WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Oct 8, 2023 – 10:08 AM 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 ESCHERICHIA 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

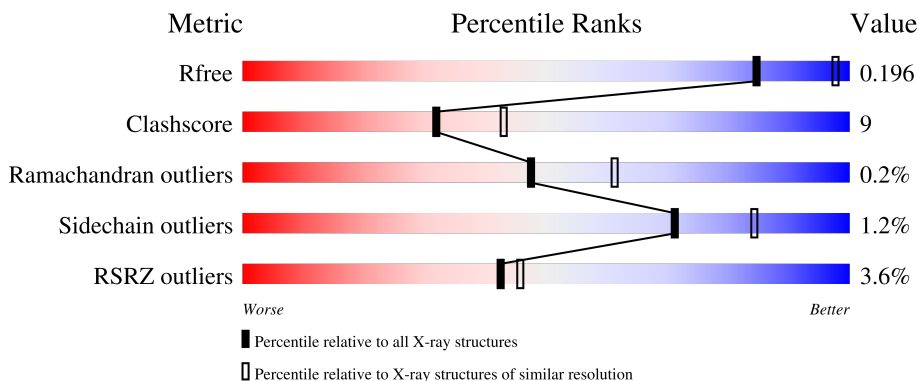|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 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}	130704	5509 (2.40-2.36)
Clashscore	141614	6082 (2.40-2.36)
Ramachandran outliers	138981	5973 (2.40-2.36)
Sidechain outliers	138945	5975 (2.40-2.36)
RSRZ outliers	127900	5397 (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 of the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	3%; 83% 14% ..
1	B	527	3%; 79% 18% ..
1	C	527	3%; 81% 17% .
1	D	527	6%; 80% 18% .

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 (i)

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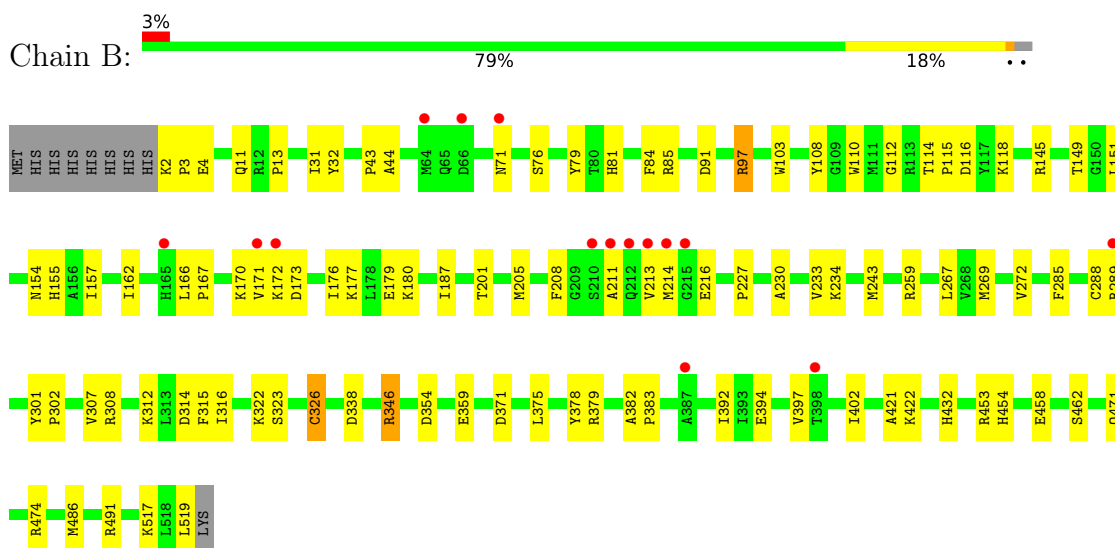| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	192	Total 192	O 192	0	0
3	C	218	Total 218	O 218	0	0
3	D	178	Total 178	O 178	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, 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.

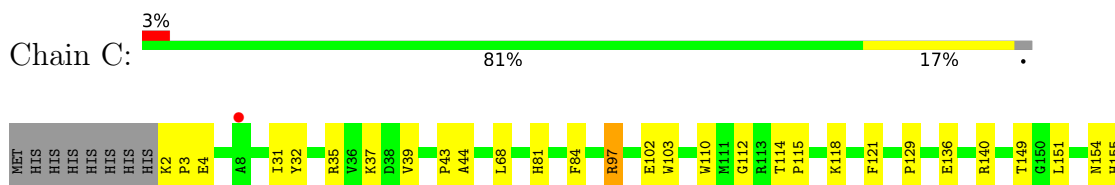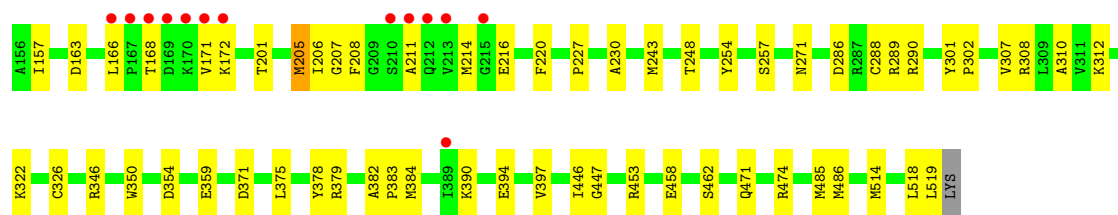- Molecule 1: 4-hydroxyphenylacetate 3-monooxygenase, oxygenase subunit

Chain A:

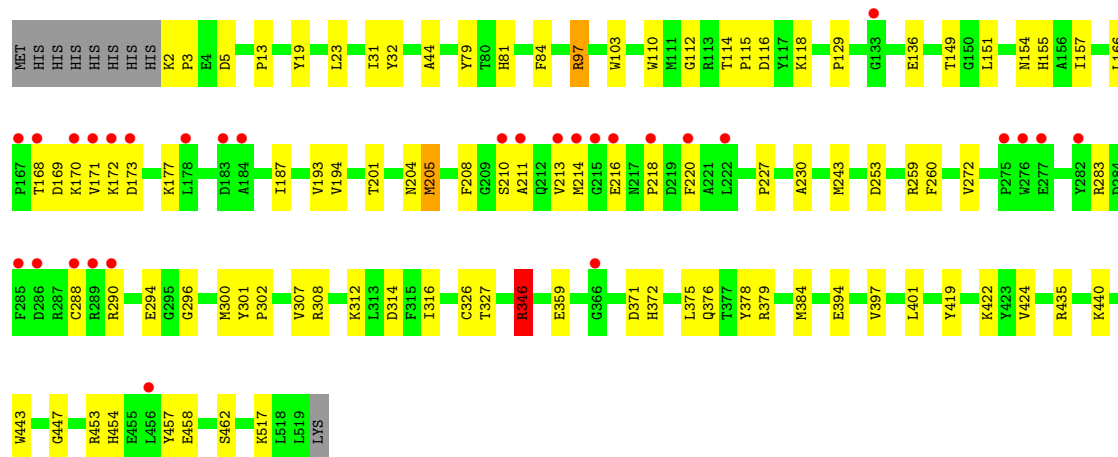- Molecule 1: 4-hydroxyphenylacetate 3-monooxygenase, oxygenase subunit

Chain B:

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

Chain C:

A156 I157 D163 L166 P167 T168 D169 K170 V171 K172 T201 M205 I206 G207 F208 G209 S210 A211 Q212 V213 M214 G215 E216 F220 P227 A230 M243 T248 Y254 S257 N271 D286 R287 C288 R289 R290 Y301 P302 V307 R308 L309 A310 V311 K312

K322 C326 R346 W350 D354 E359 D371 L375 Y378 R379 A382 P383 M384 I389 K390 E394 V397 I446 G447 R453 E458 S462 Q471 R474 M485 M486 M514 L518 L519 LYS

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

Chain D:

6%

80%   18%   •

MET HIS HIS HIS HIS HIS HIS K2 P3 E4 D5 P13 Y19 L23 I31 Y32 A44 Y79 T80 H81 F84 R97 W103 W110 M111 G112 R113 T114 P115 D116 Y117 K118 P129 G133 E136 T149 G150 L151 N154 H155 A156 I157 L166

P167 T168 D169 K170 V171 K172 D173 K177 L178 D183 A184 I187 V193 V194 T201 N204 M205 F208 G209 S210 A211 Q212 V213 M214 G215 E216 N217 P218 D219 F220 A221 L222 P227 A230 M243 D253 R259 F260 V272 P275 W276 E277 Y282 R283 D284

F285 D286 R287 C288 R289 R290 E294 G295 G296 M300 Y301 P302 V307 R308 K312 L313 D314 F315 I316 C326 T327 R346 E359 G366 D371 H372 L375 Q376 T377 Y378 R379 M384 E394 V397 L401 V419 K422 Y423 V424 R435 K440

W443 G447 R453 H454 E455 L456 Y457 E458 S462 K517 L518 L519 LYS

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	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
$< I/\sigma(I) >$ [1]	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^2)	33.3	Xtriage
Anisotropy	0.022	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 51.7	EDS
L-test for twinning [2]	$< |L| > = 0.49, < L^2 > = 0.32$	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^2)	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.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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(^{o})	Ideal(^{o})
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 ⓘ

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.

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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:4:GLU:HG2	1:C:149:THR:CG2	2.20	0.70
1:C:301:TYR:OH	1:C:379:ARG:NH2	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:2:LYS:N	1:A:3:PRO:HD2	2.16	0.60
1:A:154:ASN:HB3	1:A:204:ASN:HD21	1.67	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:43:PRO:HB2	1:B:243:MET:HG3	1.89	0.54
1:B:211:ALA:H	1:B:214:MET:CE	2.20	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:233:VAL:HG13	1:B:267:LEU:HD11	1.89	0.54
1:D:2:LYS:HA	1:D:5:ASP:OD2	2.08	0.53
1:D:118:LYS:HD3	1:D:155:HIS:HB2	1.89	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:13:PRO:HD3	1:B:79:TYR:O	2.12	0.49
1:B:259:ARG:NH1	3:B:602:HOH:O	1.99	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:31:ILE:HG12	1:B:32:TYR:CD2	2.48	0.48
1:B:172:LYS:HD3	1:B:213:VAL:O	2.14	0.48
1:C:43:PRO:HB2	1:C:243:MET:HG3	1.95	0.48
1:B:97:ARG:HG2	1:B:307:VAL:HG21	1.96	0.48
1:B:110:TRP:CZ2	1:B:316:ILE:HD11	2.48	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:B:402:ILE:HD13	1:D:457:TYR:HD1	1.80	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: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:39:VAL:HG22	3:C:918:HOH:O	2.14	0.46
1:C:301:TYR:CZ	1:C:379:ARG:NH2	2.84	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:97:ARG:HG3	1:A:307:VAL:HG21	1.97	0.46
1:A:518:LEU:CD2	1:C:514:MET:HE2	2.46	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:HD3	1:C:37:LYS:HA	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:O	1:C:453:ARG:HG2	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:CD	1:A:277:GLU:H	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:O	1:D:205:MET:HG3	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:2:LYS:N	1:C:3:PRO:HD2	2.35	0.42
1:C:205:MET:CE	1:C:207:GLY:N	2.83	0.42
1:A:384:MET:HE3	1:A:384:MET:HB3	1.87	0.42
1:B:155:HIS:CD2	1:B:157:ILE:HG23	2.55	0.42
1:B:338:ASP:HB3	1:B:392:ILE:HG23	2.01	0.42
1:B:379:ARG:HH11	1:B:462:SER:CB	2.32	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:97:ARG:O	1:D:97:ARG:HG2	2.21	0.41
1:D:379:ARG:HH11	1:D:462:SER:CB	2.33	0.41
1:A:254:TYR:HB3	1:A:257:SER:HB2	2.02	0.41
1:A:429:GLY:HA2	1:C:163:ASP:OD2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:208:PHE:CD2	1:C:288:CYS:HB3	2.55	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:A:243:MET:CE	1:B:519:LEU:HD21	2.52	0.40
1:B:112:GLY:CA	1:B:308:ARG:HD2	2.38	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:44:ALA:HB2	1:B:243:MET:HE3	2.02	0.40
1:B:170:LYS:N	1:B:170:LYS:HD3	2.36	0.40
1:B:108:TYR:HB3	1:B:315:PHE:CD1	2.56	0.40
1:B:179:GLU:O	1:B:180:LYS:HG2	2.21	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%)	47	61
1	B	516/527 (98%)	500 (97%)	15 (3%)	1 (0%)	47	61

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	516/527 (98%)	502 (97%)	13 (2%)	1 (0%)	47	61
1	D	516/527 (98%)	502 (97%)	13 (2%)	1 (0%)	47	61
All	All	2064/2108 (98%)	2007 (97%)	53 (3%)	4 (0%)	47	61

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%)	67	81
1	B	428/443 (97%)	424 (99%)	4 (1%)	78	89
1	C	428/443 (97%)	423 (99%)	5 (1%)	71	84
1	D	428/443 (97%)	422 (99%)	6 (1%)	67	81
All	All	1712/1772 (97%)	1691 (99%)	21 (1%)	71	84

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

Sometimes 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 ⓘ

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 monosaccharides in this entry.

5.6   Ligand geometry ⓘ

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	-	3,3,3	0.71	0	3,3,3	1.43	0
2	ACT	C	702	-	3,3,3	0.80	0	3,3,3	1.60	1 (33%)
2	ACT	C	701	-	3,3,3	0.79	0	3,3,3	1.50	0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	702	ACT	OXT-C-O	-2.18	114.03	122.05

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	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	46	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 ⓘ

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^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 ⓘ

There are no such residues in this entry.