11	1:F:239:MET:HE3	1.86	0.57
1:D:166:GLN:HG2	1:D:167:MET:CE	2.34	0.57
1:A:36:ASN:ND2	1:A:71:ASN:H	2.02	0.57
1:C:64:ARG:HH22	1:C:93:PRO:HG2	1.70	0.57
1:E:199:LEU:CD2	1:F:199:LEU:HD23	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:ILE:HD13	1:A:177:ARG:CZ	2.35	0.57
1:C:64:ARG:HD2	3:C:2015:HOH:O	2.02	0.57
1:A:39:ARG:H	1:A:39:ARG:NH1	2.03	0.56
1:E:106:ARG:HD2	1:E:106:ARG:N	2.20	0.56
1:A:39:ARG:N	1:A:39:ARG:HH11	2.03	0.56
1:F:204:TYR:C	1:F:205:ARG:HG2	2.30	0.56
1:D:64:ARG:HG3	1:D:64:ARG:NH1	2.20	0.56
1:E:104:ASN:HD22	1:E:106:ARG:HH21	1.55	0.55
1:B:2:LEU:HD11	1:B:239:MET:HE3	1.87	0.55
1:B:5:HIS:HD2	1:B:240:HIS:CE1	2.17	0.55
1:A:6:ILE:HG22	1:A:237:CYS:HB3	1.89	0.55
1:D:104:ASN:ND2	1:D:106:ARG:HH22	2.05	0.55
1:E:61:GLN:HG3	1:E:90:TYR:CE2	2.42	0.54
1:E:58:GLU:HG3	1:F:274:ARG:HD2	1.89	0.54
1:B:115:ARG:HH12	1:B:142:GLN:NE2	2.04	0.54
1:A:136:ILE:HD13	1:A:177:ARG:NE	2.23	0.54
1:A:199:LEU:HD23	1:B:199:LEU:HD21	1.74	0.54
1:E:174:ASN:H	1:E:174:ASN:HD22	1.54	0.54
1:D:165:ALA:HB1	1:D:226:THR:HG22	1.90	0.53
1:B:174:ASN:HD22	1:B:174:ASN:H	1.57	0.53
1:F:155:MET:O	1:F:193:CYS:HA	2.08	0.53
1:D:134:GLU:H	1:D:134:GLU:CD	2.16	0.53
1:A:155:MET:O	1:A:193:CYS:HA	2.09	0.53
1:D:205:ARG:NH1	3:D:2163:HOH:O	2.36	0.52
1:E:106:ARG:CG	1:E:106:ARG:NH1	2.49	0.52
1:E:164:ASN:C	1:E:164:ASN:HD22	2.16	0.52
1:C:271:THR:C	3:C:2052:HOH:O	2.52	0.52
1:B:167:MET:HE2	1:B:219:VAL:HG11	1.92	0.52
1:A:96:PRO:HD2	1:A:97:GLN:HE22	1.75	0.52
1:B:206:GLN:H	1:B:206:GLN:NE2	2.08	0.51
1:D:5:HIS:HE1	1:D:48:SER:OG	1.93	0.51
1:E:97:GLN:CD	1:E:97:GLN:H	2.18	0.51
1:C:97:GLN:H	1:C:97:GLN:NE2	2.09	0.51
1:D:174:ASN:HD22	1:D:174:ASN:N	1.94	0.51
1:D:263:TYR:HE2	1:D:265:GLU:HG3	1.75	0.51
1:A:5:HIS:O	1:A:237:CYS:HB2	2.11	0.51
1:D:240:HIS:HD2	1:D:249:SER:OG	1.93	0.51
1:F:204:TYR:CE2	1:F:205:ARG:HD3	2.46	0.51
1:B:64:ARG:HH22	1:B:93:PRO:HG2	1.75	0.51
1:C:155:MET:O	1:C:193:CYS:HA	2.11	0.51
1:E:177:ARG:HG2	1:E:177:ARG:NH1	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:5:HIS:HE1	1:F:48:SER:OG	1.94	0.51
1:D:5:HIS:HD2	1:D:240:HIS:CE1	2.17	0.50
1:B:240:HIS:HD2	1:B:249:SER:OG	1.94	0.50
1:D:49:GLY:HA2	1:D:77:ILE:O	2.12	0.50
1:F:115:ARG:HD2	3:F:2084:HOH:O	2.09	0.50
1:D:184:ARG:HB3	1:D:184:ARG:NH1	2.26	0.50
1:C:206:GLN:H	1:C:206:GLN:NE2	2.10	0.49
1:E:5:HIS:HE1	1:E:48:SER:OG	1.95	0.49
1:E:42:PRO:HG3	1:E:239:MET:HE1	1.94	0.49
1:A:240:HIS:HD2	1:A:249:SER:OG	1.95	0.49
1:F:252:HIS:HE1	3:F:2070:HOH:O	1.95	0.49
1:F:164:ASN:C	1:F:164:ASN:HD22	2.21	0.49
1:A:206:GLN:H	1:A:206:GLN:NE2	2.11	0.48
1:C:58:GLU:H	1:C:58:GLU:CD	2.20	0.48
1:D:206:GLN:H	1:D:206:GLN:NE2	2.10	0.48
1:F:104:ASN:ND2	1:F:106:ARG:HH22	1.91	0.48
1:C:6:ILE:HG22	1:C:237:CYS:HB3	1.95	0.48
1:C:64:ARG:HG3	1:C:64:ARG:NH1	2.29	0.48
1:F:240:HIS:HD2	1:F:249:SER:OG	1.96	0.48
1:E:206:GLN:NE2	1:E:206:GLN:H	2.12	0.47
1:E:110:ASP:OD1	1:E:115:ARG:NH1	2.47	0.47
1:A:96:PRO:HD2	1:A:97:GLN:NE2	2.29	0.47
1:C:240:HIS:CD2	1:C:247:TRP:HE1	2.32	0.47
1:C:190:ARG:HD3	1:C:208:LEU:HB3	1.96	0.47
1:D:263:TYR:CE2	1:D:265:GLU:HG3	2.48	0.47
1:D:174:ASN:ND2	1:D:174:ASN:N	2.61	0.47
1:A:203:GLN:HG3	1:B:203:GLN:HE22	1.80	0.47
1:A:252:HIS:HE1	3:A:2057:HOH:O	1.98	0.46
1:C:5:HIS:HE1	1:C:48:SER:OG	1.99	0.46
1:F:104:ASN:ND2	1:F:134:GLU:HG3	2.27	0.46
1:E:240:HIS:HD2	1:E:249:SER:OG	1.99	0.46
1:F:134:GLU:CD	1:F:134:GLU:H	2.23	0.46
1:D:141:ALA:O	1:D:145:GLU:HB3	2.16	0.45
1:F:110:ASP:OD1	1:F:149:LYS:NZ	2.42	0.45
1:B:115:ARG:HH22	1:B:142:GLN:NE2	2.14	0.45
1:A:174:ASN:H	1:A:174:ASN:ND2	2.11	0.45
1:A:97:GLN:NE2	3:A:2033:HOH:O	2.50	0.45
1:B:164:ASN:C	1:B:164:ASN:ND2	2.75	0.45
1:C:203:GLN:HE22	1:D:203:GLN:CG	2.29	0.45
1:D:84:LYS:NZ	1:D:122:SER:O	2.50	0.45
1:B:5:HIS:HE1	1:B:48:SER:OG	2.00	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:109:VAL:HB	1:B:116:LEU:HB2	1.99	0.45
1:C:109:VAL:HB	1:C:116:LEU:HB2	1.99	0.44
1:E:106:ARG:HH12	1:E:135:THR:HA	1.81	0.44
1:C:174:ASN:HD22	1:C:174:ASN:N	2.09	0.44
1:C:64:ARG:NE	3:C:2015:HOH:O	2.50	0.44
1:A:39:ARG:HH11	1:A:40:GLU:H	1.66	0.44
1:A:199:LEU:HD23	1:B:199:LEU:HD22	1.92	0.44
1:D:6:ILE:HG22	1:D:237:CYS:HB3	1.98	0.44
1:D:164:ASN:ND2	1:D:167:MET:H	2.16	0.44
1:D:2:LEU:HD11	1:D:239:MET:HE3	2.00	0.44
1:E:263:TYR:HB3	1:F:228:PRO:HB2	2.00	0.44
1:E:61:GLN:HG3	1:E:90:TYR:HE2	1.82	0.43
1:A:131:LEU:HB3	1:A:136:ILE:CD1	2.47	0.43
1:E:155:MET:O	1:E:193:CYS:HA	2.18	0.43
1:A:106:ARG:HB2	1:A:118:PHE:O	2.19	0.43
1:C:164:ASN:HD22	1:C:164:ASN:C	2.27	0.43
1:D:104:ASN:HD22	1:D:106:ARG:HH22	1.65	0.43
1:F:6:ILE:HG22	1:F:237:CYS:HB3	2.00	0.43
1:D:88:LEU:HD13	1:D:105:MET:SD	2.58	0.43
1:A:58:GLU:CD	1:A:58:GLU:N	2.77	0.42
1:A:174:ASN:HD22	1:A:174:ASN:N	2.02	0.42
1:C:42:PRO:HG3	1:C:239:MET:HE1	2.00	0.42
1:F:206:GLN:H	1:F:206:GLN:NE2	2.17	0.42
1:D:123:ARG:HD2	1:D:126:THR:CG2	2.49	0.42
1:E:252:HIS:HE1	3:E:2024:HOH:O	2.02	0.42
1:E:190:ARG:HD3	1:E:208:LEU:HB3	2.01	0.42
1:F:174:ASN:HD22	1:F:174:ASN:N	2.11	0.42
1:C:5:HIS:O	1:C:237:CYS:HB2	2.19	0.42
1:C:163:GLY:O	1:C:223:HIS:CD2	2.73	0.42
1:C:64:ARG:HH11	1:C:64:ARG:CG	2.32	0.42
1:B:167:MET:HE3	1:B:196:ASN:HA	2.02	0.42
1:D:246:GLN:NE2	3:D:2066:HOH:O	2.48	0.42
1:E:177:ARG:CG	1:E:177:ARG:NH1	2.75	0.42
1:A:131:LEU:CB	1:A:136:ILE:HD11	2.48	0.42
1:D:166:GLN:HG2	1:D:167:MET:HE2	2.01	0.42
1:E:158:PRO:HA	1:E:159:PRO:HD3	1.70	0.41
1:E:18:LEU:HD13	1:E:19:TYR:CE2	2.55	0.41
1:C:168:ASP:N	1:C:169:PRO:CD	2.83	0.41
1:C:203:GLN:HE22	1:D:203:GLN:HG3	1.85	0.41
1:B:155:MET:O	1:B:193:CYS:HA	2.20	0.41
1:D:64:ARG:HH11	1:D:64:ARG:CG	2.31	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:GLN:CG	1:B:203:GLN:HE22	2.33	0.41
1:B:174:ASN:HD22	1:B:174:ASN:N	2.18	0.41
1:D:252:HIS:HE1	3:D:2034:HOH:O	2.03	0.41
1:F:64:ARG:NE	3:F:2170:HOH:O	2.46	0.41
1:F:205:ARG:HB2	1:F:206:GLN:H	1.50	0.41
1:D:42:PRO:HG3	1:D:239:MET:HE1	2.02	0.40
1:D:155:MET:O	1:D:193:CYS:HA	2.20	0.40
1:A:199:LEU:CD2	1:B:199:LEU:HD22	2.38	0.40
1:B:6:ILE:HG22	1:B:237:CYS:HB3	2.02	0.40
1:C:163:GLY:O	1:C:223:HIS:HD2	2.04	0.40
1:D:240:HIS:CD2	1:D:247:TRP:HE1	2.39	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	272/274 (99%)	262 (96%)	9 (3%)	1 (0%)	30	22
1	B	269/274 (98%)	263 (98%)	5 (2%)	1 (0%)	30	22
1	C	269/274 (98%)	261 (97%)	8 (3%)	0	100	100
1	D	269/274 (98%)	258 (96%)	11 (4%)	0	100	100
1	E	269/274 (98%)	260 (97%)	9 (3%)	0	100	100
1	F	272/274 (99%)	264 (97%)	8 (3%)	0	100	100
All	All	1620/1644 (98%)	1568 (97%)	50 (3%)	2 (0%)	48	41

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	216	VAL
1	A	216	VAL



### 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	
1	A	235/235 (100%)	217 (92%)	18 (8%)	10	4
1	B	232/235 (99%)	217 (94%)	15 (6%)	14	7
1	C	232/235 (99%)	219 (94%)	13 (6%)	17	10
1	D	232/235 (99%)	216 (93%)	16 (7%)	13	6
1	E	232/235 (99%)	216 (93%)	16 (7%)	13	6
1	F	235/235 (100%)	222 (94%)	13 (6%)	18	10
All	All	1398/1410 (99%)	1307 (94%)	91 (6%)	14	7

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

Mol	Chain	Res	Type
1	A	3	LEU
1	A	18	LEU
1	A	39	ARG
1	A	58	GLU
1	A	106	ARG
1	A	110	ASP
1	A	123	ARG
1	A	136	ILE
1	A	139	LEU
1	A	145	GLU
1	A	164	ASN
1	A	174	ASN
1	A	179	LEU
1	A	181	LEU
1	A	187	SER
1	A	205	ARG
1	A	206	GLN
1	A	245	GLU
1	B	3	LEU
1	B	18	LEU
1	B	51	ILE
1	B	61	GLN

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Mol	Chain	Res	Type
1	B	110	ASP
1	B	123	ARG
1	B	136	ILE
1	B	139	LEU
1	B	164	ASN
1	B	174	ASN
1	B	179	LEU
1	B	181	LEU
1	B	206	GLN
1	B	238	LEU
1	B	245	GLU
1	C	3	LEU
1	C	18	LEU
1	C	58	GLU
1	C	64	ARG
1	C	97	GLN
1	C	139	LEU
1	C	145	GLU
1	C	164	ASN
1	C	174	ASN
1	C	179	LEU
1	C	181	LEU
1	C	206	GLN
1	C	238	LEU
1	D	3	LEU
1	D	18	LEU
1	D	51	ILE
1	D	64	ARG
1	D	123	ARG
1	D	134	GLU
1	D	139	LEU
1	D	145	GLU
1	D	164	ASN
1	D	174	ASN
1	D	179	LEU
1	D	181	LEU
1	D	182	VAL
1	D	184	ARG
1	D	206	GLN
1	D	245	GLU
1	E	3	LEU
1	E	5	HIS

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Mol	Chain	Res	Type
1	E	18	LEU
1	E	106	ARG
1	E	110	ASP
1	E	115	ARG
1	E	123	ARG
1	E	139	LEU
1	E	145	GLU
1	E	164	ASN
1	E	174	ASN
1	E	177	ARG
1	E	179	LEU
1	E	181	LEU
1	E	206	GLN
1	E	238	LEU
1	F	3	LEU
1	F	18	LEU
1	F	134	GLU
1	F	139	LEU
1	F	145	GLU
1	F	164	ASN
1	F	174	ASN
1	F	179	LEU
1	F	181	LEU
1	F	205	ARG
1	F	206	GLN
1	F	226	THR
1	F	245	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (78) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	HIS
1	A	28	ASN
1	A	34	GLN
1	A	36	ASN
1	A	97	GLN
1	A	103	ASN
1	A	164	ASN
1	A	174	ASN
1	A	206	GLN
1	A	223	HIS
1	A	240	HIS

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Mol	Chain	Res	Type
1	A	252	HIS
1	B	5	HIS
1	B	28	ASN
1	B	34	GLN
1	B	61	GLN
1	B	65	GLN
1	B	142	GLN
1	B	164	ASN
1	B	166	GLN
1	B	174	ASN
1	B	203	GLN
1	B	206	GLN
1	B	240	HIS
1	B	252	HIS
1	C	5	HIS
1	C	28	ASN
1	C	34	GLN
1	C	36	ASN
1	C	97	GLN
1	C	103	ASN
1	C	174	ASN
1	C	203	GLN
1	C	206	GLN
1	C	223	HIS
1	C	240	HIS
1	C	252	HIS
1	D	5	HIS
1	D	34	GLN
1	D	104	ASN
1	D	142	GLN
1	D	164	ASN
1	D	174	ASN
1	D	206	GLN
1	D	223	HIS
1	D	240	HIS
1	D	242	GLN
1	D	246	GLN
1	D	252	HIS
1	E	5	HIS
1	E	28	ASN
1	E	61	GLN
1	E	65	GLN

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Mol	Chain	Res	Type
1	E	97	GLN
1	E	104	ASN
1	E	142	GLN
1	E	164	ASN
1	E	166	GLN
1	E	174	ASN
1	E	206	GLN
1	E	223	HIS
1	E	240	HIS
1	E	251	GLN
1	E	252	HIS
1	F	5	HIS
1	F	28	ASN
1	F	34	GLN
1	F	103	ASN
1	F	104	ASN
1	F	142	GLN
1	F	164	ASN
1	F	174	ASN
1	F	203	GLN
1	F	206	GLN
1	F	240	HIS
1	F	242	GLN
1	F	251	GLN
1	F	252	HIS

### 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 oligosaccharides in this entry.

## 5.6 Ligand geometry

Of 12 ligands modelled in this entry, 12 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 [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, 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	A	274/274 (100%)	-0.48	2 (0%) 84 86	2, 4, 14, 19	0
1	B	271/274 (98%)	-0.53	1 (0%) 89 90	2, 5, 15, 19	0
1	C	271/274 (98%)	-0.46	4 (1%) 71 74	2, 5, 18, 24	0
1	D	271/274 (98%)	-0.50	4 (1%) 71 74	2, 5, 17, 26	0
1	E	271/274 (98%)	-0.36	2 (0%) 84 86	2, 9, 22, 27	0
1	F	274/274 (100%)	-0.54	1 (0%) 89 90	2, 6, 18, 26	0
All	All	1632/1644 (99%)	-0.48	14 (0%) 81 82	2, 6, 19, 27	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	227	ASP	3.1
1	A	148	ASP	3.0
1	D	148	ASP	2.7
1	E	145	GLU	2.4
1	C	229	TYR	2.4
1	D	227	ASP	2.3
1	E	229	TYR	2.3
1	C	265	GLU	2.2
1	D	40	GLU	2.2
1	B	229	TYR	2.2
1	C	144	PHE	2.2
1	A	229	TYR	2.2
1	D	265	GLU	2.1
1	F	144	PHE	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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
2	CO	C	1002	1/1	0.98	0.03	7,7,7,7	1
2	CO	E	1002	1/1	0.98	0.04	8,8,8,8	1
2	CO	C	1001	1/1	0.99	0.02	4,4,4,4	1
2	CO	A	1002	1/1	0.99	0.03	3,3,3,3	1
2	CO	D	1002	1/1	0.99	0.05	6,6,6,6	1
2	CO	E	1001	1/1	0.99	0.01	7,7,7,7	1
2	CO	B	1002	1/1	0.99	0.04	5,5,5,5	1
2	CO	F	1002	1/1	0.99	0.06	7,7,7,7	1
2	CO	A	1001	1/1	1.00	0.02	3,3,3,3	1
2	CO	D	1001	1/1	1.00	0.02	4,4,4,4	1
2	CO	F	1001	1/1	1.00	0.03	4,4,4,4	1
2	CO	B	1001	1/1	1.00	0.01	4,4,4,4	1

### 6.5 Other polymers [i](#)

There are no such residues in this entry.