

Full wwPDB X-ray Structure Validation Report (i)

Sep 17, 2024 - 08:36 PM JST

PDB ID	:	8ZI8
Title	:	Terephthalate 1,2-cis-dihydrodioldehydrogenase/Decarboxylase in complex
		with 2,5-Dihydroxybenzoate.
Authors	:	Kumar, K.A.; Pahwa, D.; Kumar, P.
Deposited on	:	2024-05-13
Resolution	:	2.65 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 (1)) 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	:	3.0
buster-report	:	1.1.7(2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.002 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.38.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 2.65 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R _{free}	164625	$1003 \ (2.66-2.66)$
Clashscore	180529	$1063 \ (2.66-2.66)$
Ramachandran outliers	177936	$1052 \ (2.66-2.66)$
Sidechain outliers	177891	$1052 \ (2.66-2.66)$

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%

Mol	Chain	Length	Quality of chain		
1	А	335	82%	11%	• 6%
1	В	335	77%	16%	• 6%
1	С	335	79%	13%	7%
1	D	335	83%	10%	6%



2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 18811 atoms, of which 9466 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.

Mol	Chain	Residues		Atoms					ZeroOcc	AltConf	Trace
1	Δ	314	Total	С	Η	Ν	0	\mathbf{S}	68	0	0
1	Л	514	4670	1445	2368	412	432	13	00		0
1	1 B 314	314	Total	С	Η	Ν	Ο	\mathbf{S}	68	0	0
1		514	4670	1445	2368	412	433	12			0
1	1 C	911	Total	С	Η	Ν	0	S	68	0	0
	311	4620	1429	2342	408	428	13	08	0	0	
1 D	214	Total	С	Н	Ν	0	S	68	0	0	
	514	4670	1445	2368	412	432	13		0	U	

• Molecule 1 is a protein called 4-hydroxythreonine-4-phosphate dehydrogenase.

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	-19	MET	-	initiating methionine	UNP B7WRJ7
А	-18	GLY	-	expression tag	UNP B7WRJ7
А	-17	SER	-	expression tag	UNP B7WRJ7
А	-16	SER	-	expression tag	UNP B7WRJ7
А	-15	HIS	-	expression tag	UNP B7WRJ7
А	-14	HIS	-	expression tag	UNP B7WRJ7
А	-13	HIS	-	expression tag	UNP B7WRJ7
А	-12	HIS	-	expression tag	UNP B7WRJ7
А	-11	HIS	-	expression tag	UNP B7WRJ7
А	-10	HIS	-	expression tag	UNP B7WRJ7
А	-9	SER	-	expression tag	UNP B7WRJ7
А	-8	SER	-	expression tag	UNP B7WRJ7
А	-7	GLY	-	expression tag	UNP B7WRJ7
А	-6	LEU	-	expression tag	UNP B7WRJ7
А	-5	VAL	-	expression tag	UNP B7WRJ7
А	-4	PRO	-	expression tag	UNP B7WRJ7
А	-3	ARG	-	expression tag	UNP B7WRJ7
А	-2	GLY	-	expression tag	UNP B7WRJ7
А	-1	SER	-	expression tag	UNP B7WRJ7
А	0	HIS	-	expression tag	UNP B7WRJ7
В	-19	MET	-	initiating methionine	UNP B7WRJ7

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Chain	Residue	Modelled	Actual	Comment	Reference
В	-18	GLY	- expression tag		UNP B7WRJ7
В	-17	SER	-	expression tag	UNP B7WRJ7
В	-16	SER	-	expression tag	UNP B7WRJ7
В	-15	HIS	_	expression tag	UNP B7WRJ7
В	-14	HIS	-	expression tag	UNP B7WRJ7
В	-13	HIS	_	expression tag	UNP B7WRJ7
В	-12	HIS	_	expression tag	UNP B7WRJ7
В	-11	HIS	_	expression tag	UNP B7WRJ7
В	-10	HIS	_	expression tag	UNP B7WRJ7
В	-9	SER	-	expression tag	UNP B7WRJ7
В	-8	SER	-	expression tag	UNP B7WRJ7
В	-7	GLY	_	expression tag	UNP B7WRJ7
В	-6	LEU	-	expression tag	UNP B7WRJ7
В	-5	VAL	_	expression tag	UNP B7WRJ7
В	-4	PRO	_	expression tag	UNP B7WRJ7
В	-3	ARG	-	expression tag	UNP B7WRJ7
В	-2	GLY	_	expression tag	UNP B7WRJ7
В	-1	SER	-	expression tag	UNP B7WRJ7
В	0	HIS	_	expression tag	UNP B7WRJ7
С	-19	MET	_	initiating methionine	UNP B7WRJ7
С	-18	GLY	-	expression tag	UNP B7WRJ7
С	-17	SER	-	expression tag	UNP B7WRJ7
С	-16	SER	-	expression tag	UNP B7WRJ7
С	-15	HIS	-	expression tag	UNP B7WRJ7
С	-14	HIS	-	expression tag	UNP B7WRJ7
С	-13	HIS	-	expression tag	UNP B7WRJ7
С	-12	HIS	-	expression tag	UNP B7WRJ7
С	-11	HIS	-	expression tag	UNP B7WRJ7
С	-10	HIS	-	expression tag	UNP B7WRJ7
С	-9	SER	-	expression tag	UNP B7WRJ7
С	-8	SER	-	expression tag	UNP B7WRJ7
С	-7	GLY	-	expression tag	UNP B7WRJ7
С	-6	LEU	-	expression tag	UNP B7WRJ7
С	-5	VAL	-	expression tag	UNP B7WRJ7
С	-4	PRO	-	expression tag	UNP B7WRJ7
C	-3	ARG	_	expression tag	UNP B7WRJ7
C	-2	GLY		expression tag	UNP B7WRJ7
C	-1	SER	-	expression tag	UNP B7WRJ7
C	0	HIS	-	expression tag	UNP B7WRJ7
D	-19	MET	-	initiating methionine	UNP B7WRJ7
D	-18	GLY	-	expression tag	UNP B7WRJ7
D	-17	SER	-	expression tag	UNP B7WRJ7

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	expression tag	UNP B7WRJ7
D	-15	HIS	-	expression tag	UNP B7WRJ7
D	-14	HIS	-	expression tag	UNP B7WRJ7
D	-13	HIS	-	expression tag	UNP B7WRJ7
D	-12	HIS	-	expression tag	UNP B7WRJ7
D	-11	HIS	-	expression tag	UNP B7WRJ7
D	-10	HIS	-	expression tag	UNP B7WRJ7
D	-9	SER	-	expression tag	UNP B7WRJ7
D	-8	SER	-	expression tag	UNP B7WRJ7
D	-7	GLY	-	expression tag	UNP B7WRJ7
D	-6	LEU	-	expression tag	UNP B7WRJ7
D	-5	VAL	-	expression tag	UNP B7WRJ7
D	-4	PRO	-	expression tag	UNP B7WRJ7
D	-3	ARG	-	expression tag	UNP B7WRJ7
D	-2	GLY	_	expression tag	UNP B7WRJ7
D	-1	SER	-	expression tag	UNP B7WRJ7
D	0	HIS	-	expression tag	UNP B7WRJ7

• Molecule 2 is CARBON DIOXIDE (three-letter code: CO2) (formula: CO₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 3 & 1 & 2 \end{array}$	0	0
2	D	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 3 1 2 \end{array}$	0	0



• Molecule 3 is 2,5-dihydroxybenzoic acid (three-letter code: GTQ) (formula: C₇H₆O₄).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	$\begin{array}{ccccc} \text{Total} & \text{C} & \text{H} & \text{O} \\ 15 & 7 & 4 & 4 \end{array}$	1	0
3	D	1	Total C H O 15 7 4 4	1	0

• Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	1	Total Zn 1 1	0	0
4	С	1	Total Zn 1 1	0	0
4	D	1	Total Zn 1 1	0	0

• Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).







Mol	Chain	Residues	Ato	oms		ZeroOcc	AltConf
5	D	1	Total C 10 2	С Н 2 б	O 2	2	0
5	D	1	Total C 10 2	С Н 2 6	O 2	2	0

• Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	D	1	Total Cl 1 1	0	0

• Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	А	54	$\begin{array}{cc} \text{Total} & \text{O} \\ 54 & 54 \end{array}$	0	0
7	В	15	Total O 15 15	0	0
7	С	10	Total O 10 10	0	0
7	D	42	$\begin{array}{cc} \text{Total} & \text{O} \\ 42 & 42 \end{array}$	0	0



3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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-hydroxythreonine-4-phosphate dehydrogenase

Chain A:	82%	11% • 6%
MET MET SER SER SER HIS HIS HIS SER RIS SER SER SER SER SER SER SER SER SER SE	836 153 163 164 164 164 164 164 164 897 897 8119 8119 81128 81128 81128	E141 H159 H163 R168 R168 H203 A204 S205
7219 7220 7220 7236 7241 7241 7244 7245 7245 7245 7245 7245 7266 7261 7261 7261 7261 7263 7282 7282 7282 7282	C234 R305 P314 VAL	
• Molecule 1: 4-hydroxythreonine	-4-phosphate dehydrogenase	
Chain B:	77% 1	<mark>6% •</mark> 6%
MET MET SER SER HIS HIS HIS HIS SER RIS RIS RER RIS RIS RER MET MET MET	127 127 128 128 153 153 153 153 153 153 153 153 153 153	1115 1116 1116 1116 1116 1118 1118 1128 1128
8161 1462 1463 8164 8165 8164 8167 8168 8167 8168 8205 8205 8205 8205 8205 8205 8205 820	6229 0234 0234 0234 0234 0241 1260 1260 1260 1260 1260 1260 1268 1260 1268 1268 1268 1268 1268 1268 1268 1268	A B B B B B B B B B B B B B B B B B B B
• Molecule 1: 4-hydroxythreonine	-4-phosphate dehydrogenase	
Chain C:	79% 1	13% 7%
MET MET SER SER HIS SER HIS HIS SER RIS RIS SER RIS SER RIS RIS SER RIS RIS RIS RIS RIS RIS RI	127 127 127 127 164 164 164 164 164 1110 7127 7127 7127 7128	1157 1158 1158 1158 1158 1158 1158 1158
A204 8205 8205 8205 7210 7210 7210 7210 7210 7210 7228 7228 7228 7228 7228 7229 7234 7234 7234 7234 7234 7234 7234 7234	1260 1261 1264 1264 1273 1278 1278 1278 1278 1278 1278 1278 1278 1278 1278 1278 1278 1278 1278 1277 1277 1277 1277 1277 1264 1277 1264 1277 1264 1277 1264 1277 1264 1277 1264 1277 1279	YAL
• Molecule 1: 4-hydroxythreonine	-4-phosphate dehydrogenase	
Chain D:	83%	10% 6%
MET MET SER SER HIS SER HIS SER HIS SER RIS RIC ME RIS RIS RIS RIS RIS RIS RIS RIS RIS RIS	127 133 856 836 852 857 857 164 164 733 873 873 873 873 873 873 873 873 873	R119 127 128 128 128 8128 R168 A204 A204 S205





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants	86.55Å 94.72Å 166.71Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Bosolution(A)	24.00 - 2.65	Depositor
Resolution (A)	24.00 - 2.65	EDS
% Data completeness	99.7 (24.00-2.65)	Depositor
(in resolution range)	99.7 (24.00-2.65)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.57 (at 2.64 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
B B.	0.260 , 0.295	Depositor
II, II free	0.305 , 0.324	DCC
R_{free} test set	2003 reflections $(4.94%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	32.4	Xtriage
Anisotropy	0.242	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.42 , 15.7	EDS
L-test for $twinning^2$	$ < L >=0.43, < L^2>=0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	18811	wwPDB-VP
Average B, all atoms $(Å^2)$	3.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The analyses of the Patterson function reveals a significant off-origin peak that is 36.49 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.9555e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

²Theoretical 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.



¹Intensities estimated from amplitudes.

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: GTQ, ZN, CL, CO2, EDO

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).

Mal	Chain	Bond lengths		Bond angles	
INIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.43	0/2339	0.76	2/3183~(0.1%)
1	В	0.36	0/2339	0.75	1/3183~(0.0%)
1	С	0.36	0/2313	0.74	1/3145~(0.0%)
1	D	0.44	0/2339	0.74	1/3183~(0.0%)
All	All	0.40	0/9330	0.75	5/12694~(0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	А	0	4
1	В	0	2
1	D	0	3
All	All	0	9

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	245	ARG	NE-CZ-NH2	-6.54	117.03	120.30
1	А	278	ARG	NE-CZ-NH1	-5.99	117.30	120.30
1	С	299	ASP	CB-CA-C	5.97	122.35	110.40
1	В	208	GLN	CB-CA-C	-5.44	99.52	110.40
1	D	7	ARG	NE-CZ-NH2	-5.27	117.67	120.30

There are no chirality outliers.

All (9) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
1	А	163	ARG	Sidechain
1	А	168	ARG	Sidechain
1	А	278	ARG	Sidechain
1	А	305	ARG	Sidechain
1	В	119	ARG	Sidechain
1	В	168	ARG	Sidechain
1	D	119	ARG	Sidechain
1	D	168	ARG	Sidechain
1	D	7	ARG	Sidechain

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	А	2302	2368	2357	24	1
1	В	2302	2368	2354	41	0
1	С	2278	2342	2330	36	0
1	D	2302	2368	2357	22	1
2	А	3	0	0	0	0
2	D	3	0	0	0	0
3	А	11	4	4	2	0
3	D	11	4	4	0	0
4	А	1	0	0	0	1
4	С	1	0	0	0	0
4	D	1	0	0	0	1
5	D	8	12	12	1	0
6	D	1	0	0	0	0
7	А	54	0	0	4	0
7	В	15	0	0	2	0
7	С	10	0	0	1	0
7	D	42	0	0	2	0
All	All	9345	9466	9418	106	2

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 6.

All (106) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.



Atom_1	Atom_2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:244:GLN:OE1	1:A:246:LYS:HE2	1.57	1.03
1:B:159:HIS:O	1:C:210:PHE:CE1	2.33	0.82
1:B:161:SER:OG	1:B:164:SER:HB2	1.83	0.78
1:B:159:HIS:O	1:C:210:PHE:CD1	2.37	0.78
1:B:161:SER:OG	1:B:164:SER:CB	2.34	0.76
1:B:200:ILE:O	7:B:401:HOH:O	2.03	0.76
1:A:246:LYS:CE	7:A:504:HOH:O	2.33	0.75
1:A:159:HIS:HB2	7:A:533:HOH:O	1.89	0.71
1:D:113:HIS:HA	5:D:404:EDO:H12	1.74	0.68
1:B:54:CYS:O	1:B:56:MET:N	2.29	0.66
1:D:129:SER:HB3	7:D:525:HOH:O	1.96	0.66
1:B:159:HIS:HB3	1:C:210:PHE:CZ	2.35	0.62
1:A:246:LYS:HE2	7:A:504:HOH:O	1.96	0.62
1:B:113:HIS:ND1	1:B:115:THR:OG1	2.32	0.62
1:A:119:ARG:NH2	1:B:229:GLY:O	2.33	0.61
1:A:244:GLN:OE1	1:A:246:LYS:CE	2.42	0.60
1:C:292:ILE:HG22	1:D:286:HIS:HB2	1.84	0.60
1:B:202:PRO:HG3	1:C:255:HIS:HB3	1.84	0.59
1:B:240:MET:HG3	1:B:241:VAL:N	2.16	0.59
1:B:265:LEU:HD11	1:C:264:LEU:HD11	1.84	0.59
1:B:239:ASP:HA	1:C:260:ILE:HA	1.85	0.57
1:C:36:SER:HA	1:C:64:ILE:HD13	1.86	0.57
1:A:259:HIS:NE2	3:A:402:GTQ:OAD	2.35	0.56
1:C:208:GLN:NE2	1:C:215:SER:HB3	2.20	0.56
1:B:162:VAL:HG23	1:C:201:ASN:HA	1.87	0.56
1:B:242:LEU:HD12	1:C:260:ILE:HG23	1.89	0.55
1:D:313:GLN:CG	1:D:314:PRO:HD2	2.36	0.55
1:B:113:HIS:CE1	1:B:115:THR:OG1	2.61	0.54
1:A:36:SER:HA	1:A:64:ILE:HD13	1.90	0.54
1:C:127:TYR:N	1:C:128:PRO:CD	2.71	0.53
1:D:313:GLN:HG2	1:D:314:PRO:HD2	1.90	0.53
1:C:299:ASP:OD1	1:D:297:VAL:O	2.26	0.53
1:B:300:ALA:HA	7:B:404:HOH:O	2.09	0.53
1:B:127:TYR:N	1:B:128:PRO:CD	2.72	0.53
1:A:286:HIS:HE1	7:A:531:HOH:O	1.93	0.52
1:A:127:TYR:N	1:A:128:PRO:CD	2.73	0.52
1:C:278:ARG:O	1:C:278:ARG:HG2	2.09	0.52
1:D:127:TYR:N	1:D:128:PRO:CD	2.72	0.52
1:C:5:HIS:HB2	1:C:312:ALA:HA	1.91	0.51
1:C:161:SER:OG	1:C:164:SER:HB2	2.11	0.51
1:B:161:SER:OG	1:B:164:SER:HB3	2.11	0.51
1:D:297:VAL:O	1:D:297:VAL:HG23	2.11	0.50
		Continue	ed on next page



	le us pagem	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:83:GLN:NE2	1:D:73:GLN:OE1	2.45	0.50
1:A:93:THR:HG22	1:A:97:ARG:CZ	2.42	0.50
1:D:270:ALA:HB3	7:D:532:HOH:O	2.10	0.50
1:D:36:SER:HA	1:D:64:ILE:HD13	1.95	0.49
1:B:210:PHE:O	1:C:161:SER:N	2.46	0.49
1:C:234:GLY:HA2	1:C:236:MET:HG3	1.94	0.49
1:C:228:ARG:O	7:C:501:HOH:O	2.19	0.49
1:B:27:LEU:HD13	1:B:63:LEU:HD11	1.96	0.48
1:A:159:HIS:HE1	3:A:402:GTQ:CAE	2.27	0.48
1:A:273:LEU:HD22	1:A:282:SER:HB2	1.96	0.48
1:C:157:THR:HG21	1:C:165:ALA:HB1	1.96	0.48
1:B:118:HIS:O	1:B:120:ALA:O	2.31	0.47
1:D:204:ALA:O	1:D:205:SER:HB2	2.14	0.47
1:A:260:ILE:N	1:A:261:PRO:HD2	2.29	0.47
1:B:110:CYS:HB3	1:B:111:PRO:CD	2.45	0.47
1:B:163:ARG:O	1:B:167:GLU:HG2	2.14	0.46
1:C:191:PRO:O	1:C:192:LYS:C	2.53	0.46
1:C:264:LEU:C	1:C:264:LEU:HD13	2.34	0.46
1:B:260:ILE:N	1:B:261:PRO:HD2	2.30	0.46
1:B:260:ILE:HG23	1:C:242:LEU:HD12	1.97	0.46
1:B:207:GLY:O	1:B:209:LEU:HG	2.14	0.46
1:B:268:ASN:N	1:B:268:ASN:OD1	2.49	0.46
1:C:204:ALA:O	1:C:205:SER:HB2	2.16	0.46
1:C:260:ILE:N	1:C:261:PRO:HD2	2.31	0.46
1:B:161:SER:HG	1:B:164:SER:HB2	1.78	0.46
1:B:273:LEU:HD22	1:B:282:SER:HB2	1.98	0.46
1:C:110:CYS:HB3	1:C:111:PRO:CD	2.46	0.46
1:B:210:PHE:O	1:C:161:SER:HB3	2.16	0.45
1:D:260:ILE:N	1:D:261:PRO:HD2	2.31	0.45
1:B:219:VAL:HB	1:B:220:PRO:HD3	1.99	0.45
1:C:273:LEU:HD22	1:C:282:SER:HB2	1.97	0.45
1:A:204:ALA:O	1:A:205:SER:HB2	2.17	0.45
1:A:53:ILE:HD13	1:A:294:GLY:HA2	1.97	0.45
1:B:222:VAL:HG21	1:B:234:GLY:HA2	1.99	0.45
1:B:52:GLN:O	1:B:53:ILE:HB	2.16	0.45
1:C:52:GLN:HA	1:C:57:GLU:OE1	2.16	0.45
1:B:207:GLY:O	1:B:208:GLN:C	2.54	0.45
1:B:204:ALA:O	1:B:205:SER:HB2	2.15	0.44
1:B:202:PRO:HB3	1:C:255:HIS:CG	2.52	0.44
1:C:294:GLY:O	1:D:268:ASN:ND2	2.49	0.44
1:D:236:MET:HB2	1:D:241:VAL:CG2	2.48	0.44

Continued on next page...



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (\AA)
1:D:297:VAL:O	1:D:297:VAL:CG2	2.65	0.44
1:A:138:ASN:HB2	1:A:141:GLU:HG2	2.00	0.44
1:A:27:LEU:HD13	1:A:63:LEU:HD11	2.00	0.43
1:D:110:CYS:HB3	1:D:111:PRO:CD	2.47	0.43
1:A:9:ALA:HB2	1:A:104:VAL:HG21	2.00	0.43
1:B:9:ALA:HB2	1:B:104:VAL:HG21	2.00	0.43
1:C:311:GLY:O	1:C:312:ALA:C	2.56	0.43
1:D:27:LEU:HD13	1:D:63:LEU:HD11	2.00	0.43
1:B:114:GLU:OE1	1:B:114:GLU:N	2.46	0.43
1:D:52:GLN:HA	1:D:57:GLU:OE1	2.19	0.42
1:C:161:SER:OG	1:C:164:SER:CB	2.67	0.42
1:A:219:VAL:HB	1:A:220:PRO:HD3	2.02	0.42
1:C:219:VAL:HB	1:C:220:PRO:HD3	2.02	0.42
1:B:36:SER:HA	1:B:64:ILE:HD13	2.02	0.41
1:C:9:ALA:HB2	1:C:104:VAL:HG21	2.02	0.41
1:D:9:ALA:HB2	1:D:104:VAL:HG21	2.01	0.41
1:B:39:LYS:HG3	1:B:64:ILE:HG22	2.03	0.41
1:A:236:MET:HB2	1:A:241:VAL:CG2	2.51	0.41
1:A:236:MET:HB3	1:A:240:MET:HE1	2.03	0.41
1:A:268:ASN:C	1:A:268:ASN:OD1	2.59	0.41
1:D:230:LEU:HD23	1:D:232:VAL:CG2	2.52	0.41
1:D:273:LEU:HD22	1:D:282:SER:HB2	2.02	0.40
1:C:27:LEU:HD13	1:C:63:LEU:HD11	2.03	0.40

All (2) 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)
1:D:203:HIS:HE2	4:A:403:ZN:ZN[4_654]	1.40	0.20
1:A:203:HIS:HE2	4:D:405:ZN:ZN[4_655]	1.47	0.13

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



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
1	А	312/335~(93%)	301~(96%)	11 (4%)	0	100	100
1	В	312/335~(93%)	297~(95%)	13~(4%)	2(1%)	22	35
1	С	307/335~(92%)	294~(96%)	12~(4%)	1 (0%)	37	53
1	D	312/335~(93%)	304~(97%)	8(3%)	0	100	100
All	All	1243/1340~(93%)	1196 (96%)	44 (4%)	3(0%)	44	61

analysed, and the total number of residues.

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	В	55	GLN
1	С	158	LEU
1	В	53	ILE

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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed Rotameric Outliers		Percentiles		
1	А	243/261~(93%)	242 (100%)	1 (0%)	89	95
1	В	243/261~(93%)	241~(99%)	2(1%)	79	89
1	С	240/261~(92%)	238~(99%)	2 (1%)	79	89
1	D	243/261~(93%)	242 (100%)	1 (0%)	89	95
All	All	969/1044~(93%)	963~(99%)	6 (1%)	84	92

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	268	ASN
1	В	58	SER
1	В	283	SER
1	С	62	ASP
1	С	138	ASN
1	D	33	THR



Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	286	HIS
1	В	286	HIS
1	С	203	HIS
1	С	208	GLN
1	D	133	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 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).

Mal	Turne	Chain	Dec	Tinle	Bo	ond leng	$_{\rm ths}$	B	ond ang	gles
	туре	Chain	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	EDO	D	404	-	3,3,3	0.16	0	2,2,2	0.35	0
3	GTQ	А	402	4	11,11,11	1.88	2 (18%)	$15,\!15,\!15$	0.98	1 (6%)
2	CO2	А	401	-	2,2,2	0.44	0	1,1,1	0.35	0
3	GTQ	D	401	4	11,11,11	1.64	1 (9%)	$15,\!15,\!15$	2.00	3 (20%)
5	EDO	D	403	-	3,3,3	0.28	0	2,2,2	0.39	0
2	CO2	D	402	-	2,2,2	0.20	0	1,1,1	0.35	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
3	GTQ	А	402	4	-	4/4/4/4	0/1/1/1
5	EDO	D	404	-	-	1/1/1/1	-
3	GTQ	D	401	4	-	4/4/4/4	0/1/1/1
5	EDO	D	403	-	-	1/1/1/1	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
3	А	402	GTQ	OAD-CAJ	-5.57	1.25	1.36
3	D	401	GTQ	OAD-CAJ	-4.92	1.26	1.36
3	А	402	GTQ	CAF-CAJ	2.03	1.43	1.39

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$\mathbf{Observed}(^{o})$	$\operatorname{Ideal}(^{o})$
3	D	401	GTQ	CAG-CAK-CAJ	4.06	122.60	118.70
3	D	401	GTQ	OAB-CAH-CAK	-3.91	112.43	121.94
3	D	401	GTQ	CAF-CAJ-CAK	-3.35	116.28	119.89
3	А	402	GTQ	CAG-CAK-CAJ	2.47	121.07	118.70

There are no chirality outliers.

All (10) torsion outlie	rs are listed below:
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Mol	Chain	Res	Type	Atoms
3	А	402	GTQ	OAA-CAH-CAK-CAJ
3	А	402	GTQ	OAB-CAH-CAK-CAJ
3	D	401	GTQ	OAA-CAH-CAK-CAJ
3	D	401	GTQ	OAB-CAH-CAK-CAJ
5	D	403	EDO	O1-C1-C2-O2
3	А	402	GTQ	OAA-CAH-CAK-CAG
3	А	402	GTQ	OAB-CAH-CAK-CAG
5	D	404	EDO	O1-C1-C2-O2
3	D	401	GTQ	OAA-CAH-CAK-CAG
3	D	401	GTQ	OAB-CAH-CAK-CAG

There are no ring outliers.

2 monomers are involved in 3 short contacts:



Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	404	EDO	1	0
3	А	402	GTQ	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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 (i)

6.1 Protein, DNA and RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

















6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

