



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2019 – 06:15 PM EDT

PDB ID : 6EB0  
Title : STRUCTURE OF 4 - H Y D R O X Y P H E N Y L A C E T A T E 3-MONOOXYGENASE (HPAB), OXYGENASE COMPONENT FROM ES-CHERICHIA COLI  
Authors : Zhou, D.; Kandavelu, P.; Zhang, H.; Wang, B.C.; Yan, Y.; Rose, J.  
Deposited on : 2018-08-03  
Resolution : 2.37 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 : 1.8.0 (224370), CSD as540be (2019)  
Xtriage (Phenix) : 1.13  
EDS : rb-20031633  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20031633

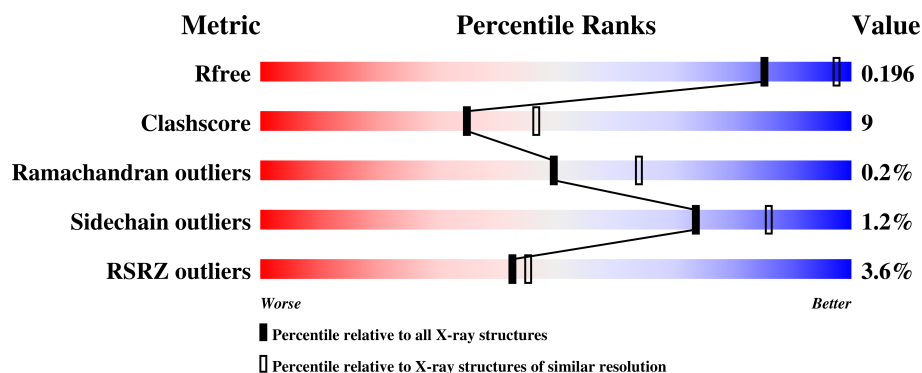
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.37 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))
$R_{free}$	111664	4850 (2.40-2.36)
Clashscore	122126	5405 (2.40-2.36)
Ramachandran outliers	120053	5324 (2.40-2.36)
Sidechain outliers	120020	5326 (2.40-2.36)
RSRZ outliers	108989	4741 (2.40-2.36)

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	A	527	<div> <div>3%</div> <div>83%</div> <div>14%</div> <div>..</div> </div>
1	B	527	<div> <div>3%</div> <div>79%</div> <div>18%</div> <div>..</div> </div>
1	C	527	<div> <div>3%</div> <div>81%</div> <div>17%</div> <div>.</div> </div>
1	D	527	<div> <div>6%</div> <div>80%</div> <div>18%</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	ACT	C	702	-	-	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17250 atoms, of which 9 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 4-hydroxyphenylacetate 3-monooxygenase, oxygenase subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	518	Total	C	N	O	S	0	0	0
			4099	2593	713	767	26			
1	B	518	Total	C	N	O	S	0	0	0
			4099	2593	713	767	26			
1	C	518	Total	C	N	O	S	0	0	0
			4099	2593	713	767	26			
1	D	518	Total	C	N	O	S	0	0	0
			4099	2593	713	767	26			

There are 32 discrepancies between the modelled and reference sequences:

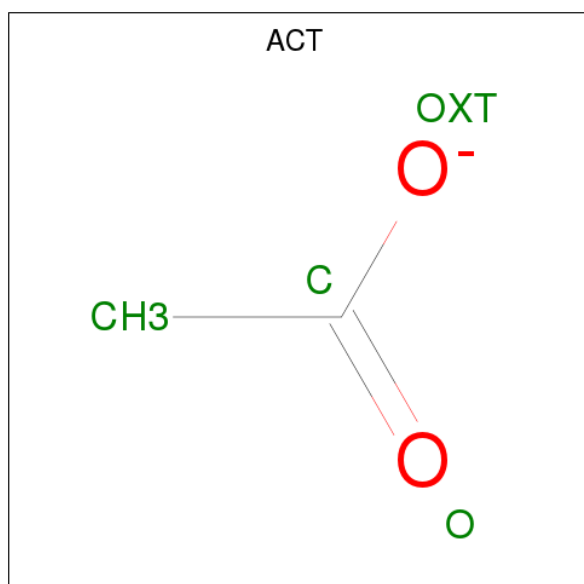
Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	initiating methionine	UNP A0A140NG21
A	-5	HIS	-	expression tag	UNP A0A140NG21
A	-4	HIS	-	expression tag	UNP A0A140NG21
A	-3	HIS	-	expression tag	UNP A0A140NG21
A	-2	HIS	-	expression tag	UNP A0A140NG21
A	-1	HIS	-	expression tag	UNP A0A140NG21
A	0	HIS	-	expression tag	UNP A0A140NG21
A	1	HIS	-	expression tag	UNP A0A140NG21
B	-6	MET	-	initiating methionine	UNP A0A140NG21
B	-5	HIS	-	expression tag	UNP A0A140NG21
B	-4	HIS	-	expression tag	UNP A0A140NG21
B	-3	HIS	-	expression tag	UNP A0A140NG21
B	-2	HIS	-	expression tag	UNP A0A140NG21
B	-1	HIS	-	expression tag	UNP A0A140NG21
B	0	HIS	-	expression tag	UNP A0A140NG21
B	1	HIS	-	expression tag	UNP A0A140NG21
C	-6	MET	-	initiating methionine	UNP A0A140NG21
C	-5	HIS	-	expression tag	UNP A0A140NG21
C	-4	HIS	-	expression tag	UNP A0A140NG21
C	-3	HIS	-	expression tag	UNP A0A140NG21
C	-2	HIS	-	expression tag	UNP A0A140NG21

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	HIS	-	expression tag	UNP A0A140NG21
C	0	HIS	-	expression tag	UNP A0A140NG21
C	1	HIS	-	expression tag	UNP A0A140NG21
D	-6	MET	-	initiating methionine	UNP A0A140NG21
D	-5	HIS	-	expression tag	UNP A0A140NG21
D	-4	HIS	-	expression tag	UNP A0A140NG21
D	-3	HIS	-	expression tag	UNP A0A140NG21
D	-2	HIS	-	expression tag	UNP A0A140NG21
D	-1	HIS	-	expression tag	UNP A0A140NG21
D	0	HIS	-	expression tag	UNP A0A140NG21
D	1	HIS	-	expression tag	UNP A0A140NG21

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			7	2	3	2		
2	C	1	Total	C	H	O	0	0
			7	2	3	2		
2	C	1	Total	C	H	O	0	0
			7	2	3	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	245	Total	O	0	0
			245	245		

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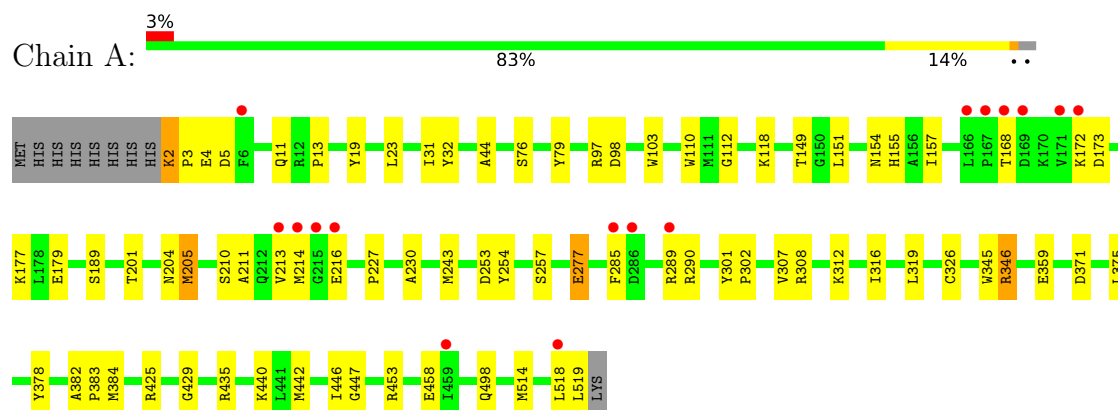
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	192	Total 192	O 192	0	0
3	C	218	Total 218	O 218	0	0
3	D	178	Total 178	O 178	0	0

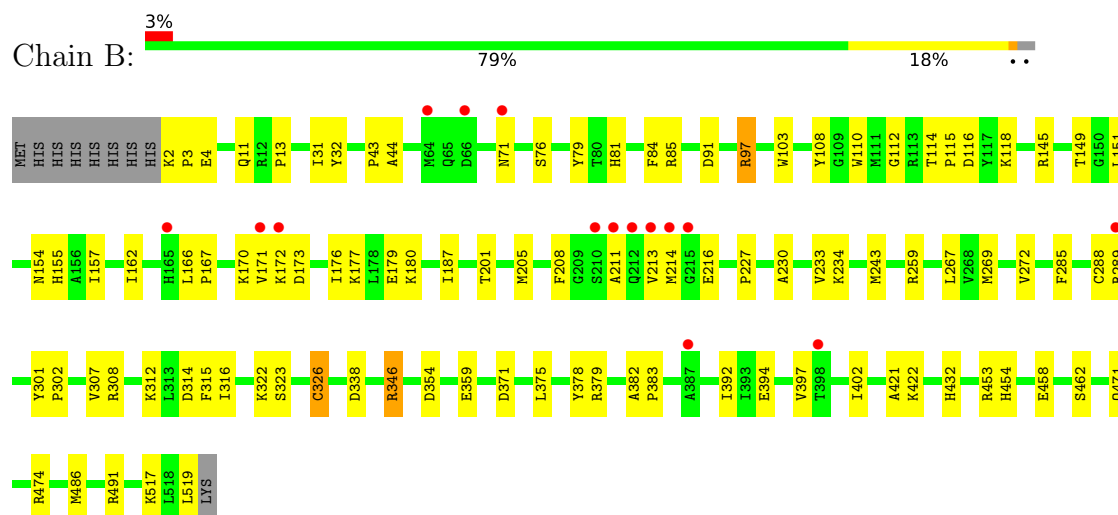
### 3 Residue-property plots

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

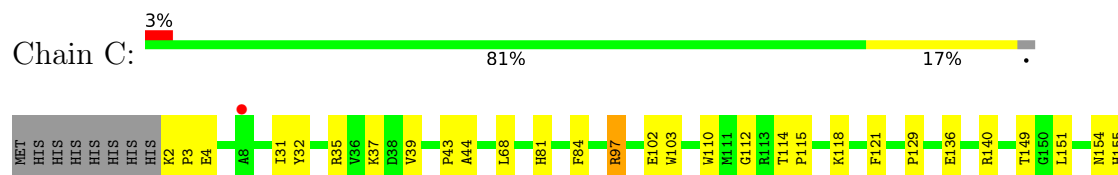
- Molecule 1: 4-hydroxyphenylacetate 3-monooxygenase, oxygenase subunit

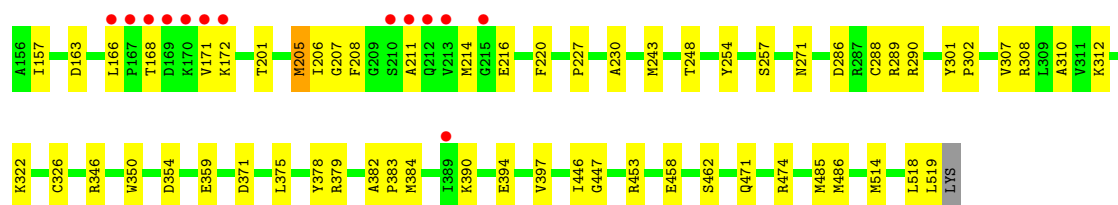


- Molecule 1: 4-hydroxyphenylacetate 3-monooxygenase, oxygenase subunit

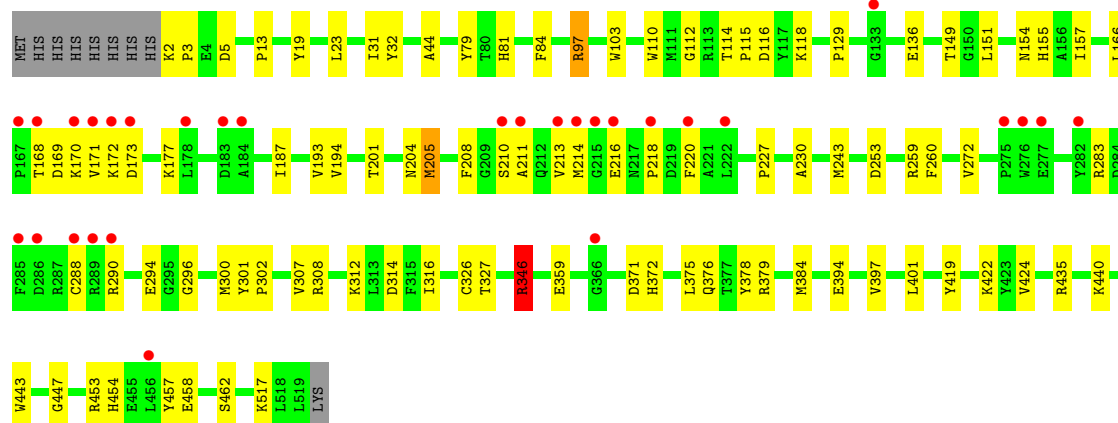
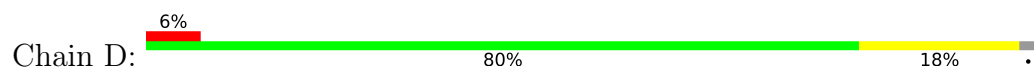


- Molecule 1: 4-hydroxyphenylacetate 3-monooxygenase, oxygenase subunit





● Molecule 1: 4-hydroxyphenylacetate 3-monooxygenase, oxygenase subunit





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	179.41Å 93.73Å 142.34Å 90.00° 108.23° 90.00°	Depositor
Resolution (Å)	46.36 – 2.37 48.71 – 2.37	Depositor EDS
% Data completeness (in resolution range)	99.2 (46.36-2.37) 95.0 (48.71-2.37)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.05 (at 2.37Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, $R_{free}$	0.160 , 0.195 0.161 , 0.196	Depositor DCC
$R_{free}$ test set	4401 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.3	Xtriage
Anisotropy	0.022	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 51.7	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	0.96	EDS
Total number of atoms	17250	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	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: ACT

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	0.41	1/4197 (0.0%)	0.55	0/5692
1	B	0.41	1/4197 (0.0%)	0.54	0/5692
1	C	0.43	1/4197 (0.0%)	0.55	0/5692
1	D	0.39	1/4197 (0.0%)	0.55	2/5692 (0.0%)
All	All	0.41	4/16788 (0.0%)	0.55	2/22768 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	326	CYS	CB-SG	-7.92	1.68	1.82
1	B	326	CYS	CB-SG	-6.91	1.70	1.82
1	A	326	CYS	CB-SG	-6.17	1.71	1.82
1	D	326	CYS	CB-SG	-6.08	1.72	1.82

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	346	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	D	97	ARG	NE-CZ-NH1	-5.22	117.69	120.30

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	4099	0	3958	70	0
1	B	4099	0	3958	79	0
1	C	4099	0	3958	80	0
1	D	4099	0	3958	80	0
2	A	4	3	3	0	0
2	C	8	6	6	0	0
3	A	245	0	0	5	0
3	B	192	0	0	6	0
3	C	218	0	0	11	0
3	D	178	0	0	10	1
All	All	17241	9	15841	288	1

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 (288) 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:C:384:MET:SD	3:C:1003:HOH:O	2.04	1.12
1:A:4:GLU:HG2	1:A:149:THR:HG21	1.42	0.97
1:B:97:ARG:NH2	1:B:354:ASP:OD1	1.98	0.96
1:C:4:GLU:HG2	1:C:149:THR:HG21	1.43	0.96
1:C:97:ARG:NH2	1:C:354:ASP:OD1	2.01	0.93
1:D:166:LEU:HD13	1:D:170:LYS:HD2	1.48	0.93
1:D:308:ARG:NH1	3:D:602:HOH:O	2.04	0.90
1:B:397:VAL:O	3:B:601:HOH:O	1.90	0.88
1:C:271:ASN:HB3	3:C:808:HOH:O	1.74	0.87
1:C:168:THR:HA	1:C:171:VAL:HG22	1.56	0.87
1:A:277:GLU:OE2	3:A:701:HOH:O	1.93	0.86
1:B:112:GLY:HA2	1:B:308:ARG:HD2	1.55	0.86
1:D:2:LYS:N	3:D:603:HOH:O	2.08	0.85
1:B:491:ARG:NH1	3:B:607:HOH:O	2.10	0.83
1:A:172:LYS:HE2	1:A:213:VAL:O	1.79	0.82
1:B:11:GLN:NE2	1:B:76:SER:O	2.12	0.81
1:B:173:ASP:OD2	1:D:422:LYS:NZ	2.13	0.81
1:B:285:PHE:HB3	1:B:289:ARG:NH1	1.96	0.80
1:D:227:PRO:HG2	1:D:230:ALA:HB2	1.62	0.79
1:B:116:ASP:OD2	3:B:603:HOH:O	2.00	0.78
1:B:394:GLU:OE2	3:B:604:HOH:O	2.01	0.78
1:D:116:ASP:OD2	3:D:601:HOH:O	2.01	0.78
1:B:155:HIS:CE1	1:B:157:ILE:HD13	2.20	0.77
1:A:2:LYS:HG3	1:A:3:PRO:HD3	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:286:ASP:OD2	1:C:290:ARG:NH1	2.18	0.77
1:D:172:LYS:HB3	1:D:220:PHE:HZ	1.51	0.76
1:C:112:GLY:HA2	1:C:308:ARG:HD2	1.68	0.76
1:C:227:PRO:HG2	1:C:230:ALA:HB2	1.67	0.75
1:A:112:GLY:HA2	1:A:308:ARG:HD2	1.66	0.75
1:D:308:ARG:NH2	3:D:602:HOH:O	2.19	0.74
1:D:173:ASP:HA	1:D:177:LYS:HE3	1.69	0.74
1:C:308:ARG:NE	3:C:806:HOH:O	2.21	0.74
1:D:112:GLY:HA2	1:D:308:ARG:HD2	1.70	0.73
1:B:4:GLU:OE2	1:B:145:ARG:HD3	1.87	0.72
1:A:210:SER:HA	1:A:214:MET:HE1	1.71	0.72
1:A:2:LYS:HG3	1:A:3:PRO:CD	2.21	0.71
1:C:302:PRO:HB2	1:C:375:LEU:HD22	1.70	0.71
1:A:254:TYR:OH	3:A:703:HOH:O	2.08	0.70
1:C:301:TYR:OH	1:C:379:ARG:NH2	2.20	0.70
1:C:4:GLU:HG2	1:C:149:THR:CG2	2.20	0.70
1:C:155:HIS:CE1	1:C:157:ILE:HD13	2.28	0.69
1:B:302:PRO:HB2	1:B:375:LEU:HD22	1.74	0.69
1:B:422:LYS:NZ	1:D:173:ASP:OD2	2.26	0.69
1:B:149:THR:OG1	1:B:151:LEU:HG	1.93	0.69
1:B:112:GLY:HA2	1:B:308:ARG:CD	2.23	0.68
1:A:118:LYS:HD3	1:A:155:HIS:HB2	1.74	0.68
1:D:308:ARG:NE	3:D:606:HOH:O	2.27	0.67
1:D:172:LYS:HB2	3:D:604:HOH:O	1.94	0.67
1:C:289:ARG:HD3	3:C:812:HOH:O	1.94	0.66
1:C:308:ARG:NH2	1:C:458:GLU:OE2	2.28	0.66
1:D:112:GLY:HA2	1:D:308:ARG:CD	2.25	0.66
1:A:308:ARG:NH2	1:A:458:GLU:OE2	2.28	0.66
1:B:173:ASP:HA	1:B:177:LYS:HE3	1.77	0.66
1:A:302:PRO:HB2	1:A:375:LEU:HD22	1.77	0.66
1:D:210:SER:HA	1:D:214:MET:HE1	1.77	0.66
1:B:402:ILE:CD1	1:D:457:TYR:HD1	2.08	0.65
1:D:97:ARG:HG3	1:D:307:VAL:HG21	1.77	0.65
1:C:471:GLN:OE1	1:C:474:ARG:NH1	2.27	0.65
1:A:168:THR:O	1:A:172:LYS:HG2	1.97	0.65
1:D:308:ARG:CZ	3:D:602:HOH:O	2.40	0.64
1:D:168:THR:HA	1:D:171:VAL:HG22	1.80	0.63
1:C:155:HIS:NE2	1:C:157:ILE:HG21	2.14	0.63
1:C:168:THR:HA	1:C:171:VAL:CG2	2.27	0.63
1:A:118:LYS:NZ	1:A:205:MET:HG2	2.14	0.62
1:A:154:ASN:HB3	1:A:204:ASN:ND2	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:PRO:HG2	1:A:230:ALA:HB2	1.81	0.62
1:A:2:LYS:HA	1:A:5:ASP:OD2	2.00	0.62
1:C:211:ALA:O	1:C:214:MET:HE2	2.00	0.62
1:C:308:ARG:NH1	3:C:807:HOH:O	2.22	0.62
1:D:97:ARG:HG3	1:D:307:VAL:CG2	2.30	0.61
1:A:4:GLU:HG2	1:A:149:THR:CG2	2.25	0.61
1:B:314:ASP:OD1	1:B:346:ARG:NH1	2.33	0.61
1:A:155:HIS:NE2	1:A:157:ILE:HG21	2.16	0.61
1:B:308:ARG:NH2	1:B:458:GLU:OE2	2.33	0.61
1:D:169:ASP:O	3:D:604:HOH:O	2.16	0.61
1:D:172:LYS:HB3	1:D:220:PHE:CZ	2.35	0.61
1:C:205:MET:HE3	1:C:206:ILE:C	2.21	0.60
1:A:154:ASN:HB3	1:A:204:ASN:HD21	1.67	0.60
1:A:2:LYS:N	1:A:3:PRO:HD2	2.16	0.60
1:C:166:LEU:HB2	1:C:171:VAL:HG12	1.83	0.60
1:A:112:GLY:HA2	1:A:308:ARG:CD	2.32	0.60
1:C:112:GLY:HA2	1:C:308:ARG:CD	2.31	0.60
1:B:155:HIS:NE2	1:B:157:ILE:HG21	2.17	0.59
1:D:302:PRO:HB2	1:D:375:LEU:HD22	1.85	0.59
1:D:110:TRP:CE3	1:D:312:LYS:HE2	2.37	0.59
1:A:518:LEU:HG	1:C:514:MET:HE3	1.84	0.58
1:A:211:ALA:H	1:A:214:MET:CE	2.17	0.58
1:D:314:ASP:OD1	1:D:346:ARG:NE	2.34	0.58
1:A:110:TRP:CE3	1:A:312:LYS:HE2	2.40	0.57
1:C:205:MET:HE3	1:C:207:GLY:N	2.18	0.57
1:D:2:LYS:N	1:D:3:PRO:HD2	2.18	0.57
1:A:514:MET:HE3	1:C:518:LEU:HG	1.86	0.57
1:A:118:LYS:HZ1	1:A:205:MET:HG2	1.71	0.56
1:A:31:ILE:HG12	1:A:32:TYR:CD2	2.41	0.56
1:A:172:LYS:CE	1:A:213:VAL:HG12	2.36	0.56
1:D:211:ALA:H	1:D:214:MET:CE	2.18	0.56
1:B:227:PRO:HG2	1:B:230:ALA:HB2	1.87	0.55
1:B:91:ASP:OD2	3:B:608:HOH:O	2.17	0.55
1:B:211:ALA:O	1:B:214:MET:HE2	2.06	0.55
1:A:44:ALA:HB2	1:A:243:MET:HE3	1.88	0.55
1:C:205:MET:HE1	1:C:207:GLY:HA3	1.89	0.55
1:A:155:HIS:CE1	1:A:157:ILE:HD13	2.43	0.54
1:D:129:PRO:HB2	1:D:136:GLU:HG3	1.88	0.54
1:B:471:GLN:OE1	1:B:474:ARG:NH1	2.37	0.54
1:B:211:ALA:H	1:B:214:MET:CE	2.20	0.54
1:B:233:VAL:HG13	1:B:267:LEU:HD11	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:PRO:HB2	1:B:243:MET:HG3	1.89	0.54
1:D:118:LYS:HD3	1:D:155:HIS:HB2	1.89	0.53
1:D:2:LYS:HA	1:D:5:ASP:OD2	2.08	0.53
1:B:162:ILE:HB	1:B:171:VAL:HG13	1.90	0.53
1:A:97:ARG:HG3	1:A:307:VAL:CG2	2.39	0.53
1:C:248:THR:OG1	3:C:801:HOH:O	1.98	0.53
1:B:166:LEU:HB2	1:B:171:VAL:CG2	2.39	0.53
1:A:243:MET:HE1	1:B:519:LEU:HD21	1.91	0.52
1:C:397:VAL:O	3:C:804:HOH:O	2.19	0.52
1:A:519:LEU:C	3:A:707:HOH:O	2.47	0.52
1:B:2:LYS:N	1:B:3:PRO:HD2	2.24	0.52
1:A:498:GLN:HG2	3:A:714:HOH:O	2.08	0.52
1:D:453:ARG:HG2	1:D:453:ARG:O	2.10	0.52
1:D:359:GLU:HB2	1:D:371:ASP:HB2	1.92	0.52
1:C:110:TRP:CE3	1:C:312:LYS:HE2	2.45	0.51
1:D:443:TRP:CZ3	1:D:447:GLY:HA3	2.46	0.51
1:D:168:THR:O	1:D:171:VAL:HG22	2.10	0.51
1:C:308:ARG:CZ	3:C:806:HOH:O	2.59	0.51
1:D:296:GLY:O	1:D:300:MET:HG3	2.11	0.51
1:D:81:HIS:HB3	1:D:84:PHE:CD1	2.46	0.51
1:D:149:THR:OG1	1:D:151:LEU:HG	2.11	0.50
1:B:285:PHE:HB3	1:B:289:ARG:HH12	1.75	0.50
1:D:301:TYR:N	1:D:302:PRO:CD	2.74	0.50
1:C:68:LEU:HD21	1:C:102:GLU:HB3	1.93	0.50
1:C:118:LYS:HD3	1:C:155:HIS:HB2	1.92	0.50
1:A:11:GLN:NE2	1:A:76:SER:O	2.45	0.50
1:C:136:GLU:OE2	1:C:140:ARG:NH2	2.39	0.50
1:D:211:ALA:H	1:D:214:MET:HE2	1.76	0.50
1:C:379:ARG:HH11	1:C:462:SER:CB	2.25	0.49
1:B:259:ARG:NH1	3:B:602:HOH:O	1.99	0.49
1:B:13:PRO:HD3	1:B:79:TYR:O	2.12	0.49
1:D:154:ASN:HB2	1:D:201:THR:HG21	1.94	0.49
1:B:155:HIS:NE2	1:B:157:ILE:CG2	2.75	0.49
1:C:359:GLU:HB2	1:C:371:ASP:HB2	1.95	0.49
1:A:173:ASP:HA	1:A:177:LYS:HE3	1.95	0.49
1:D:327:THR:HA	3:D:621:HOH:O	2.13	0.49
1:B:208:PHE:CD2	1:B:288:CYS:HB3	2.48	0.49
1:B:4:GLU:OE1	1:B:4:GLU:N	2.35	0.48
1:C:155:HIS:NE2	1:C:157:ILE:CG2	2.75	0.48
1:C:379:ARG:NH1	1:C:462:SER:OG	2.41	0.48
1:A:155:HIS:NE2	1:A:157:ILE:CG2	2.76	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:ARG:NH2	1:A:98:ASP:OD1	2.35	0.48
1:B:172:LYS:HD3	1:B:213:VAL:O	2.14	0.48
1:B:31:ILE:HG12	1:B:32:TYR:CD2	2.48	0.48
1:C:43:PRO:HB2	1:C:243:MET:HG3	1.95	0.48
1:B:110:TRP:CZ2	1:B:316:ILE:HD11	2.48	0.48
1:B:97:ARG:HG2	1:B:307:VAL:HG21	1.96	0.48
1:D:173:ASP:HA	1:D:177:LYS:CE	2.41	0.48
1:B:155:HIS:CD2	1:B:205:MET:HE3	2.49	0.48
1:D:166:LEU:HD13	1:D:170:LYS:CD	2.34	0.48
1:C:286:ASP:CG	1:C:290:ARG:HH11	2.17	0.48
1:A:19:TYR:CZ	1:A:23:LEU:HD11	2.49	0.47
1:B:71:ASN:O	1:B:85:ARG:NH1	2.43	0.47
1:B:234:LYS:NZ	1:D:419:TYR:OH	2.27	0.47
1:B:166:LEU:HB2	1:B:171:VAL:HG22	1.97	0.47
1:B:486:MET:SD	1:C:322:LYS:HE2	2.55	0.47
1:C:301:TYR:N	1:C:302:PRO:CD	2.78	0.47
1:A:425:ARG:O	1:A:435:ARG:HD2	2.14	0.47
1:A:359:GLU:HB2	1:A:371:ASP:HB2	1.96	0.47
1:D:208:PHE:CD2	1:D:288:CYS:HB3	2.50	0.47
1:C:446:ILE:HG13	1:C:447:GLY:N	2.28	0.47
1:D:110:TRP:O	1:D:454:HIS:HE1	1.99	0.47
1:B:402:ILE:HD13	1:D:457:TYR:HD1	1.80	0.47
1:C:97:ARG:HG2	1:C:307:VAL:HG21	1.96	0.46
1:D:97:ARG:CG	1:D:307:VAL:HG21	2.46	0.46
1:B:154:ASN:HB2	1:B:201:THR:HG21	1.97	0.46
1:B:301:TYR:N	1:B:302:PRO:CD	2.79	0.46
1:D:31:ILE:HG12	1:D:32:TYR:CD2	2.49	0.46
1:C:154:ASN:HB2	1:C:201:THR:HG21	1.98	0.46
1:A:345:TRP:CZ2	1:D:384:MET:HE1	2.51	0.46
1:A:518:LEU:HG	1:C:514:MET:CE	2.46	0.46
1:C:301:TYR:CZ	1:C:379:ARG:NH2	2.84	0.46
1:C:39:VAL:HG22	3:C:918:HOH:O	2.14	0.46
1:B:359:GLU:HB2	1:B:371:ASP:HB2	1.98	0.46
1:C:382:ALA:HB3	1:C:383:PRO:HD3	1.97	0.46
1:A:518:LEU:CD2	1:C:514:MET:HE2	2.46	0.46
1:A:97:ARG:HG3	1:A:307:VAL:HG21	1.97	0.46
1:C:166:LEU:HB2	1:C:171:VAL:CG1	2.45	0.46
1:C:44:ALA:HB2	1:C:243:MET:HE3	1.96	0.46
1:C:37:LYS:HA	1:C:37:LYS:HD3	1.51	0.45
1:C:81:HIS:HB3	1:C:84:PHE:CD1	2.51	0.45
1:A:319:LEU:HD21	1:A:442:MET:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:453:ARG:O	1:A:453:ARG:HG2	2.15	0.45
1:D:394:GLU:OE2	3:D:605:HOH:O	2.20	0.45
1:A:154:ASN:HB2	1:A:201:THR:HG21	1.99	0.45
1:D:173:ASP:CA	1:D:177:LYS:HE3	2.44	0.45
1:D:312:LYS:O	1:D:316:ILE:HG12	2.17	0.45
1:A:155:HIS:CD2	1:A:157:ILE:HG23	2.52	0.45
1:B:118:LYS:HD3	1:B:155:HIS:HB2	1.98	0.45
1:C:35:ARG:HD2	3:C:859:HOH:O	2.16	0.45
1:D:193:VAL:HG23	1:D:194:VAL:HG23	1.98	0.45
1:D:397:VAL:HG11	1:D:401:LEU:HG	1.99	0.45
1:B:176:ILE:CD1	1:B:269:MET:HG3	2.46	0.45
1:C:205:MET:HE2	1:C:205:MET:O	2.16	0.45
1:D:114:THR:HB	1:D:115:PRO:CD	2.46	0.45
1:C:155:HIS:CD2	1:C:157:ILE:HG23	2.52	0.45
1:D:13:PRO:HD3	1:D:79:TYR:O	2.17	0.45
1:D:44:ALA:HB2	1:D:243:MET:HE3	1.98	0.45
1:D:114:THR:HB	1:D:115:PRO:HD2	2.00	0.44
1:B:176:ILE:HD11	1:B:269:MET:HG3	1.98	0.44
1:C:31:ILE:HG12	1:C:32:TYR:CD2	2.52	0.44
1:C:519:LEU:HD21	1:D:243:MET:HE1	1.99	0.44
1:A:253:ASP:HA	1:A:440:LYS:HD3	2.00	0.44
1:B:167:PRO:HB2	1:B:170:LYS:HG2	2.00	0.44
1:B:322:LYS:HE2	1:C:486:MET:SD	2.57	0.44
1:C:172:LYS:HB3	1:C:220:PHE:HZ	1.83	0.44
1:A:211:ALA:O	1:A:214:MET:HE2	2.18	0.44
1:A:285:PHE:HB3	1:A:289:ARG:NH1	2.33	0.44
1:C:254:TYR:HB3	1:C:257:SER:HB2	2.00	0.44
1:B:382:ALA:HB3	1:B:383:PRO:HD3	2.00	0.44
1:B:421:ALA:HA	1:B:432:HIS:CG	2.53	0.44
1:C:149:THR:OG1	1:C:151:LEU:HG	2.18	0.44
1:D:155:HIS:NE2	1:D:157:ILE:CG2	2.81	0.44
1:A:519:LEU:HD21	1:B:243:MET:HE1	2.00	0.43
1:B:346:ARG:HD2	1:C:485:MET:SD	2.58	0.43
1:C:168:THR:CA	1:C:171:VAL:HG22	2.37	0.43
1:C:453:ARG:HG2	1:C:453:ARG:O	2.18	0.43
1:A:205:MET:O	1:A:205:MET:HG3	2.18	0.43
1:A:382:ALA:HB3	1:A:383:PRO:HD3	2.01	0.43
1:D:19:TYR:CZ	1:D:23:LEU:HD11	2.54	0.43
1:D:308:ARG:NH2	1:D:458:GLU:OE2	2.52	0.43
1:B:81:HIS:HB3	1:B:84:PHE:CD1	2.54	0.43
1:C:172:LYS:HB3	1:C:220:PHE:CZ	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:187:ILE:HA	1:D:272:VAL:O	2.18	0.43
1:A:301:TYR:N	1:A:302:PRO:CD	2.81	0.43
1:D:155:HIS:NE2	1:D:157:ILE:HG23	2.34	0.43
1:A:149:THR:OG1	1:A:151:LEU:HG	2.18	0.43
1:D:116:ASP:OD1	1:D:116:ASP:N	2.52	0.43
1:A:345:TRP:HZ2	1:D:384:MET:HE1	1.83	0.43
1:C:390:LYS:O	1:C:394:GLU:HG3	2.18	0.43
1:D:110:TRP:CZ3	1:D:312:LYS:HE2	2.54	0.43
1:B:110:TRP:CE3	1:B:312:LYS:HE2	2.54	0.42
1:C:114:THR:HB	1:C:115:PRO:CD	2.49	0.42
1:D:424:VAL:HG12	1:D:435:ARG:HD3	2.01	0.42
1:A:277:GLU:H	1:A:277:GLU:CD	2.22	0.42
1:B:110:TRP:O	1:B:454:HIS:HE1	2.01	0.42
1:B:187:ILE:HA	1:B:272:VAL:O	2.19	0.42
1:D:205:MET:HG3	1:D:205:MET:O	2.18	0.42
1:B:323:SER:O	1:B:326:CYS:HB2	2.20	0.42
1:C:121:PHE:CZ	1:C:205:MET:HG3	2.55	0.42
1:A:13:PRO:HD3	1:A:79:TYR:O	2.19	0.42
1:D:259:ARG:HD2	1:D:260:PHE:CZ	2.55	0.42
1:C:205:MET:CE	1:C:207:GLY:CA	2.98	0.42
1:C:205:MET:CE	1:C:207:GLY:N	2.83	0.42
1:C:2:LYS:N	1:C:3:PRO:HD2	2.35	0.42
1:A:384:MET:HB3	1:A:384:MET:HE3	1.87	0.42
1:B:155:HIS:CD2	1:B:157:ILE:HG23	2.55	0.42
1:B:379:ARG:HH11	1:B:462:SER:CB	2.32	0.42
1:B:338:ASP:HB3	1:B:392:ILE:HG23	2.01	0.42
1:D:253:ASP:HA	1:D:440:LYS:HD3	2.02	0.42
1:C:310:ALA:HB1	1:C:350:TRP:CE2	2.55	0.41
1:A:179:GLU:OE2	1:A:189:SER:HB2	2.19	0.41
1:B:211:ALA:H	1:B:214:MET:HE2	1.84	0.41
1:B:402:ILE:HD11	1:D:457:TYR:HD1	1.84	0.41
1:C:271:ASN:ND2	3:C:808:HOH:O	2.26	0.41
1:A:446:ILE:HG13	1:A:447:GLY:N	2.34	0.41
1:D:372:HIS:CD2	1:D:376:GLN:HE21	2.39	0.41
1:C:129:PRO:HB2	1:C:136:GLU:HG3	2.03	0.41
1:B:162:ILE:HB	1:B:171:VAL:CG1	2.51	0.41
1:B:114:THR:HB	1:B:115:PRO:CD	2.51	0.41
1:D:379:ARG:HH11	1:D:462:SER:CB	2.33	0.41
1:D:97:ARG:HG2	1:D:97:ARG:O	2.21	0.41
1:A:254:TYR:HB3	1:A:257:SER:HB2	2.02	0.41
1:C:208:PHE:CD2	1:C:288:CYS:HB3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:429:GLY:HA2	1:C:163:ASP:OD2	2.20	0.41
1:B:453:ARG:O	1:B:453:ARG:HG2	2.20	0.41
1:C:110:TRP:CZ3	1:C:312:LYS:HE2	2.56	0.41
1:D:2:LYS:N	1:D:3:PRO:CD	2.84	0.41
1:A:118:LYS:HZ3	1:A:205:MET:HG2	1.86	0.40
1:A:346:ARG:HD3	1:A:346:ARG:C	2.41	0.40
1:A:290:ARG:NH2	3:A:710:HOH:O	2.40	0.40
1:B:517:LYS:HE2	1:D:517:LYS:HE2	2.03	0.40
1:B:112:GLY:CA	1:B:308:ARG:HD2	2.38	0.40
1:A:243:MET:CE	1:B:519:LEU:HD21	2.52	0.40
1:C:114:THR:HB	1:C:115:PRO:HD2	2.04	0.40
1:D:218:PRO:HB2	1:D:283:ARG:HB3	2.02	0.40
1:A:110:TRP:CZ2	1:A:316:ILE:HD11	2.57	0.40
1:B:170:LYS:N	1:B:170:LYS:HD3	2.36	0.40
1:B:44:ALA:HB2	1:B:243:MET:HE3	2.02	0.40
1:B:179:GLU:O	1:B:180:LYS:HG2	2.21	0.40
1:B:108:TYR:HB3	1:B:315:PHE:CD1	2.56	0.40
1:D:290:ARG:NH2	1:D:294:GLU:OE1	2.53	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:717:HOH:O	3:D:737:HOH:O[3_555]	2.14	0.06

## 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	516/527 (98%)	503 (98%)	12 (2%)	1 (0%)	49 64
1	B	516/527 (98%)	500 (97%)	15 (3%)	1 (0%)	49 64

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	516/527 (98%)	502 (97%)	13 (2%)	1 (0%)	49 64
1	D	516/527 (98%)	502 (97%)	13 (2%)	1 (0%)	49 64
All	All	2064/2108 (98%)	2007 (97%)	53 (3%)	4 (0%)	49 64

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	216	GLU
1	C	216	GLU
1	A	216	GLU
1	D	216	GLU

### 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	428/443 (97%)	422 (99%)	6 (1%)	69 83
1	B	428/443 (97%)	424 (99%)	4 (1%)	81 90
1	C	428/443 (97%)	423 (99%)	5 (1%)	74 86
1	D	428/443 (97%)	422 (99%)	6 (1%)	69 83
All	All	1712/1772 (97%)	1691 (99%)	21 (1%)	74 86

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LYS
1	A	103	TRP
1	A	205	MET
1	A	277	GLU
1	A	346	ARG
1	A	378	TYR
1	B	97	ARG
1	B	103	TRP

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Mol	Chain	Res	Type
1	B	346	ARG
1	B	378	TYR
1	C	97	ARG
1	C	103	TRP
1	C	205	MET
1	C	346	ARG
1	C	378	TYR
1	D	103	TRP
1	D	204	ASN
1	D	205	MET
1	D	213	VAL
1	D	346	ARG
1	D	378	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	204	ASN
1	C	155	HIS

### 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](#)

3 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	ACT	A	601	-	1,3,3	2.18	1 (100%)	0,3,3	0.00	-
2	ACT	C	701	-	1,3,3	1.47	0	0,3,3	0.00	-
2	ACT	C	702	-	1,3,3	2.14	1 (100%)	0,3,3	0.00	-

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	ACT	A	601	-	-	0/0/0/0	0/0/0/0
2	ACT	C	701	-	-	0/0/0/0	0/0/0/0
2	ACT	C	702	-	-	0/0/0/0	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	702	ACT	CH3-C	2.14	1.51	1.48
2	A	601	ACT	CH3-C	2.18	1.51	1.48

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 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	518/527 (98%)	-0.00	16 (3%) 49 51	26, 31, 49, 83	0
1	B	518/527 (98%)	-0.04	15 (2%) 51 53	27, 33, 55, 95	0
1	C	518/527 (98%)	-0.07	14 (2%) 54 56	25, 31, 49, 106	0
1	D	518/527 (98%)	0.11	30 (5%) 23 25	26, 37, 58, 98	0
All	All	2072/2108 (98%)	-0.00	75 (3%) 42 45	25, 33, 54, 106	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	171	VAL	10.1
1	A	213	VAL	6.1
1	B	213	VAL	5.9
1	C	213	VAL	5.7
1	C	167	PRO	5.0
1	B	215	GLY	4.5
1	C	169	ASP	4.3
1	D	215	GLY	4.3
1	A	171	VAL	4.1
1	C	168	THR	4.0
1	A	168	THR	4.0
1	D	211	ALA	3.8
1	D	213	VAL	3.8
1	D	170	LYS	3.5
1	C	210	SER	3.5
1	D	214	MET	3.4
1	B	171	VAL	3.4
1	D	171	VAL	3.4
1	D	285	PHE	3.4
1	B	210	SER	3.3
1	D	276	TRP	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	214	MET	3.2
1	D	277	GLU	3.2
1	D	172	LYS	3.1
1	C	215	GLY	3.1
1	B	212	GLN	3.0
1	D	178	LEU	3.0
1	A	6	PHE	3.0
1	D	133	GLY	3.0
1	D	290	ARG	3.0
1	D	210	SER	3.0
1	A	215	GLY	2.9
1	D	183	ASP	2.8
1	A	214	MET	2.8
1	D	282	TYR	2.7
1	D	184	ALA	2.7
1	C	166	LEU	2.7
1	D	216	GLU	2.7
1	A	216	GLU	2.7
1	D	289	ARG	2.6
1	B	172	LYS	2.6
1	C	172	LYS	2.6
1	A	172	LYS	2.6
1	D	288	CYS	2.6
1	B	165	HIS	2.6
1	A	286	ASP	2.5
1	C	170	LYS	2.5
1	C	8	ALA	2.5
1	D	167	PRO	2.5
1	D	173	ASP	2.4
1	B	289	ARG	2.4
1	D	275	PRO	2.3
1	A	285	PHE	2.3
1	B	211	ALA	2.3
1	B	387	ALA	2.3
1	A	166	LEU	2.3
1	C	211	ALA	2.3
1	B	398	THR	2.3
1	B	66	ASP	2.2
1	C	389	ILE	2.2
1	D	222	LEU	2.2
1	B	64	MET	2.2
1	A	169	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	220	PHE	2.2
1	D	456	LEU	2.2
1	D	366	GLY	2.2
1	D	218	PRO	2.2
1	C	212	GLN	2.1
1	B	71	ASN	2.1
1	A	167	PRO	2.1
1	D	286	ASP	2.1
1	A	459	ILE	2.1
1	A	289	ARG	2.0
1	D	168	THR	2.0
1	A	518	LEU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no 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	ACT	C	702	4/4	0.61	0.45	39,51,54,62	0
2	ACT	A	601	4/4	0.70	0.34	42,47,51,51	0
2	ACT	C	701	4/4	0.90	0.31	50,51,63,63	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.