

Full wwPDB X-ray Structure Validation Report (i)

Oct 11, 2023 – 02:08 PM EDT

PDB ID	:	8EKG
Title	:	MHETase variant Thr159Val, Met192Tyr, Tyr252Phe, Tyr503Trp
Authors	:	Saunders, J.W.; Frkic, R.L.; Jackson, C.J.
Deposited on	:	2022-09-20
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	:	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 (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}	130704	1332 (2.68-2.64)
Clashscore	141614	1374(2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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	592	.% 8 5%	9%	6%
1	В	592	81%	13%	6%
1	С	592	83%	10%	6%
1	D	592	% 8 5%	9%	6%
1	Е	592	^{2%} 79%	15%	6%



Mol	Chain	Length	Quality of chain		
			3%		
1	F	592	80%	14%	• 6%



$8 \mathrm{EKG}$

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 25228 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.

Mol	Chain	Residues		I	Atom	s			ZeroOcc	AltConf	Trace	
1	А	558	Total	С	Ν	0	Р	S	0	0	0	
			4128	2583	726	791	1	27	Ŭ	Ŭ	Ŭ	
1	В	557	Total	\mathbf{C}	Ν	0	Р	\mathbf{S}	0	0	0	
1	D	557	4123	2580	725	790	1	27	0	0	0	
1	С	557	Total	С	Ν	0	Р	\mathbf{S}	0	0	0	
1	U		4123	2580	725	790	1	27			0	
1	а	557	557	Total	С	Ν	0	Р	S	0	0	0
1	D		4123	2580	725	790	1	27	0	0	0	
1	F	558	Total	С	Ν	0	Р	S	0	0	0	
1		558	4128	2583	726	791	1	27	0	0	0	
1	Б	557	Total	С	Ν	0	Р	S	0	0	0	
	I F	557	4123	2580	725	790	1	27	0	U	0	

• Molecule 1 is a protein called Mono(2-hydroxyethyl) terephthalate hydrolase.

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	12	MET	-	initiating methionine	UNP A0A0K8P8E7
А	13	GLU	-	expression tag	UNP A0A0K8P8E7
А	14	ASN	-	expression tag	UNP A0A0K8P8E7
А	15	LEU	-	expression tag	UNP A0A0K8P8E7
А	16	TYR	-	expression tag	UNP A0A0K8P8E7
А	17	PHE	-	expression tag	UNP A0A0K8P8E7
А	18	GLN	-	expression tag	UNP A0A0K8P8E7
А	19	GLY	-	expression tag	UNP A0A0K8P8E7
А	159	VAL	THR	engineered mutation	UNP A0A0K8P8E7
А	192	TYR	MET	engineered mutation	UNP A0A0K8P8E7
А	252	PHE	TYR	engineered mutation	UNP A0A0K8P8E7
А	503	TRP	TYR	engineered mutation	UNP A0A0K8P8E7
В	12	MET	-	initiating methionine	UNP A0A0K8P8E7
В	13	GLU	-	expression tag	UNP A0A0K8P8E7
В	14	ASN	-	expression tag	UNP A0A0K8P8E7
В	15	LEU	-	expression tag	UNP A0A0K8P8E7
B	16	TYR	-	expression tag	UNP A0A0K8P8E7



Chain	Residue	Modelled	Actual	Comment	Reference
В	17	PHE	-	expression tag	UNP A0A0K8P8E7
В	18	GLN	-	expression tag	UNP A0A0K8P8E7
В	19	GLY	-	expression tag	UNP A0A0K8P8E7
В	159	VAL	THR	engineered mutation	UNP A0A0K8P8E7
В	192	TYR	MET	engineered mutation	UNP A0A0K8P8E7
В	252	PHE	TYR	engineered mutation	UNP A0A0K8P8E7
В	503	TRP	TYR	engineered mutation	UNP A0A0K8P8E7
С	12	MET	_	initiating methionine	UNP A0A0K8P8E7
С	13	GLU	-	expression tag	UNP A0A0K8P8E7
С	14	ASN	-	expression tag	UNP A0A0K8P8E7
С	15	LEU	-	expression tag	UNP A0A0K8P8E7
С	16	TYR	-	expression tag	UNP A0A0K8P8E7
С	17	PHE	-	expression tag	UNP A0A0K8P8E7
С	18	GLN	-	expression tag	UNP A0A0K8P8E7
С	19	GLY	-	expression tag	UNP A0A0K8P8E7
С	159	VAL	THR	engineered mutation	UNP A0A0K8P8E7
С	192	TYR	MET	engineered mutation	UNP A0A0K8P8E7
С	252	PHE	TYR	engineered mutation	UNP A0A0K8P8E7
С	503	TRP	TYR	engineered mutation	UNP A0A0K8P8E7
D	12	MET	-	initiating methionine	UNP A0A0K8P8E7
D	13	GLU	-	expression tag	UNP A0A0K8P8E7
D	14	ASN	-	expression tag	UNP A0A0K8P8E7
D	15	LEU	-	expression tag	UNP A0A0K8P8E7
D	16	TYR	-	expression tag	UNP A0A0K8P8E7
D	17	PHE	-	expression tag	UNP A0A0K8P8E7
D	18	GLN	-	expression tag	UNP A0A0K8P8E7
D	19	GLY	-	expression tag	UNP A0A0K8P8E7
D	159	VAL	THR	engineered mutation	UNP A0A0K8P8E7
D	192	TYR	MET	engineered mutation	UNP A0A0K8P8E7
D	252	PHE	TYR	engineered mutation	UNP A0A0K8P8E7
D	503	TRP	TYR	engineered mutation	UNP A0A0K8P8E7
E	12	MET	-	initiating methionine	UNP A0A0K8P8E7
E	13	GLU	-	expression tag	UNP A0A0K8P8E7
E	14	ASN	-	expression tag	UNP A0A0K8P8E7
E	15	LEU	-	expression tag	UNP A0A0K8P8E7
E	16	TYR	-	expression tag	UNP A0A0K8P8E7
E	17	PHE	_	expression tag	UNP A0A0K8P8E7
E	18	GLN	_	expression tag	UNP A0A0K8P8E7
E	19	GLY	-	expression tag	UNP A0A0K8P8E7
E	159	VAL	THR	engineered mutation	UNP A0A0K8P8E7
E	192	TYR	MET	engineered mutation	UNP A0A0K8P8E7
E	252	PHE	TYR	engineered mutation	UNP A0A0K8P8E7



Chain	Residue	Modelled	Actual	Comment	Reference
Е	503	TRP	TYR	engineered mutation	UNP A0A0K8P8E7
F	12	MET	-	initiating methionine	UNP A0A0K8P8E7
F	13	GLU	-	expression tag	UNP A0A0K8P8E7
F	14	ASN	-	expression tag	UNP A0A0K8P8E7
F	15	LEU	-	expression tag	UNP A0A0K8P8E7
F	16	TYR	-	expression tag	UNP A0A0K8P8E7
F	17	PHE	-	expression tag	UNP A0A0K8P8E7
F	18	GLN	-	expression tag	UNP A0A0K8P8E7
F	19	GLY	-	expression tag	UNP A0A0K8P8E7
F	159	VAL	THR	engineered mutation	UNP A0A0K8P8E7
F	192	TYR	MET	engineered mutation	UNP A0A0K8P8E7
F	252	PHE	TYR	engineered mutation	UNP A0A0K8P8E7
F	503	TRP	TYR	engineered mutation	UNP A0A0K8P8E7

• Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	Total Ca 1 1	0	0
2	В	1	Total Ca 1 1	0	0
2	С	1	Total Ca 1 1	0	0
2	D	1	Total Ca 1 1	0	0
2	Ε	1	Total Ca 1 1	0	0
2	F	1	Total Ca 1 1	0	0

• Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).





Mol	Chain	Residues	Ator	ms	ZeroOcc	AltConf
3	А	1	Total 7	C O 4 3	0	0

• Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0



Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	С	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	D	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	D	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	Е	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0

• Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
5	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
5	Е	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0



Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
5	Е	1	Total 5	0 4	S 1	0	0

• Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	А	70	Total O 70 70	0	0
6	В	91	Total O 91 91	0	0
6	С	71	Total O 71 71	0	0
6	D	64	$\begin{array}{cc} \text{Total} & \text{O} \\ 64 & 64 \end{array}$	0	0
6	Е	52	$\begin{array}{cc} \text{Total} & \text{O} \\ 52 & 52 \end{array}$	0	0
6	F	55	$\begin{array}{cc} \text{Total} & \text{O} \\ 55 & 55 \end{array}$	0	0



3 Residue-property plots (i)

MET GLU GLU GLU CLEU CLEU GLY GLY CLEU CLEU PRO GLN PRO GLN PRO GLN PRO GLN PRO CGLN VAL

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: Mono(2-hydroxyethyl) terephthalate hydrolase



M433 D191 M437 M196 M437 N196 P444 S196 F443 N196 P444 S225 P463 P246 W466 A247 P463 V246 P638 Q248 P639 P263 P633 P334 P633 P335 P633 P336 P441 P3377 P3377 P3377 P4410 P337 P4410 P410 P410 P410 P429 P429 P429 P429 P4410 P410

• Molecule 1: Mono(2-hydroxyethyl) terephthalate hydrolase

Chain D:	85%	9% 6%
MET ALU ALU TYR ALU TYR PIE GLY CLZ CLY CLZ CLY CLZ CLN CLN CLN CLN CLN CLN CLN CLN CLN CLN	CLAN CLAN CLAN CLAN CLAN PRO PRO PRO PRO PRO NALA ALA ALA ALA ALA ALA ALA ALA ALA AL	L115 1160 0163 0191 8196 8196
N210 122 225 225 8246 V246 V246 V246 V246 V246 V246 V246 V	D311 P332 A335 A335 A335 A335 A335 B361 B375 B361 D379 D379 D379 D379 D379 D379 D379 C400 C400 C400 C400 C400 C400 C400 C40	F424 1447 1455 F459 8663 ¥466
L474 M484 M480 M490 L507 L507 L518 L518 L514 L514 L514 L544 L544 L544 L544 L544		
• Molecule 1: Mono(2-hydroxye	thyl) terephthalate hydrolase	
Chain E:	79%	L5% 6%
MET ALU ALU TYR ALU TYR PIE GLY CLZ CLY CLZ CLN CLZ CLN CLN CLN CLN CLN CLN CLN CLN CLN CLN	GLM GLM GLU PR0 PR0 PR0 PR0 PR0 PR0 R46 R46 R46 R46 R48 R48 R48 R48 R48 R48 R48 R48 R48 R48	S84 L88 K100 R101 E110 M127 1149
L153 1160 1161 1162 1162 1162 1162 1162 1162	v266 F221 S225 H241 H241 F252 F252 F252 Q553 V260 W263 V260	1283 1284 1284 1285 1285 1287 1299 1299 1299 1299
D311 0312 1313 1314 0314 0315 1356 1356 1356 1366 1366 1366 1366 1	13 5 13 5 13 5 13 9 13 9 13 9 13 9 14 0 14 10 14 10 14 10 14 13 14 23 14 24 14	F445 1946 1447 1452 1452 1452 8463 8465 1465 1466 1466
K483 M490 1499 1522 1522 1523 1524 1524 1524 1544 1546 1546 1557	R5 84 R5 84 R5 84 R5 86 R5 86 R5 86 R5 88 R5 88 R5 91 R5 91 R5 91 R5 91 R5 92 R5 94 R5 95 R5 94 R5 95 R5 94 R5 95 R5 94 R5 95 R5 94 R5 95 R5 95	
• Molecule 1: Mono(2-hydroxye	thyl) terephthalate hydrolase	
Chain F:	80%	14% • 6%
MET ALU ALU TYR ALU TYR PLEU GLY GLY FLEU FLEU FLEU CLN GLN GLN GLN PRO GLN	GLN GLN CLU CLU CLU PRO PRO PRO PRO PRO PRO PRO CLU CLU CLU CLU CLU CLU CLU CLU CLU CLU	K100 1111 N134 0135 0135 0142 142 153
_ •		



L18 D18(P18(R375 W376 A377

T535 M331 D536 G333 L544 G333 L544 G333 L544 G333 L544 G333 H547 R411 M573 K566 M590 N412 M566 A431 M514 V422 M514 V423 M514 M431 M566 M432 M566 M441 M566 M446 M566 M446 M566 M446 M566 M446 M566 M446 M566 M446 M546 M446 M546 M446 M466 M446 M466 M446 M466 M446 M466 M466</t



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants	63.97Å 120.51Å 126.29Å	Deperitor
a, b, c, α , β , γ	90.44° 95.15° 90.20°	Depositor
$\mathbf{P}_{\text{assolution}}(\hat{\mathbf{A}})$	43.87 - 2.65	Depositor
Resolution (A)	43.87 - 2.65	EDS
% Data completeness	96.0 (43.87-2.65)	Depositor
(in resolution range)	96.0(43.87-2.65)	EDS
R _{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.43 (at 2.65 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
D D	0.184 , 0.241	Depositor
$\mathbf{n}, \mathbf{n}_{free}$	0.183 , 0.240	DCC
R_{free} test set	4887 reflections (4.67%)	wwPDB-VP
Wilson B-factor $(Å^2)$	43.5	Xtriage
Anisotropy	0.360	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.31, 29.8	EDS
L-test for $twinning^2$	$< L >=0.49, < L^2>=0.31$	Xtriage
Estimated twinning fraction	0.004 for -h,k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	25228	wwPDB-VP
Average B, all atoms $(Å^2)$	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.56% of the height of the origin peak. No significant pseudotranslation is detected.

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: SEP, EDO, PEG, SO4, CA

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	0.26	0/4226	0.50	0/5752
1	В	0.26	0/4221	0.49	0/5745
1	С	0.25	0/4221	0.49	0/5745
1	D	0.25	0/4221	0.49	0/5745
1	Е	0.25	0/4226	0.49	0/5752
1	F	0.25	0/4221	0.50	0/5745
All	All	0.26	0/25336	0.49	0/34484

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	4128	0	3903	34	0
1	В	4123	0	3898	57	0
1	С	4123	0	3898	32	0
1	D	4123	0	3898	32	0
1	Е	4128	0	3903	55	0
1	F	4123	0	3898	48	0
2	А	1	0	0	0	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	В	1	0	0	0	0
2	С	1	0	0	0	0
2	D	1	0	0	0	0
2	Е	1	0	0	0	0
2	F	1	0	0	0	0
3	А	7	0	10	0	0
4	А	4	0	6	0	0
4	В	24	0	36	3	0
4	С	4	0	6	1	0
4	D	8	0	12	0	0
4	Ε	4	0	6	0	0
5	В	10	0	0	0	0
5	Е	10	0	0	0	0
6	А	70	0	0	0	0
6	В	91	0	0	0	0
6	С	71	0	0	1	0
6	D	64	0	0	0	0
6	Е	52	0	0	2	0
6	F	55	0	0	0	0
All	All	25228	0	23474	252	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 5.

All (252) 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:E:254:LEU:HD23	1:E:467:HIS:CD2	1.90	1.06
1:E:254:LEU:HD23	1:E:467:HIS:NE2	1.82	0.95
1:D:48:ARG:NH2	1:D:75:TRP:HD1	1.76	0.84
1:E:204:GLY:O	1:E:208:VAL:HG23	1.78	0.83
1:E:82:THR:HG22	1:E:84:SER:H	1.44	0.83
1:D:48:ARG:HH21	1:D:75:TRP:HD1	1.27	0.81
1:D:48:ARG:NH2	1:D:75:TRP:CD1	2.51	0.78
1:B:77:ASP:H	4:B:704:EDO:H11	1.55	0.72
1:E:379:ASP:H	1:E:382:MET:HE3	1.52	0.72
1:C:338:LEU:HD21	1:C:349:LEU:HD12	1.72	0.72
1:D:246:VAL:HG23	1:D:544:LEU:HD22	1.73	0.71
1:F:176:ALA:HB2	1:F:184:LEU:HD11	1.73	0.71
1:A:338:LEU:HD21	1:A:349:LEU:HD12	1.73	0.70
1:A:310:ALA:O	1:B:341:VAL:HG12	1.92	0.70



	A b b	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:F:410:GLN:HA	1:F:414:GLY:HA3	1.75	0.69
1:B:210:ARG:NH1	1:C:60:ASP:OD2	2.26	0.68
1:E:409:ALA:HB3	1:E:412:VAL:HG12	1.76	0.67
1:F:246:VAL:HG23	1:F:544:LEU:HD22	1.76	0.66
1:A:310:ALA:O	1:B:341:VAL:CG1	2.44	0.66
1:A:345:THR:HG23	1:A:347:ASP:H	1.61	0.65
1:E:260:SER:HA	1:E:364:PRO:HG3	1.79	0.65
1:F:377:ALA:HB2	1:F:498:LEU:HD11	1.79	0.65
1:B:344:LYS:HG3	1:B:350:SER:HB3	1.79	0.64
1:B:79:ALA:HB3	1:B:88:LEU:HB2	1.79	0.64
1:E:198:ASP:OD1	1:E:241:HIS:HE1	1.80	0.63
1:C:127:MET:HG3	1:C:160:ILE:HG23	1.81	0.63
1:B:266:GLN:NE2	1:B:441:MET:O	2.30	0.63
1:C:253:GLN:NE2	1:C:499:ASP:OD2	2.33	0.62
1:E:254:LEU:CD2	1:E:467:HIS:NE2	2.60	0.62
1:A:345:THR:HG22	1:A:348:CYS:SG	2.40	0.62
1:C:177:LEU:HD23	1:C:433:MET:HG2	1.80	0.62
1:E:359:ARG:NH2	6:E:802:HOH:O	2.33	0.62
1:D:79:ALA:HB3	1:D:88:LEU:HB2	1.81	0.62
1:E:246:VAL:HG23	1:E:544:LEU:HD22	1.81	0.61
1:B:264:THR:HG21	1:B:398:TRP:CG	2.35	0.61
1:E:299:ILE:HD13	1:E:378:TRP:HB3	1.82	0.61
1:F:278:GLN:NE2	1:F:434:THR:OG1	2.35	0.60
1:F:483:LYS:HD2	1:F:547:TRP:CE2	2.37	0.60
1:A:311:ASP:OD1	1:A:311:ASP:N	2.35	0.59
1:F:55:LYS:HZ2	1:F:56:ASP:H	1.47	0.59
1:B:126:PHE:HE2	1:B:222:ILE:HD12	1.68	0.59
1:C:582:ILE:HD11	1:C:603:PRO:HD3	1.86	0.58
1:B:222:ILE:HG12	1:B:246:VAL:HB	1.86	0.58
1:A:246:VAL:HG23	1:A:544:LEU:HD22	1.87	0.57
1:F:222:ILE:HG12	1:F:246:VAL:HB	1.86	0.57
1:E:100:LYS:CD	1:E:110:GLU:HB3	2.35	0.56
1:A:401:SER:H	1:A:408:ASN:HD21	1.53	0.56
1:C:506:ARG:NH1	6:C:805:HOH:O	2.35	0.56
1:D:379:ASP:OD2	1:D:490:MET:HB3	2.06	0.56
1:E:463:SER:HA	1:E:466:TRP:CE2	2.40	0.56
1:E:311:ASP:HB2	1:E:572:ARG:HH12	1.71	0.56
1:E:253:GLN:NE2	1:E:499:ASP:OD2	2.39	0.55
1:D:558:SER:HA	1:D:594:GLU:OE2	2.05	0.55
1:F:135:GLY:HA2	1:F:166:HIS:O	2.07	0.55
1:D:48:ARG:CZ	1:D:75:TRP:CD1	2.90	0.55



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:560:TRP:HB3	1:A:573:THR:HG22	1.89	0.55
1:C:429(A):GLU:OE2	1:C:451:LYS:HE3	2.07	0.55
1:E:55:LYS:HB2	1:E:73:ALA:HB3	1.90	0.54
1:C:55:LYS:HE2	1:C:73:ALA:HB3	1.88	0.54
1:F:60:ASP:OD1	1:F:60:ASP:N	2.40	0.54
1:D:115:LEU:HB2	1:D:160:ILE:HD12	1.90	0.54
1:A:401:SER:H	1:A:408:ASN:ND2	2.04	0.54
1:E:100:LYS:HD2	1:E:110:GLU:HB3	1.89	0.54
1:F:185:ASP:OD1	1:F:186:PRO:HD2	2.07	0.54
1:D:222:ILE:HD11	1:D:541:LEU:HD13	1.90	0.53
1:E:490:MET:HE2	1:E:522:LEU:HD22	1.90	0.53
1:C:397:TRP:HA	1:C:410:GLN:HB2	1.91	0.53
1:A:75:TRP:CZ2	1:A:90:GLU:HG2	2.44	0.53
1:E:149:ILE:HD12	1:E:149:ILE:H	1.73	0.52
1:F:391:ASN:ND2	1:F:393:GLY:H	2.07	0.52
1:A:111:ILE:HD13	1:A:196:SER:HA	1.92	0.52
1:C:149:ILE:HG12	4:C:702:EDO:H11	1.91	0.52
1:E:180:VAL:HG13	1:E:423:ASP:OD2	2.09	0.52
1:A:160:ILE:HD11	1:A:200:VAL:CG1	2.39	0.52
1:E:295:LEU:O	1:E:299:ILE:HG13	2.10	0.52
1:F:88:LEU:HD22	1:F:153:LEU:HD23	1.92	0.52
1:F:560:TRP:HB3	1:F:573:THR:HG22	1.92	0.52
1:C:226:GLU:OE2	1:C:229:ARG:NE	2.42	0.52
1:C:246:VAL:HG23	1:C:544:LEU:HD22	1.91	0.52
1:F:461:GLN:HB3	1:F:466:TRP:HD1	1.74	0.52
1:D:490:MET:HB2	1:D:524:PRO:HA	1.92	0.51
1:A:254:LEU:HD13	1:A:495:PHE:HE1	1.76	0.51
1:D:111:ILE:HD13	1:D:196:SER:HA	1.92	0.51
1:B:517:PHE:HB3	4:B:706:EDO:H21	1.92	0.51
1:E:254:LEU:HD23	1:E:467:HIS:HD2	1.68	0.51
1:E:273:VAL:HG22	1:E:285:LYS:HB3	1.93	0.51
1:F:254:LEU:HB3	1:F:467:HIS:HD2	1.75	0.51
1:B:254:LEU:HD22	1:B:424:PHE:CE2	2.46	0.51
1:B:263:TRP:CD2	1:B:364:PRO:HA	2.46	0.51
1:A:55:LYS:HB2	1:A:73:ALA:HB3	1.93	0.50
1:E:193:GLY:HA2	1:E:467:HIS:HD1	1.74	0.50
1:E:593:THR:HG22	1:E:595:ALA:H	1.77	0.50
1:E:229:ARG:HG3	1:E:252:PHE:HA	1.94	0.50
1:B:330:ALA:HA	1:B:337:ALA:HA	1.93	0.50
1:B:378:TRP:HA	1:B:382:MET:HE1	1.94	0.50
1:E:365:VAL:HG12	1:E:371:PRO:HA	1.94	0.50



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:D:254:LEU:HD22	1:D:424:PHE:CE2	2.47	0.49	
1:E:540:MET:HE1	1:E:557:ILE:HG21	1.94	0.49	
1:A:233:MET:HE3	1:A:234:LEU:HD22	1.94	0.49	
1:B:72:VAL:HG22	1:D:108:PRO:HG3	1.93	0.49	
1:B:492:ASP:OD2	1:B:528:HIS:HA	2.13	0.49	
1:E:180:VAL:HG12	1:E:422:VAL:HB	1.94	0.49	
1:B:126:PHE:CE2	1:B:222:ILE:HD12	2.48	0.49	
1:C:60:ASP:HB3	1:C:210:ARG:CZ	2.42	0.49	
1:B:142:GLY:HA3	1:B:152:ALA:HB3	1.93	0.49	
1:E:162:THR:HB	1:E:200:VAL:HG21	1.94	0.49	
1:F:134:ASN:O	1:F:166:HIS:NE2	2.46	0.49	
1:C:135:GLY:HA2	1:C:166:HIS:O	2.13	0.49	
1:F:261:GLY:O	1:F:265:THR:OG1	2.29	0.49	
1:F:309:LEU:HD21	1:F:591:ILE:HG22	1.95	0.48	
1:F:490:MET:HE3	1:F:522:LEU:HB3	1.95	0.48	
1:C:593:THR:HG22	1:C:595:ALA:H	1.78	0.48	
1:E:540:MET:CE	1:E:557:ILE:HG21	2.43	0.48	
1:F:526:MET:HG3	1:F:536:ASP:HB3	1.95	0.48	
1:D:455:THR:OG1	1:D:459:PHE:O	2.27	0.48	
1:D:474:LEU:HD12	1:D:507:LEU:HD11	1.94	0.48	
1:B:357:ILE:O	1:B:361:MET:HG2	2.14	0.48	
1:E:127:MET:HG3	1:E:160:ILE:HG23	1.96	0.48	
1:A:160:ILE:CD1	1:A:200:VAL:HG12	2.44	0.48	
1:A:263:TRP:CD2	1:A:364:PRO:HA	2.49	0.48	
1:E:520:LEU:HD22	1:E:522:LEU:HG	1.96	0.48	
1:D:191:ASP:HA	1:D:195:ASN:HB3	1.96	0.48	
1:E:354:VAL:O	1:E:358:LYS:HB2	2.14	0.48	
1:F:243:ASP:OD1	1:F:480:ARG:NH1	2.47	0.48	
1:E:263:TRP:CD2	1:E:364:PRO:HA	2.49	0.47	
1:C:177:LEU:HD22	1:C:418:ARG:HG2	1.97	0.47	
1:C:259:ILE:HD11	1:C:452:ILE:HD13	1.97	0.47	
1:F:265:THR:HG23	1:F:412:VAL:HG22	1.96	0.47	
1:D:47:SER:OG	1:D:48:ARG:N	2.46	0.47	
1:F:254:LEU:HD23	1:F:467:HIS:NE2	2.29	0.47	
1:A:263:TRP:HB2	1:A:364:PRO:HB3	1.96	0.47	
1:B:409:ALA:HB3	1:B:412:VAL:HG23	1.95	0.47	
1:B:334:ASN:HB3	1:B:336:GLN:OE1	2.15	0.47	
1:B:586:LYS:HE3	1:B:598:ALA:HB2	1.96	0.47	
1:D:276:ASP:OD1	1:D:278:GLN:N	2.46	0.47	
1:A:160:ILE:HD11	1:A:200:VAL:HG13	1.97	0.47	
1:E:563:THR:O	1:E:563:THR:OG1	2.29	0.47	



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:F:490:MET:HB2	1:F:524:PRO:HA	1.96	0.47
1:F:255:PRO:HD2	1:F:464:MET:HE1	1.97	0.47
1:B:124:ARG:HD3	1:B:220:TYR:HE2	1.80	0.46
1:B:229:ARG:HG3	1:B:252:PHE:HA	1.97	0.46
1:B:567:PHE:HB2	1:B:569:VAL:HG22	1.97	0.46
1:F:180:VAL:HG12	1:F:422:VAL:HB	1.97	0.46
1:B:60:ASP:HB2	1:B:210:ARG:HH21	1.80	0.46
1:B:91:HIS:NE2	1:B:116:ARG:NH1	2.64	0.46
1:E:410:GLN:HA	1:E:414:GLY:HA3	1.97	0.46
1:B:116:ARG:HD2	1:B:140:ALA:O	2.15	0.46
1:E:88:LEU:HD22	1:E:153:LEU:HD23	1.97	0.46
1:F:248:GLY:HA3	1:F:487:TYR:CZ	2.51	0.46
1:E:367:SER:OG	1:E:446:ASP:OD2	2.31	0.46
1:E:313:ILE:HD12	1:E:572:ARG:HH11	1.80	0.46
1:E:100:LYS:HD3	1:E:110:GLU:HB3	1.98	0.46
1:E:438:ALA:O	1:E:442:LYS:HG2	2.16	0.46
1:F:180:VAL:HG13	1:F:423:ASP:OD2	2.16	0.46
1:F:459:PHE:N	1:F:459:PHE:CD1	2.84	0.45
1:D:301:GLY:HA3	1:D:332:PRO:HG3	1.97	0.45
1:F:276:ASP:N	1:F:280:VAL:O	2.36	0.45
1:D:590:ASP:O	1:D:596:ASN:ND2	2.48	0.45
1:A:590:ASP:O	1:A:596:ASN:ND2	2.38	0.45
1:B:100:LYS:HE2	1:B:108:PRO:HB3	1.98	0.45
1:B:288:SER:OG	1:B:291:ASP:OD1	2.34	0.45
1:E:483:LYS:HD2	1:E:547:TRP:CE2	2.51	0.45
1:C:248:GLY:HA3	1:C:487:TYR:CZ	2.51	0.45
1:A:311:ASP:HA	1:B:341:VAL:HG12	1.98	0.45
1:A:463:SER:HA	1:A:466:TRP:CE2	2.51	0.45
1:D:222:ILE:HG12	1:D:246:VAL:HB	1.99	0.45
1:F:309:LEU:HD13	1:F:585:TYR:CD2	2.52	0.45
1:F:448:ASP:O	1:F:451:LYS:HD2	2.17	0.45
1:C:60:ASP:O	1:C:62:VAL:N	2.50	0.45
1:B:112:LYS:HB2	1:B:163:ASP:OD2	2.17	0.44
1:B:361:MET:HE3	1:B:376:TRP:HB2	2.00	0.44
1:A:222:ILE:HG12	1:A:246:VAL:HB	1.99	0.44
1:A:340:CYS:SG	1:A:349:LEU:O	2.75	0.44
1:C:191:ASP:HA	1:C:195:ASN:HB3	1.99	0.44
1:E:283:ILE:N	1:E:407:ASN:OD1	2.49	0.44
1:F:444:ASP:HB3	1:F:447:ILE:HG12	1.99	0.44
1:F:111:ILE:HG12	1:F:165:GLY:HA2	1.98	0.44
1:F:463:SER:HA	1:F:466:TRP:CE2	2.52	0.44



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:E:127:MET:HB3	1:E:221:PHE:HD2	1.82	0.44	
1:C:60:ASP:O	1:C:60:ASP:OD1	2.36	0.44	
1:B:60:ASP:HB2	1:B:210:ARG:NH2	2.32	0.44	
1:B:336:GLN:HG2	1:B:337:ALA:O	2.18	0.44	
1:F:287:PHE:HB3	1:F:292:LEU:HD23	1.98	0.44	
1:C:463:SER:HA	1:C:466:TRP:CE2	2.53	0.44	
1:D:311:ASP:OD1	1:D:311:ASP:N	2.50	0.44	
1:E:47:SER:OG	1:E:48:ARG:N	2.51	0.44	
1:B:127:MET:HG3	1:B:160:ILE:HG23	1.99	0.43	
1:B:191:ASP:HA	1:B:195:ASN:HB3	2.00	0.43	
1:D:463:SER:HA	1:D:466:TRP:CE2	2.53	0.43	
1:E:167:ASP:OD1	6:E:801:HOH:O	2.21	0.43	
1:F:227:GLY:HA2	1:F:230:GLU:HG3	2.01	0.43	
1:D:484:MET:O	1:D:518:ALA:HA	2.19	0.43	
1:B:366:ASN:HD21	1:B:370:THR:HB	1.83	0.43	
1:F:100:LYS:HA	1:F:100:LYS:HD2	1.81	0.43	
1:A:266:GLN:HA	1:A:441:MET:HE1	2.00	0.43	
1:E:444:ASP:OD2	1:E:447:ILE:HD12	2.19	0.43	
1:A:191:ASP:HA	1:A:195:ASN:HB3	2.00	0.43	
1:D:287:PHE:HB2	1:D:399:LEU:HD21	2.01	0.43	
1:D:401:SER:HB3	1:D:408:ASN:HD21	1.83	0.43	
1:F:142:GLY:HA3	1:F:152:ALA:HB3	2.01	0.43	
1:F:439:ARG:NH1	1:F:442:LYS:HE3	2.34	0.43	
1:B:88:LEU:HD23	1:B:88:LEU:HA	1.84	0.43	
1:A:135:GLY:HA2	1:A:166:HIS:O	2.19	0.43	
1:B:89:PRO:HD3	1:B:154:SER:HA	2.01	0.42	
1:B:361:MET:HE3	1:B:361:MET:HB3	1.93	0.42	
1:C:280:VAL:HG11	1:C:437:ALA:HB1	2.00	0.42	
1:E:452:ILE:HD12	1:E:464:MET:HE3	2.02	0.42	
1:A:310:ALA:O	1:B:341:VAL:HG11	2.17	0.42	
1:C:191:ASP:HB3	1:C:196:SER:HB3	2.00	0.42	
1:C:552:GLU:H	1:C:552:GLU:HG2	1.72	0.42	
1:B:71:GLU:HG2	1:B:72:VAL:HG23	2.02	0.42	
1:E:287:PHE:HB2	1:E:399:LEU:HD21	2.01	0.42	
1:B:243:ASP:OD1	1:B:480:ARG:NH1	2.53	0.42	
1:C:300:LEU:HD12	1:C:300:LEU:HA	1.89	0.42	
1:C:334:ASN:OD1	1:C:336:GLN:N	2.44	0.42	
1:B:399:LEU:C	1:B:409:ALA:HB2	2.39	0.42	
1:D:229:ARG:HG3	1:D:252:PHE:HA	2.01	0.42	
1:B:88:LEU:HD22	1:B:153:LEU:HD23	2.01	0.42	
1:B:438:ALA:O	1:B:442:LYS:HG2	2.18	0.42	



A , 1		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:311:ASP:N	1:B:311:ASP:OD1	2.53	0.42
1:D:357:ILE:O	1:D:361:MET:HG2	2.20	0.42
1:F:535:THR:HG21	1:F:574:ARG:HB2	2.01	0.42
1:A:97:ALA:HB1	1:A:110:GLU:HG3	2.01	0.41
1:B:116:ARG:HG2	1:B:116:ARG:HH11	1.84	0.41
1:B:341:VAL:HG12	1:B:341:VAL:O	2.20	0.41
1:E:101:ARG:NH2	1:E:185:ASP:OD2	2.50	0.41
1:F:317:TYR:CZ	1:F:522:LEU:HD12	2.55	0.41
1:B:382:MET:HG2	1:B:394:TRP:CE2	2.55	0.41
1:C:275:LEU:HD12	1:C:279:GLY:C	2.41	0.41
1:F:586:LYS:HG3	1:F:596:ASN:C	2.41	0.41
1:A:300:LEU:HD23	1:A:300:LEU:HA	1.93	0.41
1:C:160:ILE:HG13	1:C:161:ALA:N	2.34	0.41
1:E:263:TRP:CE3	1:E:364:PRO:HA	2.56	0.41
1:E:313:ILE:HG23	1:E:524:PRO:HB2	2.02	0.41
1:F:490:MET:HE1	1:F:522:LEU:HD13	2.02	0.41
1:A:367:SER:H	1:A:367:SER:HG	1.55	0.41
1:B:124:ARG:HD3	1:B:220:TYR:CE2	2.56	0.41
1:A:248:GLY:HA3	1:A:487:TYR:CE1	2.54	0.41
1:D:112:LYS:HB2	1:D:163:ASP:OD2	2.20	0.41
1:F:444:ASP:N	1:F:448:ASP:OD2	2.47	0.41
1:B:246:VAL:HG23	1:B:544:LEU:HD22	2.03	0.41
1:E:220:TYR:CZ	1:E:545:VAL:HG22	2.56	0.41
1:B:550:ARG:HH21	1:B:552:GLU:HG3	1.85	0.41
1:B:581:GLN:O	4:B:705:EDO:H11	2.21	0.41
1:C:444:ASP:O	1:C:448:ASP:HB2	2.21	0.41
1:F:490:MET:HE1	1:F:522:LEU:HD22	2.03	0.41
1:F:276:ASP:OD1	1:F:277:ALA:N	2.53	0.41
1:A:293:HIS:HA	1:A:383:SER:OG	2.22	0.40
1:C:377:ALA:HB2	1:C:498:LEU:HD11	2.04	0.40
1:D:399:LEU:C	1:D:409:ALA:HB2	2.41	0.40
1:B:301:GLY:HA3	1:B:332:PRO:HG2	2.03	0.40
1:D:408:ASN:OD1	1:D:408:ASN:N	2.53	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	ntiles
1	А	555/592~(94%)	529~(95%)	26~(5%)	0	100	100
1	В	554/592~(94%)	527~(95%)	27~(5%)	0	100	100
1	С	554/592~(94%)	530~(96%)	24~(4%)	0	100	100
1	D	554/592~(94%)	528~(95%)	25~(4%)	1 (0%)	47	64
1	Е	555/592~(94%)	526~(95%)	29~(5%)	0	100	100
1	F	554/592~(94%)	527~(95%)	27 (5%)	0	100	100
All	All	3326/3552~(94%)	3167 (95%)	158 (5%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	527	ASN

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 sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
1	А	403/433~(93%)	395~(98%)	8 (2%)	55	73
1	В	403/433~(93%)	398~(99%)	5 (1%)	71	84
1	С	403/433~(93%)	391~(97%)	12 (3%)	41	59
1	D	403/433~(93%)	397~(98%)	6 (2%)	65	80
1	Е	403/433~(93%)	393~(98%)	10 (2%)	47	66
1	F	403/433~(93%)	393~(98%)	10 (2%)	47	66



Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2418/2598~(93%)	2367~(98%)	51 (2%)	53 72

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	60	ASP
1	А	77	ASP
1	А	233	MET
1	А	254	LEU
1	А	359	ARG
1	А	375	ARG
1	А	467	HIS
1	А	538	PHE
1	В	241	HIS
1	В	375	ARG
1	В	403	ASN
1	В	442	LYS
1	В	538	PHE
1	С	155	ARG
1	С	210	ARG
1	С	241	HIS
1	С	295	LEU
1	С	307	ASP
1	С	338	LEU
1	С	340	CYS
1	С	344	LYS
1	С	375	ARG
1	С	442	LYS
1	С	538	PHE
1	С	550	ARG
1	D	210	ARG
1	D	240	SER
1	D	375	ARG
1	D	383	SER
1	D	490	MET
1	D	594	GLU
1	E	60	ASP
1	Ε	77	ASP
1	E	307	ASP
1	E	347	ASP
1	Е	359	ARG
1	Е	375	ARG



\mathbf{Mol}	Chain	\mathbf{Res}	Type
1	Е	379	ASP
1	Е	411	ARG
1	Е	465	ASP
1	Е	584	ARG
1	F	197	TYR
1	F	276	ASP
1	F	375	ARG
1	F	391	ASN
1	F	431	MET
1	F	433	MET
1	F	441	MET
1	F	442	LYS
1	F	478	ARG
1	F	594	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	\mathbf{Res}	Type
1	А	408	ASN
1	D	556	GLN
1	Е	241	HIS
1	F	241	HIS
1	F	278	GLN
1	F	391	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)

6 non-standard protein/DNA/RNA residues 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).



Mal	al Type Chain Res Lin		Tink	Bond lengths			Bond angles			
	Moi Type Chain	nes Link		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2	
1	SEP	F	225	1	8,9,10	1.54	1 (12%)	8,12,14	1.39	2 (25%)
1	SEP	Е	225	1	8,9,10	1.57	1 (12%)	8,12,14	1.72	2 (25%)
1	SEP	D	225	1	8,9,10	1.56	1 (12%)	8,12,14	1.57	2 (25%)
1	SEP	С	225	1	8,9,10	1.56	1 (12%)	8,12,14	1.52	2 (25%)
1	SEP	А	225	1	8,9,10	1.55	1 (12%)	8,12,14	1.74	2 (25%)
1	SEP	В	225	1	8,9,10	0.57	0	8,12,14	0.69	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
1	SEP	F	225	1	-	1/5/8/10	-
1	SEP	Е	225	1	-	1/5/8/10	-
1	SEP	D	225	1	-	2/5/8/10	-
1	SEP	С	225	1	-	1/5/8/10	-
1	SEP	А	225	1	-	2/5/8/10	-
1	SEP	В	225	1	-	4/5/8/10	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\operatorname{Ideal}(\operatorname{\AA})$
1	Е	225	SEP	P-O1P	3.43	1.61	1.50
1	D	225	SEP	P-O1P	3.42	1.61	1.50
1	С	225	SEP	P-O1P	3.41	1.61	1.50
1	А	225	SEP	P-O1P	3.38	1.61	1.50
1	F	225	SEP	P-O1P	3.34	1.61	1.50

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
1	А	225	SEP	P-OG-CB	-3.27	109.27	118.30
1	Е	225	SEP	P-OG-CB	-3.22	109.43	118.30
1	А	225	SEP	OG-CB-CA	3.17	111.23	108.14
1	Е	225	SEP	OG-CB-CA	3.12	111.19	108.14
1	D	225	SEP	P-OG-CB	-2.85	110.43	118.30
1	D	225	SEP	OG-CB-CA	2.82	110.89	108.14
1	С	225	SEP	P-OG-CB	-2.77	110.67	118.30
1	С	225	SEP	OG-CB-CA	2.65	110.72	108.14



Contre	Continued from previous page									
Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	Ideal(
1	F	225	SEP	P-OG-CB	-2.57	111.22	118.30			
1	F	225	SEP	OG-CB-CA	2.31	110.39	108.14			

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	В	225	SEP	CB-OG-P-O2P
1	В	225	SEP	CB-OG-P-O3P
1	В	225	SEP	CB-OG-P-O1P
1	А	225	SEP	N-CA-CB-OG
1	В	225	SEP	N-CA-CB-OG
1	С	225	SEP	N-CA-CB-OG
1	D	225	SEP	N-CA-CB-OG
1	Е	225	SEP	N-CA-CB-OG
1	F	225	SEP	N-CA-CB-OG
1	А	225	SEP	CB-OG-P-O1P
1	D	225	SEP	CB-OG-P-O2P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 22 ligands modelled in this entry, 6 are monoatomic - leaving 16 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	Bos	Link	B	ond leng	gths	Bond angles			
	Type	Unam	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
4	EDO	В	708	-	3,3,3	0.45	0	2,2,2	0.32	0



Mol	Type	Chain	Bos	Link	B	ond leng	gths	B	Bond angles		
WIOI	Type	Ullalli	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2	
4	EDO	E	704	-	3,3,3	0.45	0	2,2,2	0.37	0	
5	SO4	В	702	-	4,4,4	0.14	0	6,6,6	0.05	0	
5	SO4	В	703	-	4,4,4	0.14	0	$6,\!6,\!6$	0.04	0	
4	EDO	А	703	-	3,3,3	0.45	0	2,2,2	0.29	0	
4	EDO	D	703	-	3,3,3	0.45	0	2,2,2	0.34	0	
4	EDO	В	704	-	3,3,3	0.46	0	2,2,2	0.34	0	
4	EDO	В	707	-	3,3,3	0.45	0	2,2,2	0.35	0	
4	EDO	В	705	-	3,3,3	0.46	0	2,2,2	0.30	0	
3	PEG	А	702	-	6,6,6	0.10	0	$5,\!5,\!5$	0.11	0	
4	EDO	В	709	-	3,3,3	0.46	0	2,2,2	0.34	0	
4	EDO	D	702	-	3,3,3	0.11	0	2,2,2	0.10	0	
4	EDO	С	702	-	3,3,3	0.46	0	2,2,2	0.30	0	
5	SO4	Е	702	-	4,4,4	0.14	0	6,6,6	0.04	0	
4	EDO	В	706	-	3,3,3	0.45	0	2,2,2	0.32	0	
5	SO4	Е	703	-	4,4,4	0.14	0	6,6,6	0.05	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
4	EDO	В	708	-	-	0/1/1/1	-
4	EDO	Е	704	-	-	0/1/1/1	-
4	EDO	А	703	-	-	1/1/1/1	-
4	EDO	D	703	-	-	1/1/1/1	-
4	EDO	В	704	-	-	0/1/1/1	-
4	EDO	В	707	-	-	1/1/1/1	-
4	EDO	В	705	-	-	0/1/1/1	-
3	PEG	А	702	-	-	0/4/4/4	-
4	EDO	В	709	-	-	0/1/1/1	-
4	EDO	D	702	-	-	1/1/1/1	-
4	EDO	С	702	-	-	0/1/1/1	-
4	EDO	В	706	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:



Mol	Chain	Res	Type	Atoms
4	А	703	EDO	O1-C1-C2-O2
4	В	707	EDO	O1-C1-C2-O2
4	D	703	EDO	O1-C1-C2-O2
4	D	702	EDO	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	В	704	EDO	1	0
4	В	705	EDO	1	0
4	С	702	EDO	1	0
4	В	706	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	$\langle RSRZ \rangle$	#RSRZ>2	$OWAB(Å^2)$	$Q{<}0.9$
1	А	557/592~(94%)	-0.28	3 (0%) 91 91	34, 46, 66, 120	0
1	В	556/592~(93%)	-0.28	5 (0%) 84 83	30, 44, 66, 127	0
1	С	556/592~(93%)	-0.21	2 (0%) 92 93	33, 52, 80, 120	0
1	D	556/592~(93%)	-0.26	4 (0%) 87 87	34, 48, 73, 119	0
1	Ε	557/592~(94%)	-0.05	12 (2%) 62 57	37, 59, 83, 111	0
1	F	556/592~(93%)	0.06	19 (3%) 45 41	39, 65, 97, 142	0
All	All	3338/3552~(93%)	-0.17	45 (1%) 77 75	30, 51, 84, 142	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Е	46	ALA	4.1
1	F	277	ALA	3.8
1	F	412	VAL	3.8
1	С	341	VAL	3.6
1	D	333	ALA	3.5
1	F	367	SER	3.5
1	F	603	PRO	3.4
1	А	341	VAL	3.3
1	С	387	GLY	3.3
1	F	58	ASN	3.1
1	F	368	ALA	3.0
1	F	175	ASP	3.0
1	F	275	LEU	3.0
1	В	603	PRO	2.9
1	D	603	PRO	2.7
1	F	276	ASP	2.6
1	F	54	LEU	2.6
1	F	602	PRO	2.6
1	Е	315	ASP	2.6



Mol	Chain	Res	Type	RSRZ
1	А	58	ASN	2.6
1	F	445	PHE	2.6
1	D	336	GLN	2.5
1	Е	589	GLY	2.5
1	А	46	ALA	2.5
1	F	435	GLN	2.4
1	F	308	GLY	2.4
1	В	334	ASN	2.4
1	F	590	ASP	2.4
1	F	447	ILE	2.4
1	Е	603	PRO	2.3
1	F	52	GLU	2.3
1	В	330	ALA	2.3
1	В	336	GLN	2.3
1	F	57	GLY	2.3
1	Е	60	ASP	2.3
1	Е	586	LYS	2.2
1	D	447	ILE	2.2
1	Е	591	ILE	2.2
1	Е	367	SER	2.2
1	Е	588	SER	2.2
1	Е	280	VAL	2.1
1	Е	175	ASP	2.1
1	В	588	SER	2.1
1	Е	433	MET	2.0
1	F	338	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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	$B-factors(Å^2)$	Q<0.9
1	SEP	В	225	10/11	0.90	0.16	32,41,60,100	0
1	SEP	Е	225	10/11	0.92	0.14	46,52,64,98	0
1	SEP	F	225	10/11	0.92	0.12	$45,\!53,\!65,\!85$	0
1	SEP	D	225	10/11	0.94	0.12	40,49,68,91	0
1	SEP	С	225	10/11	0.95	0.16	41,52,67,77	0
1	SEP	А	225	10/11	0.95	0.11	38,48,57,80	0



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	B-factors(Å ²)	Q<0.9
5	SO4	В	702	5/5	0.76	0.32	111,112,123,132	0
3	PEG	А	702	7/7	0.80	0.28	44,63,68,70	0
4	EDO	В	705	4/4	0.82	0.24	38,44,45,49	4
5	SO4	Е	703	5/5	0.82	0.34	102,102,109,133	0
4	EDO	В	708	4/4	0.85	0.34	40,45,46,49	4
4	EDO	В	707	4/4	0.86	0.25	54,55,56,60	0
4	EDO	С	702	4/4	0.86	0.31	57,63,68,68	0
4	EDO	Е	704	4/4	0.87	0.20	59,63,64,67	0
4	EDO	D	702	4/4	0.88	0.18	44,45,62,64	0
4	EDO	А	703	4/4	0.88	0.28	38,38,48,49	4
5	SO4	E	702	5/5	0.91	0.23	$46,\!54,\!64,\!65$	5
2	CA	А	701	1/1	0.91	0.15	$55,\!55,\!55,\!55$	0
2	CA	С	701	1/1	0.92	0.15	58, 58, 58, 58	0
4	EDO	В	706	4/4	0.92	0.26	48,51,53,58	0
4	EDO	В	709	4/4	0.93	0.13	$49,\!55,\!61,\!62$	0
4	EDO	В	704	4/4	0.94	0.18	$48,\!51,\!54,\!59$	0
5	SO4	В	703	5/5	0.95	0.20	$99,\!101,\!105,\!125$	0
4	EDO	D	703	4/4	0.96	0.11	52,59,62,63	0
2	CA	В	701	1/1	0.97	0.12	53,53,53,53	0
2	CA	D	701	1/1	0.97	0.12	60,60,60,60	0
2	CA	E	701	1/1	0.98	0.07	64,64,64,64	0
2	CA	F	701	1/1	0.98	0.07	60,60,60,60	0

6.5 Other polymers (i)

There are no such residues in this entry.

