



# Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 08:29 PM GMT

PDB ID : 3UXK  
Title : P. putida mandelate racemase co-crystallized with the intermediate analogue  
benzohydroxamate  
Authors : Lietzan, A.D.; Pellmann, E.; St Maurice, M.  
Deposited on : 2011-12-05  
Resolution : 2.20 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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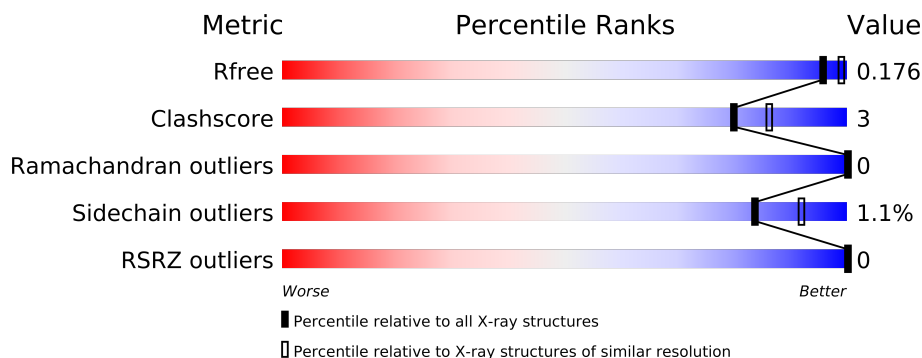
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	2938 (2.20-2.20)
Clashscore	79885	3751 (2.20-2.20)
Ramachandran outliers	78287	3681 (2.20-2.20)
Sidechain outliers	78261	3682 (2.20-2.20)
RSRZ outliers	66119	2939 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	383	
1	B	383	
1	C	383	
1	D	383	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	MG	A	360	-	X
2	MG	C	360	-	X
2	MG	D	360	-	X
3	BHO	A	361	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
3	BHO	B	361	-	X
3	BHO	C	361	-	X
3	BHO	D	361	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11566 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Mandelate racemase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	357	Total	C	N	O	S	4	2	0
			2694	1725	459	496	14			
1	B	357	Total	C	N	O	S	16	1	0
			2693	1724	461	495	13			
1	C	357	Total	C	N	O	S	9	1	0
			2690	1723	457	497	13			
1	D	357	Total	C	N	O	S	9	1	0
			2696	1726	461	496	13			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-23	MET	-	EXPRESSION TAG	UNP P11444
A	-22	ALA	-	EXPRESSION TAG	UNP P11444
A	-21	SER	-	EXPRESSION TAG	UNP P11444
A	-20	TRP	-	EXPRESSION TAG	UNP P11444
A	-19	SER	-	EXPRESSION TAG	UNP P11444
A	-18	HIS	-	EXPRESSION TAG	UNP P11444
A	-17	PRO	-	EXPRESSION TAG	UNP P11444
A	-16	GLN	-	EXPRESSION TAG	UNP P11444
A	-15	PHE	-	EXPRESSION TAG	UNP P11444
A	-14	GLU	-	EXPRESSION TAG	UNP P11444
A	-13	LYS	-	EXPRESSION TAG	UNP P11444
A	-12	GLY	-	EXPRESSION TAG	UNP P11444
A	-11	ALA	-	EXPRESSION TAG	UNP P11444
A	-10	LEU	-	EXPRESSION TAG	UNP P11444
A	-9	GLU	-	EXPRESSION TAG	UNP P11444
A	-8	VAL	-	EXPRESSION TAG	UNP P11444
A	-7	LEU	-	EXPRESSION TAG	UNP P11444
A	-6	PHE	-	EXPRESSION TAG	UNP P11444
A	-5	GLN	-	EXPRESSION TAG	UNP P11444
A	-4	GLY	-	EXPRESSION TAG	UNP P11444
A	-3	PRO	-	EXPRESSION TAG	UNP P11444

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	EXPRESSION TAG	UNP P11444
A	-1	TYR	-	EXPRESSION TAG	UNP P11444
A	0	HIS	-	EXPRESSION TAG	UNP P11444
B	-23	MET	-	EXPRESSION TAG	UNP P11444
B	-22	ALA	-	EXPRESSION TAG	UNP P11444
B	-21	SER	-	EXPRESSION TAG	UNP P11444
B	-20	TRP	-	EXPRESSION TAG	UNP P11444
B	-19	SER	-	EXPRESSION TAG	UNP P11444
B	-18	HIS	-	EXPRESSION TAG	UNP P11444
B	-17	PRO	-	EXPRESSION TAG	UNP P11444
B	-16	GLN	-	EXPRESSION TAG	UNP P11444
B	-15	PHE	-	EXPRESSION TAG	UNP P11444
B	-14	GLU	-	EXPRESSION TAG	UNP P11444
B	-13	LYS	-	EXPRESSION TAG	UNP P11444
B	-12	GLY	-	EXPRESSION TAG	UNP P11444
B	-11	ALA	-	EXPRESSION TAG	UNP P11444
B	-10	LEU	-	EXPRESSION TAG	UNP P11444
B	-9	GLU	-	EXPRESSION TAG	UNP P11444
B	-8	VAL	-	EXPRESSION TAG	UNP P11444
B	-7	LEU	-	EXPRESSION TAG	UNP P11444
B	-6	PHE	-	EXPRESSION TAG	UNP P11444
B	-5	GLN	-	EXPRESSION TAG	UNP P11444
B	-4	GLY	-	EXPRESSION TAG	UNP P11444
B	-3	PRO	-	EXPRESSION TAG	UNP P11444
B	-2	GLY	-	EXPRESSION TAG	UNP P11444
B	-1	TYR	-	EXPRESSION TAG	UNP P11444
B	0	HIS	-	EXPRESSION TAG	UNP P11444
C	-23	MET	-	EXPRESSION TAG	UNP P11444
C	-22	ALA	-	EXPRESSION TAG	UNP P11444
C	-21	SER	-	EXPRESSION TAG	UNP P11444
C	-20	TRP	-	EXPRESSION TAG	UNP P11444
C	-19	SER	-	EXPRESSION TAG	UNP P11444
C	-18	HIS	-	EXPRESSION TAG	UNP P11444
C	-17	PRO	-	EXPRESSION TAG	UNP P11444
C	-16	GLN	-	EXPRESSION TAG	UNP P11444
C	-15	PHE	-	EXPRESSION TAG	UNP P11444
C	-14	GLU	-	EXPRESSION TAG	UNP P11444
C	-13	LYS	-	EXPRESSION TAG	UNP P11444
C	-12	GLY	-	EXPRESSION TAG	UNP P11444
C	-11	ALA	-	EXPRESSION TAG	UNP P11444
C	-10	LEU	-	EXPRESSION TAG	UNP P11444
C	-9	GLU	-	EXPRESSION TAG	UNP P11444

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-8	VAL	-	EXPRESSION TAG	UNP P11444
C	-7	LEU	-	EXPRESSION TAG	UNP P11444
C	-6	PHE	-	EXPRESSION TAG	UNP P11444
C	-5	GLN	-	EXPRESSION TAG	UNP P11444
C	-4	GLY	-	EXPRESSION TAG	UNP P11444
C	-3	PRO	-	EXPRESSION TAG	UNP P11444
C	-2	GLY	-	EXPRESSION TAG	UNP P11444
C	-1	TYR	-	EXPRESSION TAG	UNP P11444
C	0	HIS	-	EXPRESSION TAG	UNP P11444
D	-23	MET	-	EXPRESSION TAG	UNP P11444
D	-22	ALA	-	EXPRESSION TAG	UNP P11444
D	-21	SER	-	EXPRESSION TAG	UNP P11444
D	-20	TRP	-	EXPRESSION TAG	UNP P11444
D	-19	SER	-	EXPRESSION TAG	UNP P11444
D	-18	HIS	-	EXPRESSION TAG	UNP P11444
D	-17	PRO	-	EXPRESSION TAG	UNP P11444
D	-16	GLN	-	EXPRESSION TAG	UNP P11444
D	-15	PHE	-	EXPRESSION TAG	UNP P11444
D	-14	GLU	-	EXPRESSION TAG	UNP P11444
D	-13	LYS	-	EXPRESSION TAG	UNP P11444
D	-12	GLY	-	EXPRESSION TAG	UNP P11444
D	-11	ALA	-	EXPRESSION TAG	UNP P11444
D	-10	LEU	-	EXPRESSION TAG	UNP P11444
D	-9	GLU	-	EXPRESSION TAG	UNP P11444
D	-8	VAL	-	EXPRESSION TAG	UNP P11444
D	-7	LEU	-	EXPRESSION TAG	UNP P11444
D	-6	PHE	-	EXPRESSION TAG	UNP P11444
D	-5	GLN	-	EXPRESSION TAG	UNP P11444
D	-4	GLY	-	EXPRESSION TAG	UNP P11444
D	-3	PRO	-	EXPRESSION TAG	UNP P11444
D	-2	GLY	-	EXPRESSION TAG	UNP P11444
D	-1	TYR	-	EXPRESSION TAG	UNP P11444
D	0	HIS	-	EXPRESSION TAG	UNP P11444

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

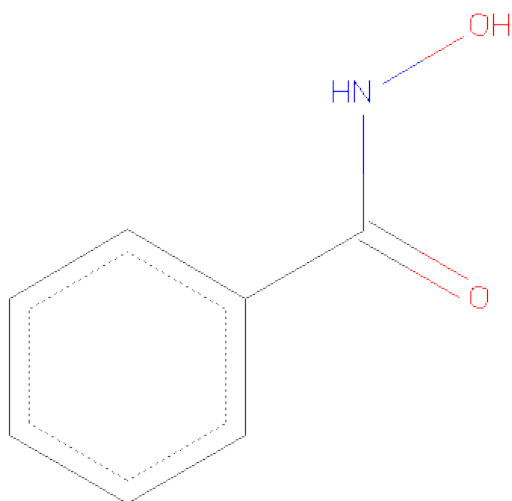
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Mg 1 1	0	0
2	A	1	Total Mg 1 1	0	0
2	D	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	1	Total	Mg	0	0
			1	1		

- Molecule 3 is BENZHYDROXAMIC ACID (three-letter code: BHO) (formula:  $C_7H_7NO_2$ ).



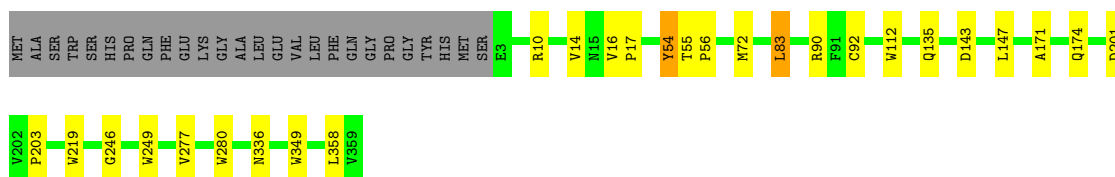
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			10	7	1	2		
3	B	1	Total	C	N	O	0	0
			10	7	1	2		
3	C	1	Total	C	N	O	0	0
			10	7	1	2		
3	D	1	Total	C	N	O	0	0
			10	7	1	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	209	Total	O	0	0
			209	209		
4	B	169	Total	O	0	0
			169	169		
4	C	161	Total	O	0	0
			161	161		
4	D	210	Total	O	0	0
			210	210		

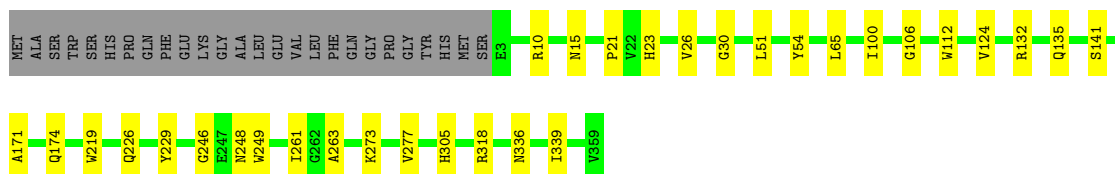
- Molecule 1: Mandelate racemase

Chain A:



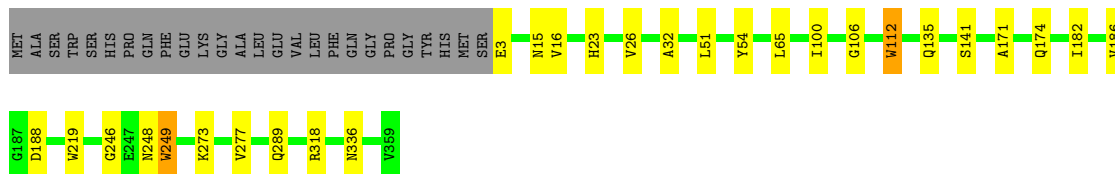
- Molecule 1: Mandelate racemase

Chain B:



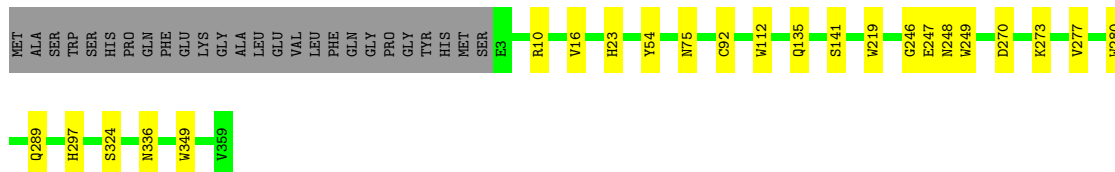
- Molecule 1: Mandelate racemase

Chain C:



- Molecule 1: Mandelate racemase

Chain D:





## 4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	148.31Å 148.31Å 169.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.20 37.21 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-2.20) 99.9 (37.21-2.20)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	7.93 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.162 , 0.193 0.159 , 0.176	Depositor DCC
$R_{free}$ test set	4618 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	16.8	Xtriage
Anisotropy	0.070	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 11.4	EDS
Estimated twinning fraction	0.486 for -h,k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	1 of 92311 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	11566	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.06% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, BHO

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	0.72	4/2756 (0.1%)	0.68	0/3756
1	B	0.68	0/2752	0.66	0/3750
1	C	0.65	2/2749 (0.1%)	0.64	0/3746
1	D	0.69	2/2755 (0.1%)	0.68	0/3753
All	All	0.69	8/11012 (0.1%)	0.66	0/15005

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	54	TYR	CE1-CZ	-7.06	1.29	1.38
1	A	349	TRP	CD2-CE2	5.64	1.48	1.41
1	D	349	TRP	CD2-CE2	5.55	1.48	1.41
1	A	280	TRP	CD2-CE2	5.35	1.47	1.41
1	C	112	TRP	CD2-CE2	5.26	1.47	1.41
1	C	249	TRP	CD2-CE2	5.24	1.47	1.41
1	D	280	TRP	CD2-CE2	5.22	1.47	1.41
1	A	54	TYR	CG-CD1	-5.10	1.32	1.39

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the

chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2694	0	2728	15	0
1	B	2693	0	2732	28	0
1	C	2690	0	2726	18	0
1	D	2696	0	2739	13	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	10	0	7	0	0
3	B	10	0	6	1	0
3	C	10	0	7	0	0
3	D	10	0	7	1	0
4	A	209	0	0	2	0
4	B	169	0	0	4	0
4	C	161	0	0	2	0
4	D	210	0	0	2	0
All	All	11566	0	10952	73	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 3.

All (73) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:54:TYR:OH	4:C:383:HOH:O	1.88	0.84
1:B:226:GLN:HG3	1:B:248:ASN:CB	2.12	0.79
1:A:135:GLN:HA	1:A:336:ASN:HD22	1.50	0.76
1:C:135:GLN:HA	1:C:336:ASN:HD22	1.50	0.76
1:D:54:TYR:OH	4:D:646:HOH:O	1.88	0.76
1:B:229:TYR:HB3	1:B:261:ILE:HD11	1.66	0.76
1:D:135:GLN:HA	1:D:336:ASN:HD22	1.52	0.74
1:B:135:GLN:HA	1:B:336:ASN:HD22	1.52	0.74
1:B:54:TYR:OH	4:B:429:HOH:O	1.87	0.73
1:B:226:GLN:NE2	4:B:443:HOH:O	2.23	0.70
1:B:124:VAL:H	1:B:305:HIS:HD2	1.39	0.68
1:B:226:GLN:HG3	1:B:248:ASN:HB3	1.80	0.64
1:C:171:ALA:H	1:C:174:GLN:HE21	1.48	0.61
1:A:112:TRP:CD1	1:A:277:VAL:HB	2.37	0.60
1:A:72:MET:HE1	1:A:90:ARG:CZ	2.31	0.59
1:D:112:TRP:CD1	1:D:277:VAL:HB	2.37	0.58
1:D:248:ASN:HD22	1:D:273:LYS:NZ	2.02	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:289:GLN:NE2	4:C:811:HOH:O	2.40	0.54
1:B:261:ILE:HD11	1:B:263:ALA:HB2	1.89	0.54
1:D:248:ASN:HD22	1:D:273:LYS:HZ3	1.54	0.54
1:B:226:GLN:CG	1:B:248:ASN:CB	2.86	0.54
1:C:112:TRP:CD1	1:C:277:VAL:HB	2.43	0.54
1:B:132:ARG:NH1	4:B:446:HOH:O	2.29	0.53
1:B:171:ALA:H	1:B:174:GLN:HE21	1.54	0.53
1:A:171:ALA:H	1:A:174:GLN:HE21	1.54	0.53
1:B:248:ASN:HD22	1:B:273:LYS:NZ	2.07	0.53
1:B:226:GLN:HG3	1:B:248:ASN:HB2	1.89	0.52
1:C:248:ASN:HD22	1:C:273:LYS:NZ	2.08	0.52
1:B:226:GLN:CG	1:B:248:ASN:HB2	2.39	0.52
1:A:83:LEU:HD13	4:A:651:HOH:O	2.09	0.52
1:C:171:ALA:H	1:C:174:GLN:NE2	2.08	0.52
1:D:246:GLY:HA2	1:D:249:TRP:CD2	2.45	0.51
1:A:246:GLY:HA2	1:A:249:TRP:CD2	2.47	0.50
1:C:246:GLY:HA2	1:C:249:TRP:CD2	2.46	0.50
1:D:289:GLN:NE2	4:D:491:HOH:O	2.44	0.50
1:B:246:GLY:HA2	1:B:249:TRP:CD2	2.46	0.50
1:B:132:ARG:NH2	4:B:446:HOH:O	2.44	0.50
1:C:51:LEU:HD21	1:C:106:GLY:CA	2.41	0.50
1:D:270:ASP:OD1	1:D:297:HIS:HD2	1.95	0.49
1:B:112:TRP:CD1	1:B:277:VAL:HB	2.47	0.49
1:B:124:VAL:H	1:B:305:HIS:CD2	2.26	0.49
1:A:92[B]:CYS:SG	1:C:26:VAL:HG21	2.53	0.48
1:B:51:LEU:HD21	1:B:106:GLY:CA	2.44	0.48
1:A:54:TYR:OH	4:A:686:HOH:O	2.16	0.47
1:A:14:VAL:HG12	1:A:358:LEU:HD23	1.95	0.47
1:B:248:ASN:HD22	1:B:273:LYS:HZ2	1.62	0.46
1:C:16:VAL:HG23	1:C:32:ALA:HB3	1.97	0.46
1:D:297:HIS:HE1	3:D:361:BHO:N	2.13	0.46
1:B:23:HIS:O	1:B:141:SER:HB2	2.16	0.45
1:B:65:LEU:HD21	1:B:100:ILE:HA	1.98	0.45
1:C:65:LEU:HD21	1:C:100:ILE:HA	1.98	0.45
1:B:21:PRO:HB3	1:B:30:GLY:HA2	1.98	0.45
1:A:135:GLN:CA	1:A:336:ASN:HD22	2.24	0.44
1:D:247:GLU:HB2	1:D:297:HIS:CD2	2.52	0.44
1:B:26:VAL:HG21	1:D:92:CYS:SG	2.58	0.44
1:C:248:ASN:HD22	1:C:273:LYS:HZ2	1.65	0.44
1:A:171:ALA:H	1:A:174:GLN:NE2	2.16	0.43
1:B:171:ALA:H	1:B:174:GLN:NE2	2.16	0.42
1:C:16:VAL:CG2	1:C:32:ALA:HB3	2.49	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:182:ILE:O	1:C:186:VAL:HG22	2.18	0.42
1:C:3:GLU:HG3	1:C:3:GLU:O	2.19	0.42
1:D:23:HIS:O	1:D:141:SER:HB2	2.19	0.42
1:C:23:HIS:O	1:C:141:SER:HB2	2.19	0.42
3:B:361:BHO:H2	3:B:361:BHO:HN	1.57	0.42
1:A:201:ASP:OD1	1:A:203:PRO:HD2	2.20	0.42
1:D:16:VAL:HG11	1:D:324:SER:HB2	2.02	0.41
1:B:248:ASN:ND2	1:B:273:LYS:HZ2	2.18	0.41
1:B:305:HIS:CE1	1:B:339:ILE:HG23	2.55	0.41
1:B:15:ASN:HA	1:B:15:ASN:HD22	1.73	0.41
1:A:143:ASP:HB3	1:A:147:LEU:HB3	2.03	0.41
1:A:16:VAL:HA	1:A:17:PRO:HD2	1.93	0.41
1:A:55:THR:OG1	1:A:56:PRO:HD2	2.21	0.41
1:C:15:ASN:HD22	1:C:15:ASN:HA	1.69	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	357/383 (93%)	345 (97%)	12 (3%)	0	100	100
1	B	356/383 (93%)	346 (97%)	10 (3%)	0	100	100
1	C	356/383 (93%)	348 (98%)	8 (2%)	0	100	100
1	D	356/383 (93%)	345 (97%)	11 (3%)	0	100	100
All	All	1425/1532 (93%)	1384 (97%)	41 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	278/301 (92%)	275 (99%)	3 (1%)	84	92
1	B	278/301 (92%)	275 (99%)	3 (1%)	84	92
1	C	278/301 (92%)	275 (99%)	3 (1%)	84	92
1	D	279/301 (93%)	276 (99%)	3 (1%)	84	92
All	All	1113/1204 (92%)	1101 (99%)	12 (1%)	84	92

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ARG
1	A	83	LEU
1	A	219	TRP
1	B	10	ARG
1	B	219	TRP
1	B	318	ARG
1	C	188	ASP
1	C	219	TRP
1	C	318	ARG
1	D	10	ARG
1	D	75	ASN
1	D	219	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	ASN
1	A	174	GLN
1	A	184	GLN
1	A	210	GLN
1	A	214	GLN
1	A	336	ASN
1	B	15	ASN
1	B	75	ASN
1	B	130	ASN
1	B	174	GLN
1	B	210	GLN
1	B	214	GLN
1	B	226	GLN

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Mol	Chain	Res	Type
1	B	240	ASN
1	B	248	ASN
1	B	305	HIS
1	B	336	ASN
1	C	15	ASN
1	C	75	ASN
1	C	130	ASN
1	C	135	GLN
1	C	174	GLN
1	C	210	GLN
1	C	214	GLN
1	C	227	HIS
1	C	233	GLN
1	C	240	ASN
1	C	248	ASN
1	C	289	GLN
1	C	336	ASN
1	D	15	ASN
1	D	130	ASN
1	D	210	GLN
1	D	214	GLN
1	D	248	ASN
1	D	289	GLN
1	D	297	HIS
1	D	336	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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	BHO	A	361	2	10,10,10	1.77	2 (20%)	12,12,12	2.38	3 (25%)
3	BHO	B	361	2	10,10,10	1.78	2 (20%)	12,12,12	2.39	3 (25%)
3	BHO	C	361	2	10,10,10	1.76	2 (20%)	12,12,12	2.38	3 (25%)
3	BHO	D	361	2	10,10,10	1.77	2 (20%)	12,12,12	2.38	3 (25%)

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
3	BHO	A	361	2	-	0/6/6/6	0/1/1/1
3	BHO	B	361	2	-	0/6/6/6	0/1/1/1
3	BHO	C	361	2	-	0/6/6/6	0/1/1/1
3	BHO	D	361	2	-	0/6/6/6	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	361	BHO	C-N	4.75	1.39	1.32
3	D	361	BHO	C-N	4.74	1.39	1.32
3	A	361	BHO	C-N	4.72	1.39	1.32
3	C	361	BHO	C-N	4.69	1.39	1.32
3	A	361	BHO	O2-N	-2.71	1.34	1.39
3	C	361	BHO	O2-N	-2.69	1.34	1.39
3	B	361	BHO	O2-N	-2.69	1.34	1.39
3	D	361	BHO	O2-N	-2.66	1.34	1.39

All (12) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	361	BHO	O2-N-C	5.77	135.44	119.64
3	D	361	BHO	O2-N-C	5.76	135.43	119.64
3	C	361	BHO	O2-N-C	5.76	135.42	119.64
3	B	361	BHO	O2-N-C	5.75	135.39	119.64
3	B	361	BHO	C1-C-N	-4.97	107.95	116.34
3	C	361	BHO	C1-C-N	-4.96	107.97	116.34
3	D	361	BHO	C1-C-N	-4.94	108.00	116.34
3	A	361	BHO	C1-C-N	-4.94	108.00	116.34
3	B	361	BHO	O1-C-C1	2.51	125.40	121.01
3	D	361	BHO	O1-C-C1	2.50	125.40	121.01
3	A	361	BHO	O1-C-C1	2.49	125.38	121.01
3	C	361	BHO	O1-C-C1	2.49	125.38	121.01

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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, 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	357/383 (93%)	-0.72	0 100 100	8, 14, 26, 38	9 (2%)
1	B	357/383 (93%)	-0.63	0 100 100	10, 18, 32, 42	14 (3%)
1	C	357/383 (93%)	-0.64	0 100 100	10, 18, 33, 46	10 (2%)
1	D	357/383 (93%)	-0.74	0 100 100	8, 14, 25, 37	12 (3%)
All	All	1428/1532 (93%)	-0.69	0 100 100	8, 15, 30, 46	45 (3%)

There are no RSRZ outliers to report.

### 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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	BHO	C	361	10/10	0.31	12.48	39,44,47,47	0
3	BHO	A	361	10/10	0.27	9.91	31,38,40,41	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	BHO	D	361	10/10	0.30	8.03	30,36,37,37	0
3	BHO	B	361	10/10	0.24	6.90	39,46,48,48	0
2	MG	A	360	1/1	0.12	6.07	11,11,11,11	0
2	MG	D	360	1/1	0.13	4.09	11,11,11,11	0
2	MG	C	360	1/1	0.12	2.82	13,13,13,13	0
2	MG	B	360	1/1	0.10	1.38	14,14,14,14	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.