



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 01:57 pm BST

PDB ID : 4E6W  
Title : ClbP in complex with 3-aminophenyl boronic acid  
Authors : Cougnoux, A.; Delmas, J.; Bonnet, R.  
Deposited on : 2012-03-16  
Resolution : 2.19 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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

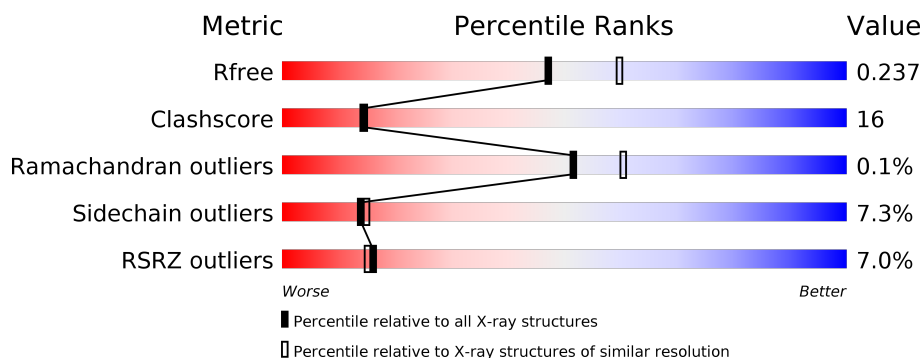
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.19 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 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	335	<div> <div>8%</div> <div>68%</div> <div>26%</div> <div>• •</div> </div>
1	B	335	<div> <div>6%</div> <div>70%</div> <div>27%</div> <div>• •</div> </div>
1	C	335	<div> <div>6%</div> <div>72%</div> <div>25%</div> <div>• •</div> </div>

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	APB	A	400	-	-	X	-
2	APB	B	400	-	-	X	-
2	APB	C	400	-	-	X	-
3	PO4	C	401	-	-	X	-

## 2 Entry composition [i](#)

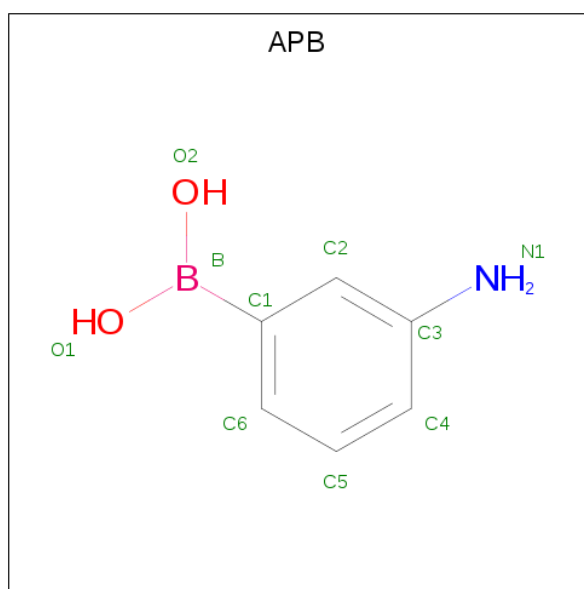
There are 4 unique types of molecules in this entry. The entry contains 8086 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ClbP peptidase.

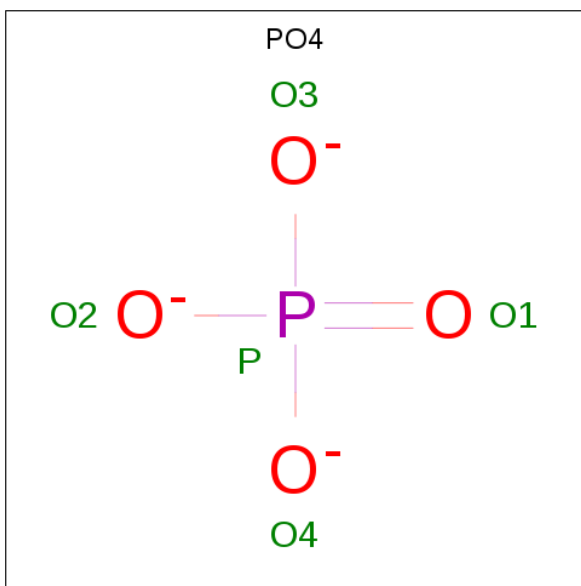
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	329	Total	C	N	O	S	0	0	0
			2537	1613	446	469	9			
1	B	332	Total	C	N	O	S	0	0	0
			2552	1622	447	474	9			
1	C	330	Total	C	N	O	S	0	0	0
			2537	1611	445	472	9			

- Molecule 2 is M-AMINOPHENYLBORONIC ACID (three-letter code: APB) (formula:  $C_6H_8BNO_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	B	C	N	O	0	0
			10	1	6	1	2		
2	B	1	Total	B	C	N	O	0	0
			10	1	6	1	2		
2	C	1	Total	B	C	N	O	0	0
			10	1	6	1	2		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		

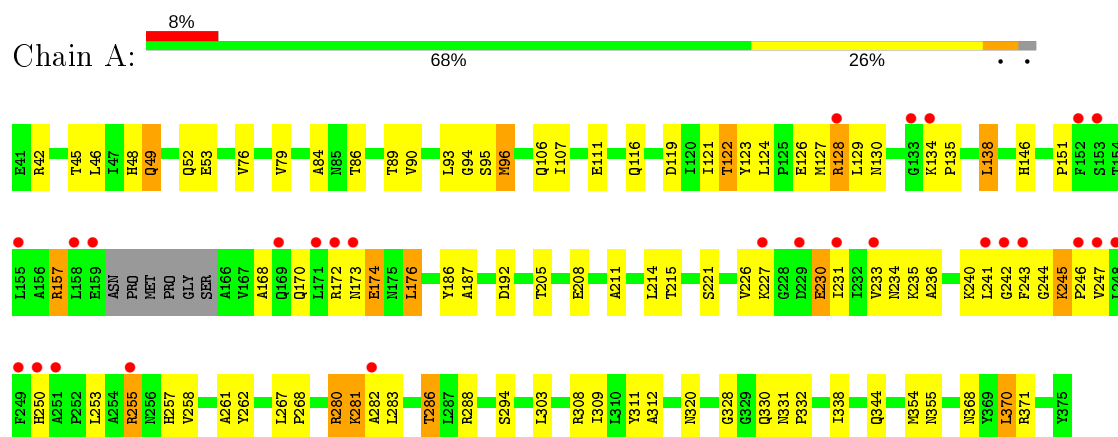
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	131	Total	O	0	0
			131	131		
4	B	128	Total	O	0	0
			128	128		
4	C	141	Total	O	0	0
			141	141		

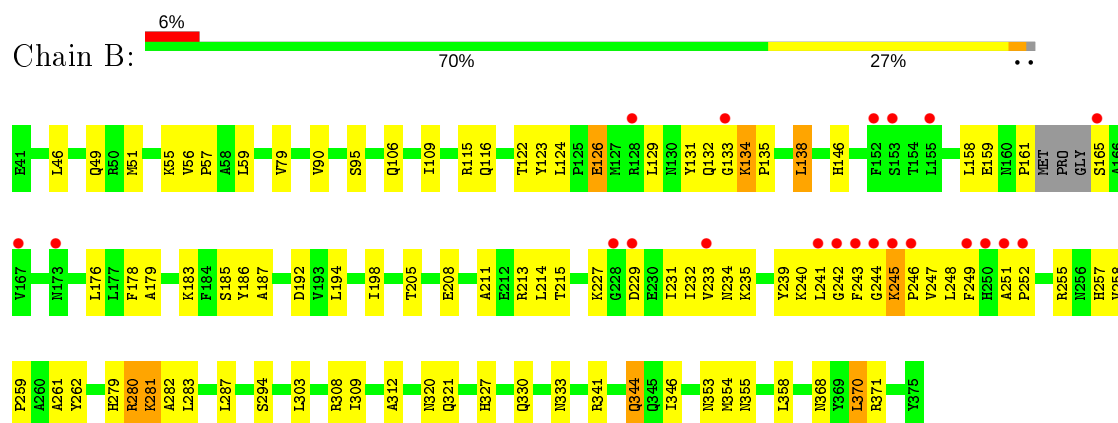
### 3 Residue-property plots [i](#)

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

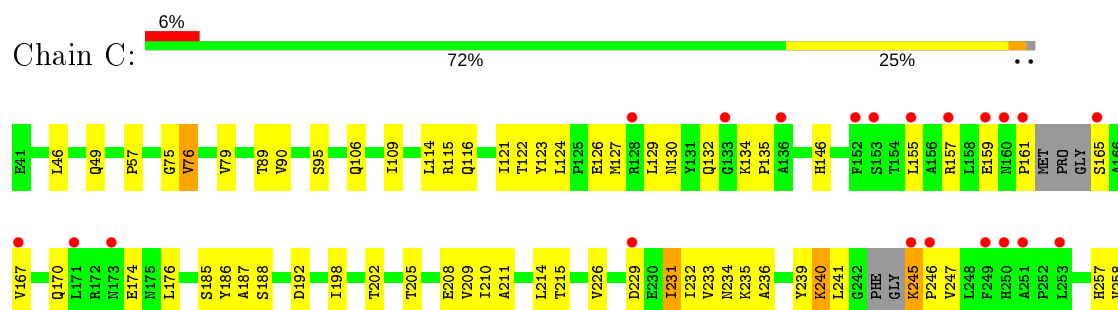
#### • Molecule 1: ClbP peptidase



#### • Molecule 1: ClbP peptidase



#### • Molecule 1: ClbP peptidase





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	104.49Å 149.36Å 88.24Å 90.00° 124.21° 90.00°	Depositor
Resolution (Å)	52.20 – 2.19 52.21 – 2.19	Depositor EDS
% Data completeness (in resolution range)	99.5 (52.20-2.19) 99.0 (52.21-2.19)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.15 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, $R_{free}$	0.195 , 0.240 0.193 , 0.237	Depositor DCC
$R_{free}$ test set	2890 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	21.8	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 26.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.015 for $-1/2^*h+1/2^*k-l, 3/2^*h+1/2^*k+l, 1/2^*h-1/2^*k$ 0.014 for $1/2^*h-1/2^*k+l, -1/2^*h+1/2^*k+l, -h$ 0.014 for $1/2^*h+1/2^*k+l, 1/2^*h+1/2^*k-l, -h$ 0.013 for $-1/2^*h-1/2^*k-l, -3/2^*h+1/2^*k-l, 1/2^*h+1/2^*k$ 0.019 for $-h, -h-2^*l, 1/2^*h-1/2^*k$ 0.013 for $-h, h+2^*l, 1/2^*h+1/2^*k$ 0.468 for $1/2^*h+1/2^*k+l, 3/2^*h-1/2^*k+l, -l$ 0.468 for $1/2^*h-1/2^*k+l, -3/2^*h-1/2^*k-l, -l$ 0.015 for $-1/2^*h+1/2^*k-l, 1/2^*h-1/2^*k-l, -1/2^*h-1/2^*k$ 0.019 for $-1/2^*h-1/2^*k-l, -1/2^*h-1/2^*k+l, -1/2^*h+1/2^*k$ 0.018 for $h, -k, -h-l$	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8086	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

<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.



Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.66% of the height of the origin peak. No significant pseudotranslation is detected.*

## 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: APB, PO4

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	0.60	0/2588	0.72	1/3517 (0.0%)
1	B	0.61	0/2604	0.74	2/3541 (0.1%)
1	C	0.62	0/2587	0.74	1/3517 (0.0%)
All	All	0.61	0/7779	0.73	4/10575 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	370	LEU	CB-CG-CD1	5.58	120.48	111.00
1	B	370	LEU	CB-CG-CD1	5.32	120.05	111.00
1	B	261	ALA	CB-CA-C	-5.23	102.25	110.10
1	C	370	LEU	CB-CG-CD1	5.02	119.53	111.00

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	2537	0	2541	92	0
1	B	2552	0	2548	90	0
1	C	2537	0	2535	62	0
2	A	10	0	8	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	10	0	8	4	0
2	C	10	0	8	4	0
3	A	10	0	0	1	0
3	B	10	0	0	1	0
3	C	10	0	0	2	0
4	A	131	0	0	3	0
4	B	128	0	0	4	0
4	C	141	0	0	2	0
All	All	8086	0	7648	238	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 16.

All (238) 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:245:LYS:CE	1:A:245:LYS:O	1.98	1.11
1:A:258:VAL:HA	1:A:262:TYR:HB2	1.08	1.08
1:B:244:GLY:O	1:B:246:PRO:HD3	1.62	1.00
1:A:245:LYS:HE2	1:A:245:LYS:O	1.60	1.00
1:C:309:ILE:HB	3:C:401:PO4:O1	1.65	0.97
1:A:245:LYS:CG	1:A:245:LYS:O	2.13	0.95
1:A:258:VAL:CA	1:A:262:TYR:HB2	1.95	0.95
1:A:245:LYS:HG2	1:A:245:LYS:O	1.64	0.94
1:C:245:LYS:N	1:C:245:LYS:CE	2.30	0.94
1:A:174:GLU:HA	1:A:174:GLU:OE1	1.71	0.88
1:C:240:LYS:O	1:C:246:PRO:HD2	1.75	0.87
1:A:211:ALA:HA	1:A:215:THR:OG1	1.75	0.87
1:A:258:VAL:HA	1:A:262:TYR:CB	2.01	0.84
1:B:57:PRO:HB2	1:B:353:ASN:HD21	1.43	0.84
1:A:127:MET:HB2	1:A:168:ALA:HB1	1.60	0.83
1:A:280:ARG:O	1:A:283:LEU:HB2	1.78	0.83
1:B:211:ALA:HA	1:B:215:THR:OG1	1.79	0.83
1:A:245:LYS:CD	1:A:245:LYS:O	2.27	0.81
1:B:245:LYS:CD	1:B:245:LYS:O	2.29	0.81
1:A:309:ILE:HB	3:A:401:PO4:O2	1.80	0.81
1:A:119:ASP:O	1:A:122:THR:HG23	1.81	0.80
1:C:245:LYS:HE2	1:C:245:LYS:N	1.96	0.80
1:B:258:VAL:HA	1:B:262:TYR:HB2	1.65	0.79
1:B:55:LYS:O	1:B:354:MET:HE3	1.83	0.78
1:B:205:THR:OG1	1:B:208:GLU:HG3	1.82	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:245:LYS:CG	1:B:245:LYS:O	2.30	0.78
1:C:245:LYS:HE3	1:C:245:LYS:N	1.99	0.78
1:B:241:LEU:HB2	1:B:354:MET:SD	2.23	0.77
1:B:281:LYS:H	1:B:281:LYS:HD3	1.48	0.77
1:A:221:SER:HA	1:C:231:ILE:HG12	1.66	0.77
1:A:227:LYS:HB3	1:A:255:ARG:HH21	1.50	0.77
1:C:258:VAL:HA	1:C:262:TYR:HB2	1.65	0.76
1:B:233:VAL:O	1:B:234:ASN:HB2	1.84	0.75
1:A:286:THR:HG22	4:A:547:HOH:O	1.87	0.73
1:A:242:GLY:HA2	1:A:243:PHE:C	2.07	0.72
1:A:241:LEU:HB2	1:A:354:MET:HE3	1.72	0.71
1:B:280:ARG:O	1:B:283:LEU:HD12	1.91	0.70
1:A:127:MET:HB2	1:A:168:ALA:CB	2.20	0.70
1:C:124:LEU:HD22	1:C:127:MET:CE	2.22	0.69
1:A:244:GLY:O	1:A:246:PRO:HD3	1.92	0.69
1:A:128:ARG:HG3	1:A:172:ARG:NH2	2.08	0.68
1:B:358:LEU:N	1:B:358:LEU:HD12	2.09	0.67
1:A:129:LEU:CD2	1:A:174:GLU:HB3	2.25	0.67
1:B:280:ARG:HA	1:B:283:LEU:HD12	1.77	0.66
1:A:205:THR:OG1	1:A:208:GLU:HG3	1.93	0.66
1:A:368:ASN:HD21	1:B:303:LEU:H	1.45	0.65
1:C:232:ILE:HD13	1:C:264:HIS:CD2	2.30	0.65
1:A:303:LEU:H	1:B:368:ASN:HD21	1.45	0.65
1:C:129:LEU:HD23	1:C:174:GLU:HB3	1.78	0.65
1:C:95:SER:HB2	2:C:400:APB:C1	2.25	0.65
1:C:130:ASN:HA	1:C:135:PRO:HA	1.78	0.64
1:A:233:VAL:O	1:A:234:ASN:HB2	1.97	0.64
1:B:146:HIS:HB3	1:B:185:SER:O	1.98	0.64
1:B:244:GLY:O	1:B:246:PRO:CD	2.42	0.64
1:A:157:ARG:NH1	1:A:170:GLN:O	2.31	0.64
1:A:172:ARG:O	1:A:173:ASN:HB2	1.97	0.63
1:B:245:LYS:HB2	1:B:354:MET:CE	2.29	0.62
1:C:90:VAL:HB	1:C:235:LYS:HA	1.81	0.62
1:B:281:LYS:HD3	1:B:281:LYS:N	2.13	0.62
1:C:186:TYR:OH	2:C:400:APB:H2	2.00	0.62
1:C:233:VAL:O	1:C:234:ASN:HB2	1.98	0.62
1:B:245:LYS:HG2	1:B:245:LYS:O	1.99	0.62
1:C:205:THR:OG1	1:C:208:GLU:HG3	2.00	0.61
1:C:57:PRO:HB2	1:C:353:ASN:HD21	1.65	0.61
1:A:94:GLY:O	1:A:261:ALA:HA	2.00	0.61
1:A:95:SER:HB2	2:A:400:APB:C1	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:358:LEU:CD1	1:B:358:LEU:N	2.64	0.61
1:A:186:TYR:OH	2:A:400:APB:H2	2.01	0.60
1:C:126:GLU:CD	1:C:126:GLU:H	2.06	0.60
1:C:215:THR:HG21	4:C:584:HOH:O	2.01	0.60
1:C:124:LEU:CD2	1:C:127:MET:HE2	2.33	0.59
1:A:245:LYS:HE3	1:A:245:LYS:O	1.99	0.59
1:B:243:PHE:N	1:B:243:PHE:CD1	2.69	0.59
1:B:249:PHE:HA	1:B:333:ASN:ND2	2.17	0.59
1:A:89:THR:CG2	1:A:236:ALA:HB2	2.32	0.59
1:B:95:SER:HB2	2:B:400:APB:C1	2.32	0.59
1:C:95:SER:OG	1:C:186:TYR:OH	2.21	0.58
1:C:330:GLN:NE2	1:C:355:ASN:OD1	2.36	0.58
1:A:281:LYS:O	1:A:282:ALA:HB3	2.03	0.58
1:B:95:SER:OG	1:B:186:TYR:OH	2.20	0.58
1:A:90:VAL:HB	1:A:235:LYS:HA	1.86	0.58
1:B:245:LYS:HD3	1:B:245:LYS:O	2.02	0.58
1:A:126:GLU:HG2	1:A:168:ALA:CB	2.34	0.58
1:A:328:GLY:O	2:A:400:APB:C3	2.52	0.57
1:A:129:LEU:HD23	1:A:174:GLU:HB3	1.86	0.57
1:B:243:PHE:N	1:B:243:PHE:HD1	2.02	0.57
1:C:76:VAL:HG21	1:C:79:VAL:HA	1.87	0.57
1:B:126:GLU:CD	1:B:126:GLU:H	2.08	0.56
1:A:303:LEU:H	1:B:368:ASN:ND2	2.04	0.56
1:B:232:ILE:HG22	1:B:235:LYS:HB2	1.88	0.55
1:B:281:LYS:O	1:B:282:ALA:HB3	2.06	0.54
1:B:281:LYS:CD	1:B:281:LYS:H	2.19	0.54
1:A:95:SER:OG	1:A:186:TYR:OH	2.26	0.54
1:A:93:LEU:O	1:A:96:MET:HB2	2.08	0.54
1:B:309:ILE:HB	3:B:401:PO4:O1	2.08	0.54
1:C:202:THR:HG21	1:C:209:VAL:HG21	1.90	0.54
1:C:95:SER:CB	2:C:400:APB:C2	2.86	0.54
1:B:321:GLN:NE2	4:B:600:HOH:O	2.41	0.53
1:A:241:LEU:HD13	1:A:354:MET:HE1	1.89	0.53
1:B:123:TYR:C	1:B:124:LEU:HD12	2.28	0.53
1:C:239:TYR:O	1:C:354:MET:HG3	2.07	0.53
1:B:245:LYS:HB2	1:B:354:MET:HE1	1.90	0.53
1:C:106:GLN:HE22	1:C:116:GLN:HE21	1.56	0.53
1:B:57:PRO:HG3	1:B:245:LYS:HG3	1.90	0.53
1:C:159:GLU:O	1:C:161:PRO:HD3	2.09	0.52
1:A:106:GLN:HE22	1:A:116:GLN:HE21	1.57	0.52
1:B:186:TYR:OH	2:B:400:APB:H2	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:ILE:O	1:A:111:GLU:HG3	2.10	0.52
1:B:131:TYR:CE1	1:B:178:PHE:HA	2.45	0.52
1:C:89:THR:CG2	1:C:236:ALA:HB2	2.39	0.52
1:C:245:LYS:HB3	1:C:354:MET:SD	2.50	0.52
1:A:129:LEU:HD12	1:A:138:LEU:HD13	1.91	0.52
1:B:245:LYS:HB2	1:B:354:MET:HE2	1.91	0.52
1:B:249:PHE:HA	1:B:333:ASN:HD22	1.75	0.51
1:B:330:GLN:CG	1:B:355:ASN:OD1	2.58	0.51
1:A:126:GLU:HG2	1:A:168:ALA:HB3	1.92	0.51
1:C:241:LEU:HD12	1:C:245:LYS:HE2	1.91	0.51
1:A:250:HIS:HA	4:A:626:HOH:O	2.11	0.51
1:C:211:ALA:HA	1:C:215:THR:OG1	2.11	0.51
1:B:294:SER:O	1:B:312:ALA:HB1	2.11	0.51
1:A:368:ASN:ND2	1:B:303:LEU:H	2.07	0.50
1:C:124:LEU:HD22	1:C:127:MET:HE2	1.90	0.50
1:A:89:THR:HG23	1:A:236:ALA:HB2	1.93	0.50
1:A:146:HIS:CD2	1:A:187:ALA:H	2.29	0.50
1:C:46:LEU:HD23	1:C:46:LEU:C	2.32	0.50
1:B:79:VAL:HG11	1:B:245:LYS:HE3	1.94	0.50
1:C:146:HIS:CD2	1:C:187:ALA:H	2.30	0.50
1:A:174:GLU:OE1	1:A:174:GLU:CA	2.53	0.50
1:B:134:LYS:HB3	1:B:135:PRO:HD2	1.93	0.50
1:A:45:THR:O	1:A:49:GLN:HB2	2.12	0.49
1:B:242:GLY:HA2	1:B:243:PHE:C	2.30	0.49
1:B:79:VAL:HG21	1:B:245:LYS:HE3	1.94	0.49
1:B:106:GLN:HE22	1:B:116:GLN:HE21	1.60	0.49
1:B:330:GLN:CD	1:B:355:ASN:OD1	2.51	0.49
1:B:239:TYR:CD2	1:B:245:LYS:HG2	2.47	0.49
1:B:341:ARG:HB3	1:B:346:ILE:HB	1.94	0.49
1:B:90:VAL:HB	1:B:235:LYS:HA	1.94	0.49
1:A:226:VAL:O	1:A:258:VAL:HG21	2.13	0.49
1:B:245:LYS:O	1:B:245:LYS:CE	2.60	0.48
1:B:245:LYS:CB	1:B:354:MET:HE1	2.43	0.48
1:C:226:VAL:O	1:C:258:VAL:HG21	2.13	0.48
1:B:279:HIS:HB3	1:B:281:LYS:NZ	2.28	0.48
1:A:123:TYR:C	1:A:124:LEU:HD12	2.34	0.48
1:C:57:PRO:O	1:C:75:GLY:HA3	2.14	0.48
1:A:368:ASN:HD22	1:A:371:ARG:HH21	1.62	0.48
1:B:248:LEU:CB	4:B:617:HOH:O	2.62	0.48
1:C:124:LEU:HD22	1:C:127:MET:HE1	1.92	0.47
1:C:95:SER:HB3	1:C:327:HIS:CE1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:ASN:HA	1:A:135:PRO:HA	1.96	0.47
1:B:368:ASN:HD22	1:B:371:ARG:HH21	1.62	0.47
1:B:129:LEU:HD12	1:B:138:LEU:HD13	1.96	0.47
1:A:242:GLY:CA	1:A:243:PHE:C	2.79	0.47
1:A:250:HIS:N	1:A:250:HIS:CD2	2.83	0.47
1:A:243:PHE:N	1:A:243:PHE:HD1	2.12	0.47
1:A:192:ASP:OD1	1:A:257:HIS:HA	2.15	0.47
1:B:280:ARG:CA	1:B:283:LEU:HD12	2.44	0.47
1:C:123:TYR:C	1:C:124:LEU:HD12	2.35	0.46
1:A:294:SER:O	1:A:312:ALA:HB1	2.15	0.46
1:B:251:ALA:HA	1:B:252:PRO:HD3	1.75	0.46
1:A:76:VAL:HG21	1:A:79:VAL:HA	1.98	0.46
1:C:286:THR:HG22	4:C:575:HOH:O	2.16	0.46
1:A:240:LYS:O	1:A:246:PRO:HD2	2.14	0.46
1:B:330:GLN:H	2:B:400:APB:H6	1.80	0.46
1:A:243:PHE:N	1:A:243:PHE:CD1	2.83	0.46
1:B:95:SER:HB3	1:B:327:HIS:CE1	2.51	0.46
1:C:198:ILE:O	1:C:202:THR:HG23	2.16	0.46
1:B:79:VAL:HG21	1:B:245:LYS:CE	2.46	0.46
1:C:356:SER:HB3	1:C:359:ILE:HG12	1.98	0.46
1:B:146:HIS:CD2	1:B:187:ALA:H	2.34	0.46
1:A:257:HIS:HB3	1:A:262:TYR:CE2	2.51	0.46
1:A:311:TYR:CD2	1:A:312:ALA:O	2.69	0.45
1:B:234:ASN:ND2	4:B:563:HOH:O	2.42	0.45
1:C:210:ILE:O	1:C:215:THR:HG23	2.17	0.45
1:B:344:GLN:HB2	1:B:344:GLN:HE21	1.64	0.45
1:C:333:ASN:OD1	1:C:333:ASN:N	2.50	0.45
1:A:126:GLU:HG2	1:A:168:ALA:HB1	1.97	0.45
1:B:131:TYR:CE2	1:B:179:ALA:HB2	2.51	0.45
1:C:167:VAL:HA	1:C:170:GLN:HB3	1.97	0.45
1:C:267:LEU:HB3	1:C:268:PRO:HD3	1.99	0.45
1:C:155:LEU:HD13	1:C:188:SER:HB3	1.99	0.44
1:A:250:HIS:H	1:A:250:HIS:CD2	2.35	0.44
1:C:146:HIS:HD2	1:C:187:ALA:H	1.66	0.44
1:C:192:ASP:OD1	1:C:257:HIS:HA	2.18	0.44
1:A:138:LEU:HD11	1:A:176:LEU:HD21	2.00	0.44
1:B:56:VAL:HG12	1:B:354:MET:HB3	1.99	0.44
1:C:294:SER:O	1:C:312:ALA:HB1	2.17	0.44
1:A:95:SER:CB	2:A:400:APB:C2	2.96	0.44
1:C:95:SER:HB3	1:C:327:HIS:HE1	1.81	0.44
1:B:192:ASP:OD1	1:B:257:HIS:HA	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:MET:HE3	1:A:338:ILE:HB	2.00	0.43
1:A:146:HIS:HD2	1:A:187:ALA:H	1.65	0.43
1:A:331:ASN:HB3	1:A:332:PRO:HD2	2.01	0.43
1:B:109:ILE:HD13	1:B:116:GLN:HG3	2.00	0.43
1:A:129:LEU:HD23	1:A:174:GLU:CB	2.48	0.43
1:A:241:LEU:HB2	1:A:354:MET:CE	2.47	0.43
1:A:283:LEU:O	1:A:288:ARG:NH1	2.52	0.43
1:A:42:ARG:HA	1:A:42:ARG:HD3	1.90	0.43
1:C:114:LEU:O	1:C:115:ARG:HG3	2.19	0.43
1:B:280:ARG:HA	1:B:283:LEU:CD1	2.46	0.43
1:B:132:GLN:HB3	1:B:133:GLY:H	1.51	0.43
1:C:146:HIS:HB3	1:C:185:SER:O	2.19	0.42
1:B:240:LYS:O	1:B:246:PRO:HD2	2.19	0.42
1:B:46:LEU:HD23	1:B:46:LEU:C	2.40	0.42
1:B:51:MET:HB2	1:B:59:LEU:CD2	2.49	0.42
1:A:320:ASN:HB2	1:B:308:ARG:HB2	2.02	0.42
1:B:258:VAL:N	1:B:259:PRO:CD	2.81	0.42
1:B:51:MET:HB2	1:B:59:LEU:HD23	2.00	0.42
1:C:315:TRP:CE3	1:C:325:ILE:HG22	2.54	0.42
1:A:227:LYS:H	1:A:227:LYS:HG3	1.70	0.42
1:B:46:LEU:HD23	1:B:46:LEU:O	2.19	0.42
1:A:126:GLU:CG	1:A:168:ALA:HB3	2.50	0.42
1:B:159:GLU:O	1:B:161:PRO:HD3	2.19	0.42
1:C:109:ILE:HD13	1:C:116:GLN:HG3	2.02	0.42
1:C:240:LYS:HB2	1:C:240:LYS:HE3	1.29	0.42
1:A:48:HIS:O	1:A:52:GLN:HG3	2.20	0.42
1:B:227:LYS:HG2	1:B:255:ARG:HH21	1.83	0.42
1:A:330:GLN:NE2	1:A:355:ASN:OD1	2.51	0.42
1:B:115:ARG:NH1	4:B:622:HOH:O	2.53	0.41
1:A:308:ARG:HB2	1:B:320:ASN:HB2	2.02	0.41
1:C:124:LEU:HD23	1:C:127:MET:HE2	2.02	0.41
1:C:368:ASN:HD22	1:C:371:ARG:HH21	1.68	0.41
1:A:84:ALA:O	1:A:86:THR:HG23	2.21	0.41
2:B:400:APB:O1	2:B:400:APB:C6	2.66	0.41
1:C:258:VAL:N	1:C:259:PRO:CD	2.83	0.41
1:A:129:LEU:HD22	1:A:174:GLU:HB3	2.02	0.41
1:B:194:LEU:O	1:B:198:ILE:HG13	2.21	0.41
1:C:95:SER:HB2	2:C:400:APB:C2	2.51	0.41
1:A:46:LEU:C	1:A:46:LEU:HD23	2.41	0.41
1:A:49:GLN:NE2	1:A:53:GLU:OE1	2.52	0.41
1:B:333:ASN:OD1	1:B:333:ASN:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:GLU:HG3	4:A:607:HOH:O	2.20	0.41
1:B:183:LYS:HE2	1:B:183:LYS:HB2	1.79	0.41
1:B:158:LEU:O	1:B:257:HIS:HB2	2.21	0.41
1:C:309:ILE:CB	3:C:401:PO4:O1	2.53	0.41
1:A:267:LEU:HB3	1:A:268:PRO:HD3	2.03	0.41
1:A:245:LYS:HB2	1:A:354:MET:SD	2.61	0.40
1:A:151:PRO:CD	1:A:174:GLU:HG3	2.51	0.40
1:B:131:TYR:CE1	1:B:178:PHE:CA	3.05	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	325/335 (97%)	318 (98%)	7 (2%)	0	100	100
1	B	328/335 (98%)	314 (96%)	14 (4%)	0	100	100
1	C	324/335 (97%)	315 (97%)	8 (2%)	1 (0%)	41	46
All	All	977/1005 (97%)	947 (97%)	29 (3%)	1 (0%)	51	60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	132	GLN

### 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	268/276 (97%)	246 (92%)	22 (8%)	11	11
1	B	270/276 (98%)	252 (93%)	18 (7%)	16	18
1	C	269/276 (98%)	250 (93%)	19 (7%)	14	16
All	All	807/828 (98%)	748 (93%)	59 (7%)	14	15

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	GLN
1	A	96	MET
1	A	121	ILE
1	A	122	THR
1	A	128	ARG
1	A	134	LYS
1	A	138	LEU
1	A	157	ARG
1	A	174	GLU
1	A	176	LEU
1	A	214	LEU
1	A	230	GLU
1	A	231	ILE
1	A	245	LYS
1	A	247	VAL
1	A	253	LEU
1	A	255	ARG
1	A	280	ARG
1	A	281	LYS
1	A	286	THR
1	A	344	GLN
1	A	370	LEU
1	B	49	GLN
1	B	122	THR
1	B	126	GLU
1	B	134	LYS
1	B	138	LEU
1	B	165	SER
1	B	176	LEU
1	B	213	ARG
1	B	214	LEU
1	B	229	ASP

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Mol	Chain	Res	Type
1	B	231	ILE
1	B	245	LYS
1	B	247	VAL
1	B	280	ARG
1	B	281	LYS
1	B	287	LEU
1	B	344	GLN
1	B	370	LEU
1	C	49	GLN
1	C	76	VAL
1	C	121	ILE
1	C	122	THR
1	C	134	LYS
1	C	157	ARG
1	C	165	SER
1	C	176	LEU
1	C	214	LEU
1	C	229	ASP
1	C	231	ILE
1	C	240	LYS
1	C	245	LYS
1	C	247	VAL
1	C	286	THR
1	C	287	LEU
1	C	343	ASP
1	C	344	GLN
1	C	370	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	82	GLN
1	A	116	GLN
1	A	146	HIS
1	A	190	ASN
1	A	250	HIS
1	A	368	ASN
1	B	82	GLN
1	B	116	GLN
1	B	146	HIS
1	B	190	ASN
1	B	234	ASN

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Mol	Chain	Res	Type
1	B	321	GLN
1	B	330	GLN
1	B	344	GLN
1	B	368	ASN
1	C	116	GLN
1	C	130	ASN
1	C	146	HIS
1	C	160	ASN
1	C	169	GLN
1	C	190	ASN
1	C	250	HIS
1	C	321	GLN
1	C	330	GLN
1	C	344	GLN
1	C	368	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

9 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
3	PO4	C	402	-	4,4,4	0.58	0	6,6,6	0.79	0
2	APB	B	400	1	10,10,10	3.08	3 (30%)	13,13,13	1.97	6 (46%)
3	PO4	A	402	-	4,4,4	0.82	0	6,6,6	1.02	0
3	PO4	C	401	-	4,4,4	0.95	0	6,6,6	1.17	0
3	PO4	B	401	-	4,4,4	0.77	0	6,6,6	1.12	0
3	PO4	A	401	-	4,4,4	0.65	0	6,6,6	0.61	0
2	APB	C	400	1	10,10,10	3.17	3 (30%)	13,13,13	1.83	4 (30%)
2	APB	A	400	1	10,10,10	3.08	3 (30%)	13,13,13	1.90	4 (30%)
3	PO4	B	402	-	4,4,4	1.04	0	6,6,6	0.46	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	APB	B	400	1	-	2/4/4/4	0/1/1/1
2	APB	A	400	1	-	2/4/4/4	0/1/1/1
2	APB	C	400	1	-	2/4/4/4	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	400	APB	B-C1	-6.85	1.43	1.57
2	B	400	APB	B-C1	-6.63	1.44	1.57
2	A	400	APB	B-C1	-6.59	1.44	1.57
2	B	400	APB	B-O1	6.28	1.47	1.36
2	C	400	APB	B-O1	6.26	1.47	1.36
2	A	400	APB	B-O1	6.08	1.46	1.36
2	C	400	APB	B-O2	3.45	1.42	1.36
2	A	400	APB	B-O2	3.39	1.42	1.36
2	B	400	APB	B-O2	2.95	1.41	1.36

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	400	APB	O2-B-O1	-3.37	108.34	119.67
2	B	400	APB	O1-B-C1	-3.33	110.02	119.95
2	A	400	APB	O2-B-O1	-3.26	108.69	119.67
2	C	400	APB	O2-B-C1	-3.20	110.39	119.95
2	C	400	APB	O1-B-C1	-3.16	110.50	119.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	400	APB	O1-B-C1	-3.10	110.68	119.95
2	A	400	APB	O2-B-C1	-3.07	110.80	119.95
2	C	400	APB	O2-B-O1	-2.97	109.68	119.67
2	B	400	APB	O2-B-C1	-2.67	111.99	119.95
2	B	400	APB	B-C1-C2	2.65	124.30	121.05
2	B	400	APB	C4-C3-N1	-2.22	116.78	120.91
2	C	400	APB	B-C1-C2	2.17	123.72	121.05
2	B	400	APB	B-C1-C6	-2.16	118.54	121.56
2	A	400	APB	B-C1-C2	2.16	123.70	121.05

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	400	APB	O2-B-C1-C2
2	B	400	APB	O2-B-C1-C6
2	C	400	APB	O2-B-C1-C2
2	C	400	APB	O2-B-C1-C6
2	A	400	APB	O2-B-C1-C2
2	A	400	APB	O2-B-C1-C6

There are no ring outliers.

6 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	400	APB	4	0
3	C	401	PO4	2	0
3	B	401	PO4	1	0
3	A	401	PO4	1	0
2	C	400	APB	4	0
2	A	400	APB	4	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, 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	329/335 (98%)	0.07	27 (8%)	11 10	7, 21, 69, 79	0
1	B	332/335 (99%)	0.00	21 (6%)	20 19	7, 21, 68, 89	0
1	C	330/335 (98%)	0.02	21 (6%)	19 18	6, 21, 72, 94	0
All	All	991/1005 (98%)	0.03	69 (6%)	16 15	6, 21, 69, 94	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	249	PHE	11.9
1	C	249	PHE	8.5
1	B	249	PHE	6.8
1	C	250	HIS	6.4
1	C	152	PHE	5.6
1	A	152	PHE	5.2
1	A	250	HIS	5.1
1	B	152	PHE	5.0
1	C	251	ALA	4.9
1	A	246	PRO	4.8
1	B	243	PHE	4.7
1	A	242	GLY	4.6
1	B	133	GLY	4.6
1	A	229	ASP	4.3
1	A	248	LEU	4.3
1	C	246	PRO	4.3
1	B	155	LEU	4.1
1	C	133	GLY	4.0
1	A	241	LEU	3.9
1	B	241	LEU	3.8
1	B	251	ALA	3.8
1	A	243	PHE	3.7
1	C	173	ASN	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	136	ALA	3.7
1	C	161	PRO	3.6
1	A	247	VAL	3.5
1	C	153	SER	3.5
1	A	251	ALA	3.5
1	A	155	LEU	3.4
1	B	250	HIS	3.2
1	A	282	ALA	3.1
1	C	160	ASN	3.0
1	B	242	GLY	3.0
1	B	246	PRO	3.0
1	C	171	LEU	2.9
1	A	227	LYS	2.9
1	B	153	SER	2.9
1	A	169	GLN	2.8
1	C	128	ARG	2.7
1	A	153	SER	2.7
1	C	165	SER	2.7
1	A	173	ASN	2.7
1	B	165	SER	2.7
1	B	244	GLY	2.7
1	C	167	VAL	2.6
1	A	128	ARG	2.6
1	C	229	ASP	2.6
1	A	133	GLY	2.6
1	A	171	LEU	2.6
1	A	134	LYS	2.5
1	C	155	LEU	2.5
1	A	255	ARG	2.4
1	B	128	ARG	2.4
1	A	233	VAL	2.4
1	B	173	ASN	2.3
1	B	167	VAL	2.3
1	A	172	ARG	2.2
1	B	229	ASP	2.2
1	C	157	ARG	2.2
1	B	252	PRO	2.2
1	C	159	GLU	2.1
1	B	233	VAL	2.1
1	C	245	LYS	2.1
1	B	245	LYS	2.1
1	B	228	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	231	ILE	2.0
1	C	253	LEU	2.0
1	A	158	LEU	2.0
1	A	159	GLU	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. 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	APB	A	400	10/10	0.82	0.22	18,21,24,29	10
2	APB	C	400	10/10	0.84	0.18	22,24,26,34	10
3	PO4	C	402	5/5	0.85	0.17	30,33,37,37	5
3	PO4	B	402	5/5	0.86	0.16	33,37,37,38	5
2	APB	B	400	10/10	0.89	0.17	18,21,24,30	10
3	PO4	A	402	5/5	0.93	0.16	26,31,33,34	5
3	PO4	A	401	5/5	0.96	0.17	26,27,28,34	5
3	PO4	B	401	5/5	0.96	0.15	26,28,29,36	5
3	PO4	C	401	5/5	0.97	0.18	25,26,27,35	5

## 6.5 Other polymers [i](#)

There are no such residues in this entry.