

Full wwPDB X-ray Structure Validation Report (i)

May 29, 2020 – 10:58 pm BST

PDB ID	:	3TKK
Title	:	Crystal Structure Analysis of a recombinant predicted acetamidase/ formami-
		dase from the thermophile thermoanaerobacter tengcongensis
Authors	:	Qian, M.; Huang, Q.; Wu, G.; Lai, L.; Tang, Y.; Pei, J.; Kusunoki, M.
Deposited on	:	2011-08-26
Resolution	:	1.99 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 as 541 be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 1.99 Å.

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



Metric	Whole archive $(\#Entries)$	Similar resolution $(\#Entries, resolution range(Å))$
R _{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=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	301	67%	28%	
1	В	301	73%	23%	•
1	С	301	72%	24%	5%
1	D	301	67%	27%	5%



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 9872 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	Atoms					ZeroOcc	AltConf	Trace
1	Δ	201	Total	С	Ν	Ο	S	0	0	0
	1 A 301	301	2257	1436	369	442	10	0	0	0
1	р	201	Total	С	Ν	Ο	S	0	0	0
	D	301	2257	1436	369	442	10	0	0	U
1	C	201	Total	С	Ν	0	S	0	0	0
		301	2257	1436	369	442	10	0	0	U
1	П	201	Total	С	Ν	Ο	S	0	0	0
		301	2257	1436	369	442	10	0	0	0

• Molecule 1 is a protein called Predicted acetamidase/formamidase.

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	-2	SER	-	EXPRESSION TAG	UNP Q8R8S5
А	-1	HIS	-	EXPRESSION TAG	UNP Q8R8S5
В	-2	SER	-	EXPRESSION TAG	UNP Q8R8S5
В	-1	HIS	-	EXPRESSION TAG	UNP Q8R8S5
С	-2	SER	-	EXPRESSION TAG	UNP Q8R8S5
С	-1	HIS	-	EXPRESSION TAG	UNP Q8R8S5
D	-2	SER	-	EXPRESSION TAG	UNP Q8R8S5
D	-1	HIS	-	EXPRESSION TAG	UNP Q8R8S5

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

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



• Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	292	Total O 292 292	0	0
4	В	153	Total O 153 153	0	0
4	С	254	Total O 254 254	0	0
4	D	136	Total O 136 136	0	0



3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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 colorcoded 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: Predicted acetamidase/formamidase



• Molecule 1: Predicted acetamidase/formamidase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	41.23Å 152.88 Å 100.25 Å	Deperitor
a, b, c, α , β , γ	90.00° 99.49° 90.00°	Depositor
Posolution(A)	50.00 - 1.99	Depositor
Resolution (A)	40.67 - 1.99	EDS
% Data completeness	94.7 (50.00-1.99)	Depositor
(in resolution range)	94.7(40.67 - 1.99)	EDS
R _{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.61 (at 2.00 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.4.0077	Depositor
D D	0.174 , 0.237	Depositor
$\mathbf{n}, \mathbf{n}_{free}$	0.240 , 0.283	DCC
R_{free} test set	3985 reflections $(5.03%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	26.1	Xtriage
Anisotropy	0.692	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.33 , 30.0	EDS
L-test for $twinning^2$	$< L >=0.50, < L^2>=0.34$	Xtriage
Estimated twinning fraction	0.023 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9872	wwPDB-VP
Average B, all atoms $(Å^2)$	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.19% 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: CSD, ZN, 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		
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	1.52	25/2285~(1.1%)	1.22	6/3088~(0.2%)	
1	В	1.03	0/2285	0.98	5/3088~(0.2%)	
1	С	1.29	5/2285~(0.2%)	1.11	7/3088~(0.2%)	
1	D	1.04	3/2285~(0.1%)	0.95	1/3088~(0.0%)	
All	All	1.24	33/9140~(0.4%)	1.07	19/12352~(0.2%)	

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	1

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(Å)
1	D	192	VAL	CB-CG1	-11.70	1.28	1.52
1	А	137	VAL	CB-CG2	6.98	1.67	1.52
1	А	69	ALA	CA-CB	6.56	1.66	1.52
1	С	198	GLU	CG-CD	6.54	1.61	1.51
1	С	146	CYS	CB-SG	-6.31	1.71	1.82
1	D	198	GLU	CG-CD	6.31	1.61	1.51
1	А	274	SER	CB-OG	6.11	1.50	1.42
1	А	233	GLU	CG-CD	6.11	1.61	1.51
1	А	202	LYS	CE-NZ	6.07	1.64	1.49
1	А	86	GLU	CB-CG	-5.98	1.40	1.52
1	А	195	SER	CB-OG	5.84	1.49	1.42
1	A	122	GLU	CD-OE2	5.77	1.31	1.25
1	A	202	LYS	CD-CE	5.73	1.65	1.51
1	А	220	VAL	CB-CG2	5.61	1.64	1.52



Mol	Chain	Res	Type	Atoms	Z	Observed(A)	Ideal(Å)
1	А	219	VAL	CB-CG1	5.55	1.64	1.52
1	С	259	GLU	CD-OE1	5.54	1.31	1.25
1	А	166	GLU	CD-OE2	-5.49	1.19	1.25
1	А	31	GLU	CG-CD	5.48	1.60	1.51
1	С	224	GLU	CG-CD	5.38	1.60	1.51
1	А	240	GLU	CD-OE2	5.34	1.31	1.25
1	А	281	LYS	CB-CG	5.33	1.67	1.52
1	А	224	GLU	CB-CG	5.29	1.62	1.52
1	А	281	LYS	N-CA	5.23	1.56	1.46
1	С	231	SER	CB-OG	5.23	1.49	1.42
1	D	198	GLU	CB-CG	5.19	1.62	1.52
1	А	159	THR	CB-CG2	5.18	1.69	1.52
1	А	240	GLU	CG-CD	5.17	1.59	1.51
1	А	198	GLU	CD-OE2	5.16	1.31	1.25
1	А	2	LYS	CE-NZ	5.16	1.61	1.49
1	A	191	GLU	CB-CG	5.14	1.61	1.52
1	А	197	VAL	CB-CG1	5.05	1.63	1.52
1	A	259	GLU	CB-CG	-5.05	1.42	1.52
1	A	89	VAL	CB-CG2	5.03	1.63	1.52

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	С	8	ASP	CB-CG-OD1	7.59	125.14	118.30
1	А	202	LYS	CD-CE-NZ	6.92	127.61	111.70
1	В	284	ARG	NE-CZ-NH1	-6.66	116.97	120.30
1	С	235	LEU	CB-CG-CD2	-6.41	100.11	111.00
1	А	157	ASP	CB-CG-OD1	6.16	123.85	118.30
1	С	284	ARG	NE-CZ-NH2	6.15	123.37	120.30
1	В	278	ASP	CB-CG-OD2	5.96	123.66	118.30
1	С	157	ASP	CB-CG-OD2	5.89	123.60	118.30
1	А	146	CYS	CA-CB-SG	-5.82	103.53	114.00
1	В	157	ASP	CB-CG-OD2	5.74	123.47	118.30
1	В	213	LEU	CA-CB-CG	5.64	128.28	115.30
1	D	124	LEU	CA-CB-CG	5.52	127.99	115.30
1	С	210	ILE	CB-CA-C	-5.37	100.86	111.60
1	С	292	LEU	CB-CG-CD1	5.35	120.09	111.00
1	А	182	ASP	CB-CG-OD2	5.31	123.08	118.30
1	А	177	LEU	CB-CG-CD2	5.27	119.96	111.00
1	С	8	ASP	CB-CG-OD2	-5.17	113.64	118.30
1	A	94	LYS	CD-CE-NZ	-5.16	99.84	111.70
1	В	198	GLU	OE1-CD-OE2	5.06	129.38	123.30



There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	А	160	LEU	Mainchain

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	2257	0	2294	74	1
1	В	2257	0	2292	90	0
1	С	2257	0	2293	75	0
1	D	2257	0	2293	107	0
2	А	2	0	0	0	0
2	В	1	0	0	0	0
2	С	1	0	0	0	0
2	D	1	0	0	0	0
3	А	1	0	0	0	0
3	В	1	0	0	0	0
3	С	1	0	0	0	0
3	D	1	0	0	0	0
4	А	292	0	0	14	1
4	В	153	0	0	9	0
4	C	254	0	0	14	0
4	D	136	0	0	11	0
All	All	9872	0	9172	327	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

All (327) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:ASN:HB3	1:B:110:VAL:CG2	1.22	1.57
1:A:135:ILE:CG1	1:A:135:ILE:CD1	1.78	1.56
1:A:161:ILE:CD1	1:A:161:ILE:CG1	1.76	1.56
1:B:45:ASN:CB	1:B:110:VAL:HG23	1.54	1.33



	1	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:B:45:ASN:CB	1:B:110:VAL:CG2	2.05	1.33
1:B:216:LYS:HD2	4:B:506:HOH:O	1.45	1.12
1:A:31:GLU:OE1	1:A:202:LYS:HE2	1.49	1.11
1:B:45:ASN:HB2	1:B:110:VAL:HG23	1.31	1.09
1:B:45:ASN:HB3	1:B:110:VAL:HG21	1.10	1.09
1:B:43:GLN:HG3	1:B:87:LYS:NZ	1.68	1.06
1:B:43:GLN:O	1:B:110:VAL:HG21	1.53	1.06
1:C:51:GLU:HB2	4:C:786:HOH:O	1.57	1.05
1:A:143:SER:O	4:A:455:HOH:O	1.76	1.02
1:D:58:ASN:HB3	1:D:146:CYS:SG	2.02	1.00
1:B:44:SER:O	1:B:45:ASN:ND2	1.96	0.98
1:D:254:THR:HG22	1:D:256:LEU:H	1.27	0.98
1:D:15:SER:HB2	1:D:143:SER:HB2	1.46	0.97
1:D:44:SER:HB2	1:D:48:LYS:HG2	1.46	0.97
1:D:45:ASN:HA	4:D:651:HOH:O	1.63	0.96
1:A:49:LEU:HD12	1:A:50:ASP:H	1.28	0.95
1:D:45:ASN:HB2	1:D:110:VAL:HG23	1.48	0.95
1:C:29:GLU:OE2	1:C:80:LYS:NZ	2.00	0.94
1:A:31:GLU:OE1	1:A:202:LYS:CE	2.17	0.93
1:B:45:ASN:HB3	1:B:110:VAL:CB	2.01	0.91
1:A:114:LYS:HE3	4:A:398:HOH:O	1.71	0.91
1:B:43:GLN:HG3	1:B:87:LYS:HZ3	1.28	0.90
1:C:144:ILE:H	1:C:144:ILE:HD12	1.37	0.90
1:A:7:ALA:O	1:A:10:HIS:HD2	1.54	0.90
1:A:41:GLN:HE22	1:A:53:ASP:H	1.14	0.90
1:C:212:GLY:O	1:D:46:GLU:HG3	1.72	0.89
1:A:31:GLU:HB3	1:A:202:LYS:HE3	1.55	0.88
1:C:220:VAL:HG23	1:C:229:ILE:HD11	1.56	0.87
1:B:53:ASP:O	1:B:55:ASN:N	2.08	0.86
1:A:44:SER:O	1:A:48:LYS:HB2	1.74	0.86
1:D:299:PHE:OXT	4:D:658:HOH:O	1.92	0.86
1:C:121:ASN:HD22	1:C:121:ASN:C	1.79	0.86
1:D:44:SER:O	1:D:45:ASN:HB3	1.76	0.85
1:D:12:PHE:O	1:D:146:CYS:HB2	1.75	0.85
1:A:43:GLN:H	1:A:48:LYS:HD3	1.41	0.84
1:D:50:ASP:HB3	1:D:106:LEU:HD13	1.59	0.84
1:D:58:ASN:CB	1:D:146:CYS:SG	2.65	0.83
1:A:256:LEU:HD21	4:C:466:HOH:O	1.79	0.82
1:B:53:ASP:O	1:B:53:ASP:OD1	1.98	0.81
1:D:276:VAL:HB	1:D:281:LYS:HE3	1.60	0.81
1:B:278:ASP:HB3	1:B:279:PRO:HD2	1.60	0.81



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:45:ASN:HB2	1:D:110:VAL:CG2	2.10	0.81
1:D:249:LEU:HD21	1:D:299:PHE:HZ	1.46	0.80
1:B:248:GLU:OE2	1:B:252:LYS:HE3	1.81	0.80
1:C:121:ASN:ND2	1:C:123:LYS:H	1.80	0.80
1:B:43:GLN:HG3	1:B:87:LYS:HZ1	1.47	0.79
1:C:121:ASN:ND2	1:C:124:LEU:H	1.79	0.79
1:C:45:ASN:OD1	4:C:603:HOH:O	2.00	0.79
1:A:255:ASP:OD2	4:A:414:HOH:O	2.01	0.79
1:D:299:PHE:HB2	4:D:799:HOH:O	1.83	0.79
1:C:211:LYS:O	4:C:706:HOH:O	2.02	0.78
1:B:43:GLN:CG	1:B:87:LYS:NZ	2.46	0.77
1:D:249:LEU:HD21	1:D:299:PHE:CZ	2.19	0.77
1:D:50:ASP:O	1:D:51:GLU:HB3	1.84	0.76
1:B:235:LEU:HB2	1:D:236:ASP:OD1	1.86	0.76
1:A:104:GLU:OE2	4:A:392:HOH:O	2.03	0.75
1:B:237:LYS:HE2	1:B:241:ILE:HG13	1.70	0.74
1:A:135:ILE:CB	1:A:135:ILE:CD1	2.66	0.74
1:B:45:ASN:CB	1:B:110:VAL:HG21	1.96	0.74
1:C:139:PRO:HG3	1:C:144:ILE:HD11	1.69	0.74
1:C:117:LYS:NZ	4:C:627:HOH:O	2.14	0.73
1:C:220:VAL:CG2	1:C:229:ILE:HD11	2.19	0.73
1:B:278:ASP:HB3	1:B:279:PRO:CD	2.19	0.73
1:D:44:SER:HB2	1:D:48:LYS:CG	2.18	0.73
1:C:139:PRO:CG	1:C:144:ILE:HD11	2.20	0.72
1:C:44:SER:HB2	1:C:48:LYS:HE2	1.72	0.71
1:D:254:THR:CG2	1:D:256:LEU:HB2	2.19	0.71
1:A:279:PRO:O	4:A:334:HOH:O	2.07	0.71
1:A:41:GLN:NE2	1:A:53:ASP:H	1.86	0.71
1:C:220:VAL:HG23	1:C:229:ILE:CD1	2.20	0.71
1:D:254:THR:HG22	1:D:256:LEU:N	2.04	0.70
1:C:7:ALA:O	1:C:10:HIS:HD2	1.74	0.70
1:D:264:LEU:O	1:D:268:THR:HG22	1.90	0.70
1:D:46:GLU:OE1	1:D:46:GLU:HA	1.90	0.70
1:B:2:LYS:HE2	1:B:31:GLU:HG3	1.73	0.69
1:C:144:ILE:N	1:C:144:ILE:HD12	2.02	0.69
1:B:42:ILE:HD13	1:B:48:LYS:O	1.91	0.69
1:B:43:GLN:CG	1:B:87:LYS:HZ1	2.05	0.68
1:C:121:ASN:OD1	4:C:466:HOH:O	2.12	0.68
1:C:248:GLU:OE2	1:C:252:LYS:HD2	1.92	0.68
1:B:24:VAL:O	1:B:67:GLU:HG3	1.94	0.68
1:D:239:VAL:CG2	4:D:597:HOH:O	2.41	0.68



	1.5	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:237:LYS:HE3	1:B:237:LYS:O	1.95	0.67
1:B:78:LYS:HG3	1:B:166:GLU:HG2	1.76	0.67
1:B:237:LYS:HE3	1:B:237:LYS:HA	1.77	0.66
1:B:123:LYS:NZ	1:D:294:SER:O	2.27	0.66
1:D:214:ASN:HB3	4:D:481:HOH:O	1.95	0.66
1:A:49:LEU:HD12	1:A:50:ASP:N	2.07	0.65
1:D:44:SER:O	1:D:45:ASN:CB	2.43	0.65
1:D:254:THR:HG21	1:D:256:LEU:HB2	1.76	0.65
1:C:121:ASN:HD21	1:C:124:LEU:H	1.41	0.65
1:C:44:SER:O	1:C:46:GLU:N	2.26	0.64
1:B:45:ASN:CG	1:B:46:GLU:N	2.51	0.64
1:D:276:VAL:CB	1:D:281:LYS:HE3	2.28	0.64
1:C:43:GLN:OE1	4:C:819:HOH:O	2.14	0.64
1:D:112:ASP:OD2	4:D:329:HOH:O	2.14	0.64
1:A:248:GLU:OE2	1:A:252:LYS:HD2	1.98	0.64
1:B:237:LYS:CA	1:B:237:LYS:HE3	2.28	0.63
1:A:12:PHE:CE1	1:A:56:ARG:HA	2.33	0.63
1:D:240:GLU:O	1:D:244:HIS:HD2	1.81	0.63
1:C:278:ASP:HB3	1:C:279:PRO:HD2	1.80	0.63
1:D:1:MET:HG2	1:D:3:TYR:CZ	2.34	0.62
1:D:140:LYS:HG2	1:D:172:PHE:HB3	1.81	0.62
1:D:94:LYS:HE2	1:D:95:GLY:N	2.15	0.62
1:A:41:GLN:HE22	1:A:53:ASP:N	1.93	0.61
1:D:48:LYS:CE	4:D:666:HOH:O	2.49	0.61
1:C:240:GLU:O	1:C:244:HIS:HD2	1.83	0.61
1:C:121:ASN:ND2	1:C:121:ASN:C	2.51	0.60
1:A:122:GLU:H	1:A:122:GLU:CD	2.04	0.60
1:C:78:LYS:HD3	1:C:166:GLU:HG2	1.82	0.60
1:D:7:ALA:H	1:D:33:GLU:CG	2.14	0.60
1:B:56:ARG:HG2	1:B:56:ARG:HH11	1.67	0.60
1:D:259:GLU:O	1:D:263:THR:HB	2.00	0.60
1:D:15:SER:HB2	1:D:143:SER:CB	2.29	0.59
1:A:278:ASP:HB3	1:A:279:PRO:CD	2.32	0.59
1:D:278:ASP:HB3	1:D:279:PRO:CD	2.33	0.59
1:B:144:ILE:HG12	1:B:152:HIS:CE1	2.37	0.59
1:C:10:HIS:HE1	4:C:417:HOH:O	1.87	0.58
1:D:47:ASP:O	1:D:49:LEU:N	2.29	0.58
1:C:236:ASP:O	1:C:240:GLU:HG3	2.04	0.57
1:A:141:GLU:HB2	4:A:337:HOH:O	2.04	0.57
1:A:43:GLN:HB2	1:A:48:LYS:HZ2	1.69	0.57
1:B:240:GLU:O	1:B:244:HIS:HD2	1.86	0.57



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	${ m distance}~({ m \AA})$	overlap (Å)
1:B:43:GLN:H	1:B:48:LYS:HE3	1.69	0.57
1:D:276:VAL:CA	1:D:281:LYS:HE3	2.35	0.57
1:A:-1:HIS:N	4:A:543:HOH:O	2.37	0.57
1:A:205:LEU:C	1:A:205:LEU:HD12	2.25	0.57
1:B:97:GLY:HA2	1:B:277:VAL:HG12	1.87	0.57
1:A:7:ALA:O	1:A:10:HIS:CD2	2.46	0.56
1:D:278:ASP:HB3	1:D:279:PRO:HD2	1.85	0.56
1:B:216:LYS:CD	4:B:506:HOH:O	2.24	0.56
1:C:121:ASN:ND2	1:C:123:LYS:N	2.51	0.56
1:A:113:ILE:C	1:A:114:LYS:HG2	2.26	0.56
1:C:42:ILE:HG22	1:C:42:ILE:O	2.06	0.56
1:C:212:GLY:O	1:D:46:GLU:C	2.44	0.56
1:A:240:GLU:O	1:A:244:HIS:HD2	1.89	0.55
1:A:36:ASP:H	1:A:40:ASN:ND2	2.04	0.55
1:B:2:LYS:HE2	1:B:31:GLU:CG	2.36	0.55
1:C:44:SER:C	1:C:46:GLU:H	2.10	0.55
1:D:290:TRP:HA	1:D:293:GLU:HG3	1.87	0.55
1:D:7:ALA:N	1:D:33:GLU:HG2	2.22	0.55
1:B:157:ASP:HB2	1:B:275:GLN:HG2	1.89	0.55
1:D:7:ALA:HB2	1:D:33:GLU:HG3	1.89	0.55
1:D:7:ALA:H	1:D:33:GLU:HG2	1.72	0.55
1:B:122:GLU:H	1:B:122:GLU:CD	2.09	0.55
1:B:67:GLU:OE1	4:B:363:HOH:O	2.18	0.55
1:B:119:ILE:H	1:B:119:ILE:HD12	1.71	0.54
1:B:36:ASP:H	1:B:40:ASN:HD21	1.55	0.54
1:A:78:LYS:HB2	1:A:78:LYS:NZ	2.23	0.54
1:A:6:SER:HB3	4:A:360:HOH:O	2.07	0.54
1:A:51:GLU:O	1:A:51:GLU:HG3	2.06	0.54
1:C:121:ASN:HD21	1:C:124:LEU:N	2.04	0.54
1:D:37:CSD:HB3	1:D:198:GLU:OE1	2.07	0.54
1:D:239:VAL:HG23	1:D:240:GLU:N	2.21	0.54
1:D:251:LYS:O	4:D:556:HOH:O	2.18	0.54
1:C:248:GLU:OE2	1:C:252:LYS:CD	2.55	0.54
1:A:119:ILE:N	1:A:119:ILE:HD13	2.23	0.53
1:C:272:GLN:HE21	1:C:284:ARG:HE	1.55	0.53
1:C:212:GLY:C	1:D:46:GLU:HG3	2.28	0.53
1:D:7:ALA:O	1:D:10:HIS:HD2	1.91	0.53
1:A:213:LEU:HD22	1:A:299:PHE:HB3	1.91	0.53
1:B:36:ASP:H	1:B:40:ASN:ND2	2.07	0.53
1:D:94:LYS:HE2	1:D:95:GLY:H	1.73	0.52
1:A:264:LEU:O	1:A:268:THR:HG22	2.08	0.52



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:135:ILE:HG23	1:C:135:ILE:O	2.07	0.52
1:C:237:LYS:HD2	1:C:237:LYS:O	2.09	0.52
1:C:205:LEU:C	1:C:205:LEU:HD12	2.30	0.52
1:D:157:ASP:OD2	1:D:191:GLU:OE1	2.28	0.52
1:B:144:ILE:HD13	1:B:148:THR:O	2.10	0.52
1:B:41:GLN:CD	1:B:52:MET:HB3	2.30	0.51
1:D:117:LYS:HA	1:D:126:LEU:O	2.11	0.51
1:A:278:ASP:HB3	1:A:279:PRO:HD2	1.92	0.51
1:D:38:PHE:O	1:D:56:ARG:O	2.29	0.51
1:A:244:HIS:HE1	1:C:101:ASN:OD1	1.93	0.51
1:C:206:GLU:HG2	1:C:207:VAL:N	2.25	0.51
1:D:50:ASP:O	1:D:51:GLU:CB	2.58	0.51
1:B:70:LYS:HB2	1:B:73:ASP:OD2	2.11	0.50
1:D:205:LEU:HD12	1:D:205:LEU:C	2.31	0.50
1:D:38:PHE:O	1:D:39:SER:HB2	2.10	0.50
1:B:7:ALA:O	1:B:10:HIS:HD2	1.95	0.50
1:D:29:GLU:OE2	1:D:80:LYS:NZ	2.33	0.50
1:A:193:GLY:O	1:A:194:VAL:HB	2.11	0.50
1:B:49:LEU:HB2	1:B:51:GLU:HG2	1.94	0.50
1:B:42:ILE:HG23	1:B:89:VAL:HG21	1.94	0.50
1:C:44:SER:HB2	1:C:48:LYS:HG2	1.94	0.50
1:D:44:SER:C	1:D:46:GLU:H	2.14	0.50
1:D:46:GLU:HB2	4:D:649:HOH:O	2.10	0.50
1:A:78:LYS:HD2	1:A:80:LYS:HE2	1.93	0.49
1:B:101:ASN:OD1	1:D:244:HIS:HE1	1.95	0.49
1:C:272:GLN:NE2	1:C:284:ARG:HE	2.09	0.49
1:D:276:VAL:HB	1:D:281:LYS:CE	2.37	0.49
1:B:45:ASN:HB3	1:B:110:VAL:HB	1.90	0.49
1:D:43:GLN:OE1	1:D:43:GLN:N	2.45	0.49
1:C:278:ASP:HB3	1:C:279:PRO:CD	2.43	0.49
1:D:122:GLU:CD	1:D:122:GLU:H	2.15	0.49
1:D:52:MET:O	1:D:53:ASP:HB2	2.12	0.49
1:B:144:ILE:HD12	1:B:144:ILE:O	2.11	0.49
1:B:42:ILE:HG23	4:B:356:HOH:O	2.12	0.49
1:D:239:VAL:HG21	4:D:597:HOH:O	2.07	0.49
1:A:122:GLU:CD	1:A:122:GLU:N	2.66	0.49
1:B:220:VAL:CG1	1:B:229:ILE:HD11	2.42	0.49
1:D:38:PHE:O	1:D:39:SER:CB	2.61	0.49
1:C:46:GLU:C	1:C:48:LYS:H	2.15	0.49
1:D:87:LYS:O	1:D:87:LYS:HG2	2.13	0.49
1:C:299:PHE:HD1	4:C:335:HOH:O	1.95	0.48



	louis pagem	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:20:PRO:HB3	1:C:65:PHE:HB2	1.95	0.48
1:D:45:ASN:OD1	1:D:109:LYS:HA	2.13	0.48
1:D:254:THR:HG22	1:D:256:LEU:HB2	1.94	0.48
1:D:219:VAL:HG11	1:D:299:PHE:CE1	2.49	0.48
1:C:50:ASP:HB2	1:C:106:LEU:HD12	1.94	0.48
1:D:98:VAL:HB	1:D:192:VAL:HG13	1.96	0.48
1:A:-1:HIS:HE1	4:A:634:HOH:O	1.95	0.48
1:A:237:LYS:O	1:A:238:ALA:C	2.50	0.47
1:A:43:GLN:CB	1:A:48:LYS:HZ2	2.27	0.47
1:C:113:ILE:O	1:C:114:LYS:HD3	2.14	0.47
1:D:58:ASN:HB2	1:D:146:CYS:SG	2.51	0.47
1:B:158:THR:HG22	1:B:274:SER:CB	2.44	0.47
1:D:254:THR:HG22	1:D:255:ASP:N	2.29	0.47
1:A:161:ILE:CB	1:A:161:ILE:CD1	2.79	0.47
1:B:251:LYS:O	1:B:251:LYS:HG2	2.13	0.47
1:B:90:LEU:HD13	1:D:263:THR:HG23	1.97	0.47
1:A:46:GLU:CD	1:B:212:GLY:HA2	2.35	0.47
1:D:121:ASN:ND2	4:D:529:HOH:O	2.45	0.47
1:B:193:GLY:H	1:D:266:SER:HB2	1.78	0.47
1:C:87:LYS:CE	4:C:373:HOH:O	2.60	0.47
1:A:114:LYS:CE	4:A:398:HOH:O	2.46	0.46
1:B:237:LYS:O	1:B:237:LYS:CE	2.63	0.46
1:C:6:SER:HB2	1:C:8:ASP:OD1	2.16	0.46
1:A:113:ILE:O	1:A:114:LYS:HG2	2.14	0.46
1:C:240:GLU:O	1:C:244:HIS:CD2	2.67	0.46
1:D:156:MET:O	1:D:157:ASP:C	2.54	0.46
1:A:253:HIS:HE1	4:A:408:HOH:O	1.99	0.46
1:C:12:PHE:CE1	1:C:56:ARG:HA	2.50	0.46
1:B:220:VAL:HG12	1:B:229:ILE:HD11	1.98	0.46
1:A:94:LYS:HG3	1:A:103:MET:O	2.16	0.46
1:B:46:GLU:C	1:B:48:LYS:H	2.19	0.46
1:C:52:MET:HE1	1:C:57:VAL:HG12	1.96	0.46
1:C:139:PRO:HG2	1:C:144:ILE:HD11	1.96	0.46
1:C:174:GLU:HG2	4:C:741:HOH:O	2.15	0.46
1:C:43:GLN:HB3	1:C:43:GLN:HE21	1.52	0.46
1:B:94:LYS:NZ	4:B:646:HOH:O	2.48	0.46
1:A:36:ASP:H	1:A:40:ASN:HD21	1.62	0.45
1:B:244:HIS:HE1	1:D:101:ASN:OD1	1.98	0.45
1:B:193:GLY:H	1:D:266:SER:CB	2.29	0.45
1:B:119:ILE:HD12	1:B:119:ILE:N	2.31	0.45
1:B:233:GLU:HG3	4:B:430:HOH:O	2.16	0.45



		Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlan(Å)
1:C:240:GLU:OE2	4:C:362:HOH:O	2 21	$\frac{0.45}{0.45}$
1:A:46:GLU:HG2	1:B:214:ASN:ND2	2.31	0.45
1:D:65:PHE:CE1	1:D:175:GLY:HA3	2.52	0.45
1:D:44:SEB:CB	1:D:48:LYS:HG2	2.33	0.45
1:A:51:GLU:O	1:A:51:GLU:CG	2.65	0.44
1:D:7:ALA:O	1:D:10:HIS:CD2	2.69	0.44
1:A:94:LYS:HE2	1:A:104:GLU:OE1	2.16	0.44
1:C:212:GLY:O	1:D:46:GLU:O	2.36	0.44
1:A:214:ASN:ND2	4:A:769:HOH:O	2.41	0.44
1:A:180:LEU:HD23	1:A:180:LEU:N	2.32	0.44
1:A:82:ILE:HG21	1:A:82:ILE:HD13	1.75	0.44
1:B:144:ILE:HD11	1:B:152:HIS:NE2	2.32	0.44
1:B:7:ALA:HB1	1:B:35:MET:HG3	1.99	0.44
1:A:228:THR:HB	4:A:304:HOH:O	2.18	0.44
1:A:101:ASN:OD1	1:C:244:HIS:HE1	2.00	0.44
1:B:237:LYS:C	1:B:237:LYS:HE3	2.38	0.44
1:A:39:SER:O	1:A:40:ASN:HB2	2.18	0.43
1:C:114:LYS:HD3	1:C:114:LYS:HA	1.73	0.43
1:C:248:GLU:HG3	1:C:252:LYS:HD3	1.99	0.43
1:B:41:GLN:OE1	1:B:52:MET:HB3	2.18	0.43
1:D:1:MET:HG2	1:D:3:TYR:CE2	2.53	0.43
1:B:158:THR:HG22	1:B:274:SER:HB3	2.00	0.43
1:A:31:GLU:CB	1:A:202:LYS:HE3	2.38	0.43
1:B:186:LEU:HG	1:D:267:ILE:O	2.19	0.43
1:B:216:LYS:HB3	4:B:432:HOH:O	2.18	0.43
1:C:35:MET:HB2	1:C:59:PRO:HG2	2.00	0.43
1:D:45:ASN:CG	1:D:110:VAL:H	2.21	0.43
1:D:6:SER:HA	1:D:33:GLU:HG2	2.01	0.43
1:A:2:LYS:HE2	1:A:31:GLU:OE2	2.19	0.43
1:C:206:GLU:OE1	4:C:336:HOH:O	2.21	0.43
1:B:156:MET:O	1:B:158:THR:HG22	2.18	0.43
1:D:14:PHE:O	1:D:143:SER:HA	2.18	0.43
1:B:45:ASN:CG	1:B:110:VAL:HB	2.38	0.42
1:B:81:LYS:HB2	1:B:204:LEU:HB3	2.00	0.42
1:C:7:ALA:O	1:C:10:HIS:CD2	2.63	0.42
1:D:12:PHE:CE1	1:D:56:ARG:HA	2.54	0.42
1:D:1:MET:HG2	1:D:3:TYR:OH	2.20	0.42
1:D:54:TRP:C	1:D:56:ARG:H	2.22	0.42
1:D:81:LYS:HE3	1:D:81:LYS:HB2	1.56	0.42
1:D:83:GLU:OE2	1:D:202:LYS:HE3	2.20	0.42
1:C:45:ASN:HA	1:C:110:VAL:HG23	2.02	0.42



A 4 1	A 4 0	Interatomic	Clash	
Atom-1	Atom-2	${ m distance}~({ m \AA})$	overlap (Å)	
1:D:288:PRO:HD2	1:D:291:ILE:HG13	2.02	0.42	
1:D:76:LYS:HE2	1:D:208:GLU:OE2	2.20	0.42	
1:A:-1:HIS:CE1	4:A:634:HOH:O	2.72	0.42	
1:A:227:ALA:HA	1:A:285:PHE:O	2.20	0.42	
1:B:45:ASN:CB	1:B:110:VAL:HB	2.49	0.42	
1:B:144:ILE:HD12	1:B:145:ASN:O	2.19	0.42	
1:B:193:GLY:HA2	4:B:319:HOH:O	2.20	0.42	
1:B:215:LEU:HD23	1:B:215:LEU:HA	1.91	0.42	
1:B:236:ASP:OD2	1:D:234:SER:HB2	2.19	0.41	
1:B:236:ASP:OD1	1:D:281:LYS:NZ	2.38	0.41	
1:C:123:LYS:HB2	1:C:123:LYS:NZ	2.35	0.41	
1:A:43:GLN:H	1:A:48:LYS:CD	2.20	0.41	
1:C:227:ALA:HA	1:C:285:PHE:O	2.20	0.41	
1:B:237:LYS:NZ	1:B:240:GLU:OE1	2.52	0.41	
1:D:74:VAL:HG21	1:D:213:LEU:HD23	2.01	0.41	
1:A:121:ASN:HB2	1:A:122:GLU:OE1	2.20	0.41	
1:B:122:GLU:N	1:B:122:GLU:CD	2.74	0.41	
1:B:236:ASP:OD1	1:D:235:LEU:HB2	2.20	0.41	
1:D:37:CSD:O	1:D:58:ASN:N	2.47	0.41	
1:C:264:LEU:HD21	1:C:291:ILE:CG2	2.50	0.41	
1:C:43:GLN:C	1:C:45:ASN:N	2.74	0.41	
1:A:119:ILE:N	1:A:119:ILE:CD1	2.84	0.41	
1:B:38:PHE:O	1:B:41:GLN:HG3	2.21	0.41	
1:D:240:GLU:O	1:D:244:HIS:CD2	2.68	0.41	
1:C:274:SER:HA	4:C:304:HOH:O	2.21	0.41	
1:A:182:ASP:O	1:A:182:ASP:CG	2.58	0.40	
1:C:123:LYS:CB	1:C:123:LYS:NZ	2.84	0.40	
1:C:114:LYS:HB2	1:C:119:ILE:HD11	2.03	0.40	
1:D:254:THR:CG2	1:D:255:ASP:N	2.83	0.40	
1:A:19:LYS:HA	1:A:20:PRO:HD3	1.91	0.40	
1:B:67:GLU:HB3	4:B:363:HOH:O	2.20	0.40	
1:C:235:LEU:HA	1:C:235:LEU:HD23	1.81	0.40	
1:A:106:LEU:HD13	1:A:107:TYR:H	1.86	0.40	
1:A:193:GLY:O	1:A:194:VAL:CB	2.69	0.40	
1:A:3:TYR:O	1:A:30:LEU:HA	2.21	0.40	
1:D:1:MET:HE3	1:D:1:MET:HB2	1.89	0.40	

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:LYS:NZ	4:A:455:HOH:O[1_455]	1.55	0.65

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	А	298/301~(99%)	276~(93%)	19~(6%)	3 (1%)	15 9
1	В	298/301~(99%)	273~(92%)	21 (7%)	4 (1%)	12 6
1	С	298/301~(99%)	277~(93%)	17~(6%)	4 (1%)	12 6
1	D	298/301~(99%)	276~(93%)	16~(5%)	6 (2%)	7 3
All	All	1192/1204~(99%)	1102 (92%)	73~(6%)	17 (1%)	11 5

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	194	VAL
1	В	44	SER
1	В	194	VAL
1	С	52	MET
1	С	194	VAL
1	D	39	SER
1	D	48	LYS
1	D	51	GLU
1	D	53	ASP
1	D	194	VAL
1	А	50	ASP
1	В	46	GLU
1	В	54	TRP
1	С	46	GLU
1	С	145	ASN
1	А	45	ASN
1	D	55	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	Rotameric Outliers	
1	А	245/245~(100%)	229~(94%)	16 (6%)	17 12
1	В	245/245~(100%)	226~(92%)	19 (8%)	12 8
1	С	245/245~(100%)	224~(91%)	21 (9%)	10 6
1	D	245/245~(100%)	227~(93%)	18 (7%)	14 9
All	All	980/980~(100%)	906~(92%)	74 (8%)	13 8

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	\mathbf{Res}	Type
1	А	4	SER
1	А	47	ASP
1	А	49	LEU
1	А	52	MET
1	А	57	VAL
1	А	81	LYS
1	А	106	LEU
1	А	114	LYS
1	А	119	ILE
1	А	122	GLU
1	А	123	LYS
1	А	194	VAL
1	А	249	LEU
1	А	259	GLU
1	А	266	SER
1	А	292	LEU
1	В	17	GLU
1	В	22	ILE
1	В	42	ILE
1	В	43	GLN
1	В	45	ASN
1	В	46	GLU
1	В	52	MET
1	В	78	LYS



Mol	Chain	Res	Type
1	В	83	GLU
1	В	86	GLU
1	В	122	GLU
1	В	124	LEU
1	В	140	LYS
1	В	158	THR
1	В	180	LEU
1	В	194	VAL
1	В	235	LEU
1	В	237	LYS
1	В	249	LEU
1	С	16	LYS
1	С	43	GLN
1	С	78	LYS
1	С	106	LEU
1	С	107	TYR
1	С	108	SER
1	С	115	ASP
1	С	121	ASN
1	С	123	LYS
1	С	140	LYS
1	С	144	ILE
1	С	145	ASN
1	С	155	ASN
1	С	180	LEU
1	С	194	VAL
1	С	233	GLU
1	С	249	LEU
1	С	256	LEU
1	С	266	SER
1	C	281	LYS
1	C	292	LEU
1	D	1	MET
1	D	4	SER
1	D	8	ASP
1	D	25	LYS
1	D	43	GLN
1	D	51	GLU
1	D	52	MET
1	D	87	LYS
1	D	94	LYS
1	D	122	GLU



Continucu from previous puye							
Mol	Chain	\mathbf{Res}	Type				
1	D	123	LYS				
1	D	143	SER				
1	D	180	LEU				
1	D	194	VAL				
1	D	211	LYS				
1	D	256	LEU				
1	D	259	GLU				
1	D	263	THR				

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	10	HIS
1	А	40	ASN
1	А	41	GLN
1	А	244	HIS
1	В	10	HIS
1	В	40	ASN
1	В	43	GLN
1	В	214	ASN
1	В	244	HIS
1	В	253	HIS
1	С	10	HIS
1	С	43	GLN
1	С	45	ASN
1	С	101	ASN
1	С	121	ASN
1	С	145	ASN
1	С	244	HIS
1	С	272	GLN
1	D	10	HIS
1	D	244	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

4 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).

Ма	Mal Truna Chain Ba		Dec	T :nl.	Bond lengths			Bond angles		
wor Type Chain	Chain	lites		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2	
1	CSD	А	37	1,3	3,7,8	2.23	1 (33%)	$1,\!8,\!10$	7.72	1 (100%)
1	CSD	В	37	1,3	3,7,8	0.83	0	$1,\!8,\!10$	<mark>5.78</mark>	1 (100%)
1	CSD	С	37	1,3	3,7,8	0.60	0	$1,\!8,\!10$	9.74	1 (100%)
1	CSD	D	37	1,3	3,7,8	2.30	1 (33%)	$1,\!8,\!10$	6.47	1 (100%)

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	\mathbf{Res}	Link	Chirals	Torsions	Rings
1	CSD	А	37	1,3	-	2/2/6/8	-
1	CSD	В	37	1,3	-	2/2/6/8	-
1	CSD	С	37	1,3	-	1/2/6/8	-
1	CSD	D	37	1,3	-	0/2/6/8	-

All	(2)	bond	length	outliers	are	listed	below:
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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\operatorname{Ideal}(\operatorname{\AA})$
1	D	37	CSD	CB-SG	3.72	1.99	1.79
1	А	37	CSD	CB-SG	3.20	1.97	1.79

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	С	37	CSD	OD1-SG-CB	9.74	124.07	105.54
1	А	37	CSD	OD1-SG-CB	7.72	120.23	105.54
1	D	37	CSD	OD1-SG-CB	6.47	117.85	105.54
1	В	37	CSD	OD1-SG-CB	5.78	116.54	105.54

There are no chirality outliers.

All (5) torsion outliers are listed below:



Mol	Chain	Res	Type	Atoms
1	А	37	CSD	N-CA-CB-SG
1	А	37	CSD	CA-CB-SG-OD1
1	В	37	CSD	N-CA-CB-SG
1	В	37	CSD	CA-CB-SG-OD1
1	С	37	CSD	CA-CB-SG-OD1

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	37	CSD	2	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (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.

6.5 Other polymers (i)

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

