

# Full wwPDB X-ray Structure Validation Report (i)

#### Nov 8, 2021 – 02:32 PM EST

PDB ID	:	6VK4
Title	:	Crystal Structure of Methylosinus trichosporium OB3b Soluble Methane
		Monooxygenase Hydroxylase and Regulatory Component Complex
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Deposited on	:	2020-01-18
Resolution	:	2.35  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 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	:	2.23.2
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)	:	2.23.2

## 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 2.35 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.



Motrie	Whole archive	Similar resolution
WIEUTIC	$(\# { m Entries})$	$(\# { m Entries},  { m resolution}  { m range}({ m \AA}))$
$R_{free}$	130704	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	$1211 \ (2.36-2.36)$
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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	А	526	83%	15%	
-	_	020	4%	1370	
1	E	526	85%	12%	••
2	В	395	89%	10%	<b>.</b>
2	F	395	5%	09/	
	T	000	2%	9%	•
3	С	169	89%	9%	••



Mol	Chain	Length	Quality of chain		
3	G	169	5% 91%		8% •
4	D	138	4%	12%	6%
4	Н	138	2% 86%	9%	6%



## 2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 19709 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

• Molecule 1 is a protein called Methane monooxygenase component A alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	А	515	Total 4175	C 2676	N 723	О 764	S 12	0	0	0
1	Е	515	Total 4175	C 2676	N 723	О 764	S 12	0	0	0

• Molecule 2 is a protein called Methane monooxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	o B	391	Total	С	Ν	Ο	$\mathbf{S}$	0	0	0
	D		3177	2029	554	589	5			
0	Б	201	Total	С	Ν	0	S	0	0	0
2 Г	391	3177	2029	554	589	5	0	U	U	

• Molecule 3 is a protein called Methane monooxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	С	167	Total 1357	C 871	N 233	O 252	S 1	0	0	0
3	G	167	Total 1357	C 871	N 233	O 252	S 1	0	0	0

• Molecule 4 is a protein called Methane monooxygenase regulatory protein B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4		120	Total	С	Ν	0	S	0	0	0
4 D	150	985	630	157	195	3	0	0	0	
4	TT	130	Total	С	Ν	0	S	0	0	0
4 П	130	985	630	157	195	3			0	

• Molecule 5 is FE (III) ION (three-letter code: FE) (formula: Fe).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	2	Total Fe 2 2	0	0

• Molecule 6 is BENZOIC ACID (three-letter code: BEZ) (formula:  $C_7H_6O_2$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 9 & 7 & 2 \end{array}$	0	0
6	Е	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 9 & 7 & 2 \end{array}$	0	0

• Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).





Mol	Chain	Residues	Ate	oms		ZeroOcc	AltConf
7	С	1	Total 4	$\begin{array}{c} \mathrm{C} \\ \mathrm{2} \end{array}$	O 2	0	0

• Molecule 8 is FE (II) ION (three-letter code: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	Е	2	Total Fe 2 2	0	0

• Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	А	71	Total O 71 71	0	0
9	В	55	$\begin{array}{cc} \text{Total} & \text{O} \\ 55 & 55 \end{array}$	0	0
9	С	17	Total O 17 17	0	0
9	D	4	Total O 4 4	0	0
9	Ε	61	$\begin{array}{cc} \text{Total} & \text{O} \\ 61 & 61 \end{array}$	0	0
9	F	62	$\begin{array}{cc} \text{Total} & \text{O} \\ 62 & 62 \end{array}$	0	0
9	G	17	Total O 17 17	0	0
9	Н	8	Total O 8 8	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 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: Methane monooxygenase component A alpha chain







## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	102.86Å $105.21$ Å $300.88$ Å	Deperitor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
$\mathbf{P}_{\text{assolution}}(\hat{\mathbf{A}})$	52.59 - 2.35	Depositor
Resolution (A)	97.33 - 2.35	EDS
% Data completeness	96.3 (52.59-2.35)	Depositor
(in resolution range)	96.4 (97.33-2.35)	EDS
R <sub>merge</sub>	0.15	Depositor
R <sub>sym</sub>	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.42 (at 2.34 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.20rc2_4400	Depositor
D D.	0.190 , $0.228$	Depositor
$\Pi, \Pi_{free}$	0.198 , $0.231$	DCC
$R_{free}$ test set	6694 reflections $(5.09%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	57.5	Xtriage
Anisotropy	0.345	Xtriage
Bulk solvent $k_{sol}(e/A^3)$ , $B_{sol}(A^2)$	0.33, $39.4$	EDS
L-test for twinning <sup>2</sup>	$< L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	0.088 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	19709	wwPDB-VP
Average B, all atoms $(Å^2)$	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.32% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;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.



<sup>&</sup>lt;sup>1</sup>Intensities 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: FE2, FE, BEZ, 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	
		RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	А	0.33	0/4305	0.53	0/5850
1	Ε	0.32	0/4305	0.53	0/5850
2	В	0.31	0/3270	0.54	0/4446
2	F	0.31	0/3270	0.53	0/4446
3	С	0.33	0/1383	0.52	0/1870
3	G	0.31	0/1383	0.53	0/1870
4	D	0.30	0/1001	0.47	0/1354
4	Н	0.31	0/1001	0.47	0/1354
All	All	0.32	0/19918	0.52	0/27040

There are no bond length outliers.

There are no bond angle outliers.

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	А	4175	0	3972	50	0
1	Е	4175	0	3972	40	0
2	В	3177	0	3019	23	0
2	F	3177	0	3019	25	0
3	С	1357	0	1395	10	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	1357	0	1395	10	0
4	D	985	0	977	11	0
4	Н	985	0	977	8	0
5	А	2	0	0	0	0
6	А	9	0	5	0	0
6	Е	9	0	5	0	0
7	С	4	0	6	1	0
8	Е	2	0	0	0	0
9	А	71	0	0	1	0
9	В	55	0	0	1	0
9	С	17	0	0	0	0
9	D	4	0	0	0	0
9	Е	61	0	0	1	0
9	F	62	0	0	0	0
9	G	17	0	0	1	0
9	Н	8	0	0	0	0
All	All	19709	0	18742	151	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (151) 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:214:ASN:OD1	4:D:110:SER:OG	2.07	0.70
4:H:54:ASP:HB2	4:H:94:LEU:HD21	1.76	0.66
2:B:259:PHE:HA	2:B:335:LEU:HD21	1.79	0.64
1:E:201:SER:HA	1:E:205:GLN:HG3	1.79	0.64
2:B:42:ILE:HD13	2:B:57:CYS:HB2	1.80	0.63
1:E:44:THR:HB	1:E:127:SER:HA	1.81	0.63
1:E:52:MET:HE2	1:E:257:ILE:HA	1.80	0.63
1:E:52:MET:HE1	1:E:257:ILE:HG12	1.82	0.62
1:A:442:ASN:O	1:A:442:ASN:ND2	2.34	0.59
1:A:396:GLU:OE1	1:A:502:ARG:NH2	2.35	0.58
4:D:93:GLU:HB3	2:F:48:ARG:HG3	1.85	0.58
3:C:168:GLN:HG3	7:C:201:EDO:H22	1.86	0.58
1:E:320:ARG:HH12	1:E:323:LYS:HE2	1.69	0.58
2:B:225:PRO:HA	2:B:228:SER:HB2	1.86	0.57
3:G:26:VAL:HG23	3:G:72:LYS:HD3	1.86	0.56
1:E:214:ASN:OD1	4:H:110:SER:OG	2.16	0.56
4:D:69:VAL:HG22	4:D:78:ILE:HG12	1.87	0.55



	lous pagem	Interatomic	Clash		
Atom-1	Atom-2	distance (Å)	overlap (Å)		
1:E:187:VAL:HG23	1:E:278:GLN:HA	1.88	0.55		
2:F:42:ILE:HD13	2:F:57:CYS:HB2	1.88	0.55		
1:E:66:GLU:OE2	1:E:69:ARG:NH1	2.39	0.55		
2:B:79:PHE:HB2	2:B:83:ARG:HB3	1.87	0.55		
2:B:121:ARG:HD3	2:F:118:GLU:OE2	2.06	0.55		
2:B:381:ASP:HB3	2:B:384:GLN:HB3	1.89	0.55		
4:D:101:VAL:HG22	4:D:120:THR:HA	1.89	0.54		
1:E:316:ILE:HG12	4:H:37:ALA:O	2.07	0.54		
1:E:182:LYS:NZ	9:E:701:HOH:O	2.31	0.54		
1:A:447:SER:HB3	1:A:523:LEU:HD21	1.90	0.54		
3:C:57:ILE:O	3:C:61:ILE:HG13	2.09	0.53		
1:E:196:ASP:HB3	1:E:199:GLU:HB2	1.89	0.53		
2:B:144:ARG:NH1	2:B:207:VAL:HG11	2.24	0.52		
1:E:124:LEU:HD21	1:E:200:CYS:HB2	1.91	0.52		
1:E:119:ALA:HB1	2:F:171:ARG:HD2	1.92	0.52		
4:D:54:ASP:HB2	4:D:94:LEU:HD21	1.90	0.52		
1:A:276:TRP:CE3	1:A:331:SER:HB2	2.46	0.51		
1:A:354:TRP:CG	1:A:355:PRO:HD3	2.45	0.51		
1:A:147:HIS:CD2	1:A:239:VAL:HG13	2.46	0.51		
2:F:272:ALA:HB1	2:F:277:ASP:HB3	1.91	0.51		
1:A:207:VAL:O	1:A:211:CYS:HB3	2.10	0.51		
2:F:47:LYS:HD3	2:F:47:LYS:H	1.75	0.51		
1:A:298:VAL:HG13	2:B:10:THR:HG21	1.93	0.51		
3:C:5:GLU:OE2	3:C:11:SER:OG	2.24	0.50		
2:F:151:TYR:OH	2:F:344:LYS:NZ	2.25	0.50		
1:E:118:ILE:HD13	1:E:145:ILE:HG12	1.93	0.50		
1:E:185:LYS:O	1:E:189:ALA:HB3	2.12	0.50		
1:A:185:LYS:O	1:A:189:ALA:HB3	2.12	0.49		
1:A:224:ALA:HB1	1:A:229:ASP:HB3	1.94	0.49		
1:A:281:TYR:CZ	1:A:285:VAL:HG21	2.48	0.49		
2:F:12:ARG:NH2	4:H:73:ALA:O	2.45	0.49		
1:A:322:GLY:HA2	1:A:326:VAL:O	2.13	0.49		
1:E:140:GLN:HG3	1:E:246:HIS:CE1	2.47	0.49		
2:F:11:LYS:O	2:F:19:ARG:NH1	2.46	0.49		
1:A:60:PHE:O	1:A:62:VAL:HG13	2.13	0.49		
2:F:116:LYS:NZ	2:F:191:ASP:OD2	2.43	0.48		
1:A:50:TYR:HD1	1:A:263:SER:HB2	1.78	0.48		
1:A:218:VAL:O	1:A:221:THR:HB	2.14	0.48		
1:A:324:TYR:OH	4:D:132:ASP:OD1	2.31	0.48		
1:E:211:CYS:HB2	1:E:313:TRP:CD1	2.49	0.48		
2:B:78:LYS:HG2	2:B:84:PRO:HA	1.96	0.47		



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:E:207:VAL:O	1:E:211:CYS:HB3	2.14	0.47	
1:A:193:ILE:HD11	2:B:85:SER:HB3	1.97	0.47	
2:B:118:GLU:OE2	2:F:121:ARG:HD3	2.14	0.47	
1:A:243:GLU:O	1:A:247:MET:HG3	2.14	0.47	
2:F:189:LYS:HD3	2:F:189:LYS:HA	1.74	0.47	
2:B:164:ASN:HB3	2:B:238:TRP:CE2	2.50	0.47	
1:A:398:PRO:HA	1:A:507:TRP:CE2	2.49	0.47	
1:E:211:CYS:HB2	1:E:313:TRP:CE2	2.50	0.47	
1:A:203:ASN:OD1	1:A:204:LEU:N	2.47	0.46	
1:E:215:PRO:HA	1:E:219:ALA:HB3	1.97	0.46	
2:B:191:ASP:O	2:B:195:MET:HG2	2.16	0.46	
1:A:59:GLN:HG3	1:A:248:ALA:HB1	1.97	0.46	
1:A:320:ARG:HB3	4:D:128:LEU:HD11	1.96	0.46	
2:B:173:CYS:HA	2:B:244:TRP:CE2	2.51	0.46	
3:C:56:TYR:CZ	3:C:60:LYS:HD2	2.50	0.46	
1:E:146:ARG:HB2	2:F:109:HIS:CE1	2.51	0.46	
1:E:265:LYS:HE2	1:E:266:PHE:CZ	2.50	0.46	
1:A:211:CYS:HB2	1:A:313:TRP:CE2	2.51	0.46	
2:F:79:PHE:HB2	2:F:83:ARG:HB3	1.96	0.46	
2:B:118:GLU:HG2	2:F:118:GLU:HG2	1.98	0.46	
1:E:396:GLU:OE1	1:E:502:ARG:NH2	2.45	0.45	
1:A:441:PHE:HB2	3:C:162:VAL:HG12	1.97	0.45	
2:F:89:GLU:OE2	3:G:116:ARG:NH2	2.46	0.45	
1:A:297:LYS:HD2	1:A:371:TRP:CZ3	2.51	0.45	
2:B:301:LEU:O	2:B:305:CYS:HB2	2.16	0.45	
1:E:255:VAL:HG13	4:H:131:LEU:HG	1.98	0.45	
1:A:187:VAL:HG23	1:A:278:GLN:HA	1.97	0.45	
1:A:221:THR:HG21	1:A:237:LEU:HD11	1.97	0.45	
1:A:415:VAL:HG22	1:A:426:ILE:HG12	1.99	0.45	
3:C:116:ARG:O	3:C:120:LYS:HB2	2.17	0.45	
3:G:147:ASP:OD1	3:G:150:GLY:HA3	2.17	0.45	
2:F:47:LYS:H	2:F:47:LYS:CD	2.30	0.45	
1:A:140:GLN:O	1:A:144:GLU:HG2	2.17	0.44	
1:A:146:ARG:HB2	2:B:109:HIS:CE1	2.52	0.44	
1:A:36:ASN:HB2	1:A:131:ALA:HB2	1.98	0.44	
1:A:206:LEU:O	1:A:210:ALA:HB3	2.18	0.44	
2:F:358:SER:HB2	2:F:390:LEU:HD11	1.99	0.44	
3:G:41:THR:HG22	3:G:54:TYR:CE2	2.51	0.44	
1:A:109:PHE:O	1:A:112:VAL:HG12	2.18	0.44	
1:E:147:HIS:CD2	1:E:239:VAL:HG13	2.52	0.44	
1:E:32:LEU:HD12	1:E:32:LEU:HA	1.82	0.44	



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
2:B:140:ASP:HB3	2:B:143:TRP:HB3	2.00	0.44	
2:F:148:LEU:O	2:F:152:PHE:HB3	2.17	0.44	
1:A:354:TBP:CH2	1.A.499.PRO.HD3	2.53	0.44	
1:A:466:CYS:HB2	2·B·76·THB·HA	2.00	0.44	
1:A:49:LYS:HG2	3:C:142:GLU:HG2	2.00	0.43	
2:B:225:PRO:O	2:B:337:ASP:HB3	2.17	0.43	
1:E:435:SEB:OG	1:E:437:ARG:NH2	2.50	0.43	
4:D:39:VAL:HB	4:D:112:VAL:HB	2.00	0.43	
2:F:139:ILE:HG13	2:F:277:ASP:HA	2.00	0.43	
1·A·181·TRP·NE1	$1 \cdot A \cdot 185 \cdot LYS \cdot HD2$	2.34	0.43	
2·B·62·ASN·HB2	$2 \cdot B \cdot 99 \cdot TYB \cdot OH$	2.18	0.43	
1·E·398·PBO·HA	$1 \cdot E \cdot 507 \cdot TBP \cdot CE2$	2.53	0.43	
1:A:348:LEU:HD13	1:A:429:LEU:HD13	2.00	0.43	
1.E.354.TRP.CG	1:E:355:PRO:HD3	2.53	0.43	
3·G·16·TBP·CG	3·G·57·ILE·HD13	2.53	0.43	
1·A·94·LYS·HE2	9·B·453·HOH·O	2.00	0.43	
3·C·137·GLY·O	3·C·141·MET·HB2	2.10	0.43	
2·F·315·HIS·NE2	3·G·66·SEB·OG	2.43	0.43	
$\frac{1 \cdot E \cdot 281 \cdot TYB \cdot CZ}{1 \cdot E \cdot 281 \cdot TYB \cdot CZ}$	1.E.285.VAL.HG21	2.53	0.43	
1.E.466.CYS.HB2	2·F·76·THB·HA	2.00	0.42	
1.A.333.ABG.NH2	4·D·27·GLU·OE2	2.52	0.42	
4·H·48·ILE·HD13	4·H·48·ILE:HA	1.92	0.42	
1:A·284·PRO·HA	1·A·343·HIS·HB3	2.01	0.42	
2:B:272:ALA:HB1	2:B:277:ASP:HB3	1.99	0.42	
1:E:187:VAL:HG13	1:E:188:PHE:N	2.35	0.42	
3:G:110:ARG:HA	3:G:110:ARG:HD2	1.87	0.42	
1:A:175:ARG:HD2	1:A:181:TRP:CZ3	2.54	0.42	
1:E:140:GLN:HG3	1:E:246:HIS:NE2	2.35	0.42	
1:A:200:CYS:HA	1:A:203:ASN:OD1	2.20	0.42	
1:E:125:TRP:CZ3	1:E:138:LEU:HD13	2.55	0.41	
1:A:67:TYR:CZ	1:A:71:GLU:HG3	2.55	0.41	
2:F:47:LYS:HB2	2:F:47:LYS:HE2	1.67	0.41	
1:A:89:LEU:HD21	1:E:230:GLU:HG3	2.02	0.41	
3:G:60:LYS:HD3	3:G:60:LYS:HA	1.79	0.41	
1:E:140:GLN:O	1:E:144:GLU:HG2	2.21	0.41	
2:F:80:HIS:HB3	3:G:140:LEU:HD23	2.03	0.41	
3:C:110:ARG:HD2	3:C:110:ARG:HA	1.81	0.41	
4:D:68:VAL:O	4:D:78:ILE:HA	2.21	0.41	
2:F:204:ALA:HB2	2:F:212:ALA:HB2	2.03	0.41	
1:A:74:LYS:HE2	4:D:106:ILE:HA	2.02	0.41	
1:E:12:ASP:OD2	1:E:15:LYS:N	2.47	0.41	



Atom-1	Atom-2	Interatomic	Clash
		distance (A)	overlap (A)
3:G:12:ILE:HD13	9:G:208:HOH:O	2.20	0.41
1:A:25:PRO:HA	1:A:63:ILE:HD13	2.03	0.40
4:H:9:ASN:O	4:H:14:GLN:HG2	2.21	0.40
2:B:301:LEU:O	2:B:306:LEU:HG	2.21	0.40
1:E:354:TRP:CH2	1:E:499:PRO:HD3	2.55	0.40
4:H:3:SER:HB3	4:H:66:SER:HA	2.03	0.40
1:A:46:TYR:HB3	9:A:713:HOH:O	2.21	0.40
1:A:297:LYS:HD2	1:A:371:TRP:CE3	2.57	0.40
1:E:104:LYS:NZ	1:E:166:ALA:O	2.50	0.40
1:E:90:GLY:O	1:E:94:LYS:HD3	2.22	0.40
3:C:121:PRO:HD3	3:C:129:PHE:CG	2.57	0.40

There are no symmetry-related clashes.

### 5.3 Torsion angles (i)

#### 5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
1	А	513/526~(98%)	497 (97%)	16 (3%)	0	100	100
1	Е	513/526~(98%)	495 (96%)	18 (4%)	0	100	100
2	В	389/395~(98%)	378~(97%)	11 (3%)	0	100	100
2	F	389/395~(98%)	375~(96%)	14 (4%)	0	100	100
3	С	165/169~(98%)	160 (97%)	5(3%)	0	100	100
3	G	165/169~(98%)	160 (97%)	5(3%)	0	100	100
4	D	128/138~(93%)	121 (94%)	6~(5%)	1 (1%)	19	20
4	Н	128/138~(93%)	121 (94%)	7~(6%)	0	100	100
All	All	2390/2456~(97%)	2307 (96%)	82 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
4	D	73	ALA

#### 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	Perce	ntiles
1	А	426/433~(98%)	420 (99%)	6 (1%)	67	78
1	Ε	426/433~(98%)	417 (98%)	9(2%)	53	65
2	В	323/327~(99%)	319~(99%)	4 (1%)	71	82
2	F	323/327~(99%)	315~(98%)	8 (2%)	47	58
3	С	145/146~(99%)	144 (99%)	1 (1%)	84	91
3	G	145/146~(99%)	145 (100%)	0	100	100
4	D	103/110~(94%)	102~(99%)	1 (1%)	76	85
4	Н	103/110~(94%)	102 (99%)	1 (1%)	76	85
All	All	1994/2032~(98%)	1964 (98%)	30 (2%)	65	76

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	52	MET
1	А	61	LYS
1	А	142	LEU
1	А	221	THR
1	А	307	ARG
1	А	442	ASN
2	В	163	PHE
2	В	176	ASP
2	В	270	ARG
2	В	274	VAL
3	С	141	MET
4	D	14	GLN
1	Е	16	VAL
1	Е	52	MET
1	Е	69	ARG



Mol	Chain	Res	Type
1	Е	105	VAL
1	Е	205	GLN
1	Е	273	ASN
1	Ε	307	ARG
1	Ε	337	ARG
1	Ε	437	ARG
2	F	8	GLN
2	F	47	LYS
2	F	95	THR
2	F	156	LEU
2	F	163	PHE
2	F	176	ASP
2	F	270	ARG
2	F	274	VAL
4	Н	114	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

#### 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 monosaccharides in this entry.

### 5.6 Ligand geometry (i)

Of 7 ligands modelled in this entry, 4 are monoatomic - leaving 3 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



Mal Trme Chain B		Dec	Tink	Bond lengths			Bond angles			
IVIOI	Type	Unain	nes		Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z >2
6	BEZ	А	603	5	7,9,9	1.21	1 (14%)	8,11,11	0.45	0
7	EDO	С	201	-	3,3,3	0.52	0	2,2,2	0.19	0
6	BEZ	E	603	8	7,9,9	1.67	1 (14%)	8,11,11	0.30	0

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).

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
6	BEZ	А	603	5	-	0/0/4/4	0/1/1/1
7	EDO	С	201	-	-	0/1/1/1	-
6	BEZ	Е	603	8	-	0/0/4/4	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
6	Е	603	BEZ	C1-C	4.27	1.51	1.47
6	А	603	BEZ	C1-C	3.00	1.50	1.47

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	201	EDO	1	0

## 5.7 Other polymers (i)

There are no such residues in this entry.

### 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



## 6 Fit of model and data (i)

## 6.1 Protein, DNA and RNA chains (i)

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,  $95^{th}$  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	$OWAB(Å^2)$	Q<0.9
1	А	515/526~(97%)	0.47	27 (5%) 27 39	47, 60, 85, 117	0
1	Е	515/526~(97%)	0.66	22 (4%) 35 47	50, 61, 81, 107	0
2	В	391/395~(98%)	0.34	7 (1%) 68 77	49, 60, 77, 105	0
2	F	391/395~(98%)	0.61	21 (5%) 25 37	52, 61, 78, 118	0
3	С	167/169~(98%)	0.31	3 (1%) 68 77	56, 67, 79, 89	0
3	G	167/169~(98%)	0.58	9 (5%) 25 37	59, 69, 83, 99	0
4	D	130/138~(94%)	0.68	5 (3%) 40 53	63, 74, 96, 118	0
4	Н	130/138~(94%)	0.61	3 (2%) 60 70	57, 72, 92, 108	0
All	All	2406/2456~(97%)	0.53	97 (4%) 38 51	47, 63, 84, 118	0

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	4	PRO	6.0
2	F	332	VAL	4.9
2	F	364	VAL	4.6
1	А	216	LEU	4.2
1	А	257	ILE	4.0
2	F	147	ILE	3.9
1	А	271	LEU	3.5
1	Е	53	ALA	3.4
2	F	392	GLY	3.4
2	В	6	SER	3.4
1	А	374	ALA	3.4
2	F	155	LEU	3.4
1	А	321	LEU	3.3
1	Е	257	ILE	3.3
1	Е	47	PRO	3.3
2	F	347	LYS	3.2



Mol	Chain	Res	Type	RSRZ
3	G	33	ILE	3.2
1	А	459	ILE	3.2
2	F	160	TYR	3.2
1	Е	324	TYR	3.2
2	F	226	ILE	3.1
3	G	75	VAL	3.0
1	А	266	PHE	3.0
2	F	149	ASN	3.0
4	D	3	SER	3.0
1	А	202	VAL	3.0
3	G	156	LEU	3.0
1	А	60	PHE	3.0
2	F	319	PHE	3.0
1	А	121	SER	2.9
4	D	7	ALA	2.9
2	В	4	PRO	2.9
1	А	323	LYS	2.9
1	А	282	PHE	2.9
2	F	380	VAL	2.8
3	С	20	ILE	2.8
4	Н	131	LEU	2.8
2	F	162	LEU	2.7
1	Е	48	THR	2.7
3	С	156	LEU	2.7
4	Н	52	ILE	2.6
2	F	385	LYS	2.5
4	Н	3	SER	2.5
1	А	439	HIS	2.5
1	Е	251	TYR	2.5
1	Е	202	VAL	2.5
1	Е	415	VAL	2.5
2	F	227	TYR	2.5
1	А	218	VAL	2.5
1	А	207	VAL	2.4
1	Е	171	ALA	2.4
1	Е	356	LEU	2.4
1	А	16	VAL	2.4
2	F	339	VAL	2.4
3	С	162	VAL	2.4
3	G	103	LYS	2.4
1	А	290	PHE	2.4
1	Е	478	LEU	2.3



Mol	Chain	Res	Type	RSRZ
3	G	143	ILE	2.3
1	Е	353	MET	2.3
2	F	384	GLN	2.3
2	F	327	TYR	2.3
2	В	7	SER	2.3
1	Е	355	PRO	2.3
1	Е	219	ALA	2.3
2	В	386	VAL	2.3
3	G	102	ALA	2.3
1	Е	432	GLY	2.2
1	А	332	LEU	2.2
1	А	325	GLY	2.2
1	А	212	PHE	2.2
1	Е	262	ALA	2.2
4	D	26	ALA	2.2
1	Е	220	VAL	2.1
1	Е	60	PHE	2.1
1	А	248	ALA	2.1
1	Е	52	MET	2.1
1	Е	201	SER	2.1
2	В	206	LEU	2.1
1	А	62	VAL	2.1
2	F	345	VAL	2.1
3	G	119	TYR	2.1
4	D	67	ILE	2.1
3	G	118	LEU	2.1
1	А	482	ILE	2.1
1	А	478	LEU	2.1
1	А	324	TYR	2.1
2	В	347	LYS	2.1
1	А	415	VAL	2.1
2	F	372	TYR	2.1
1	А	15	LYS	2.0
1	Е	383	TYR	2.0
4	D	110	SER	2.0
2	F	9	VAL	2.0
2	В	271	LEU	2.0
1	Е	497	ALA	2.0
3	G	89	ALA	2.0

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### 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 monosaccharides 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,  $95^{th}$  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	${f B} ext{-factors}({ m \AA}^2)$	Q < 0.9
7	EDO	С	201	4/4	0.93	0.11	$63,\!63,\!64,\!65$	0
6	BEZ	Е	603	9/9	0.96	0.31	$61,\!63,\!67,\!69$	0
6	BEZ	А	603	9/9	0.96	0.23	58,61,64,65	0
5	FE	А	602	1/1	0.98	0.14	70,70,70,70	0
5	FE	А	601	1/1	0.98	0.14	64,64,64,64	0
8	FE2	Е	601	1/1	0.98	0.22	66,66,66,66	0
8	FE2	Е	602	1/1	0.99	0.18	57,57,57,57	0

## 6.5 Other polymers (i)

There are no such residues in this entry.

