

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

Feb 13, 2023 – 12:21 pm GMT

:	7Z6E
:	Structure of the C1-PH-CNH regulatory module of MRCK1
:	Truebestein, L.; Leonard, T.A.
:	2022-03-11
:	2.14 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
Xtriage (Phenix)	:	1.13
EDS	:	2.32.1
buster-report	:	1.1.7(2018)
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)	:	2.32.1

# 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 2.14 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 $(\#Entries, resolution range(Å))$
D	120704	
$\Lambda_{free}$	150704	2323(2.10-2.12)
Clashscore	141614	2653 (2.16-2.12)
Ramachandran outliers	138981	2618 (2.16-2.12)
Sidechain outliers	138945	2617 (2.16-2.12)
RSRZ outliers	127900	2485 (2.16-2.12)

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	Λ	582	2%	120/ 110/
	Π	562	4%	13% • 11%
1	В	582	77%	14% • 9%
1	C	582	10%	10% . 8%
-		002	6%	1970 • 070
1	D	582	71%	17% • 10%
1	Е	582	78%	10% • 11%



## 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 21821 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					AltConf	Trace
1	Δ	510	Total	С	Ν	0	$\mathbf{S}$	0	0	0
1	Л	519	4095	2606	708	753	28	0	0	0
1	В	530	Total	С	Ν	0	S	0	0	0
1	D	550	4188	2659	725	776	28	0		0
1	C	524	Total	С	Ν	0	$\mathbf{S}$	0	0	0
1		004	4208	2672	729	778	29			
1	П	525	Total	С	Ν	Ο	S	0	0	0
1	D	525	4140	2632	714	766	28	0		0
1	F	517	Total	С	Ν	0	S	0	0	0
	E	E 517	4085	2596	702	758	29	0	0	0

• Molecule 1 is a protein called Serine/threenine-protein kinase mrck-1.

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	953	ALA	-	expression tag	UNP 001583
А	954	ARG	-	expression tag	UNP 001583
В	953	ALA	-	expression tag	UNP O01583
В	954	ARG	-	expression tag	UNP 001583
С	953	ALA	-	expression tag	UNP 001583
С	954	ARG	-	expression tag	UNP 001583
D	953	ALA	-	expression tag	UNP 001583
D	954	ARG	-	expression tag	UNP 001583
E	953	ALA	-	expression tag	UNP 001583
E	954	ARG	-	expression tag	UNP O01583

• Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	2	Total Zn 2 2	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	В	2	Total Zn 2 2	0	0
2	С	2	Total Zn 2 2	0	0
2	D	2	Total Zn 2 2	0	0
2	Ε	2	Total Zn 2 2	0	0

• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	298	Total O 298 298	0	0
3	В	268	Total O   268 268	0	0
3	С	180	Total O 180 180	0	0
3	D	168	Total O   168 168	0	0
3	Е	181	Total O 181 181	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: Serine/threonine-protein kinase mrck-1

 $\bullet$  Molecule 1: Serine/threenine-protein kinase mrck-1



ALA ARG GLU

ALA ARG GLU







## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants	69.14Å 97.47Å 131.41Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$81.38^{\circ}$ $77.77^{\circ}$ $80.39^{\circ}$	Depositor
Bosolution (Å)	49.60 - 2.14	Depositor
	49.60 - 2.14	EDS
% Data completeness	94.0 (49.60-2.14)	Depositor
(in resolution range)	94.0(49.60-2.14)	EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.67 (at 2.14 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R R.	0.194 , $0.244$	Depositor
II, II, <i>free</i>	0.194 , $0.241$	DCC
$R_{free}$ test set	8482 reflections $(4.98%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	36.5	Xtriage
Anisotropy	0.503	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.32 , $42.3$	EDS
L-test for $twinning^2$	$ < L >=0.48, < L^2>=0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	21821	wwPDB-VP
Average B, all atoms $(Å^2)$	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.32% 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: ZN

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	Chain Bond lengths		Bond angles		
1VIOI	Unain	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	А	0.44	0/4174	0.66	1/5645~(0.0%)	
1	В	0.45	0/4270	0.65	0/5775	
1	С	0.40	0/4287	0.64	1/5795~(0.0%)	
1	D	0.39	0/4222	0.61	0/5710	
1	Е	0.39	0/4165	0.63	1/5632~(0.0%)	
All	All	0.42	0/21118	0.64	3/28557~(0.0%)	

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

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

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
1	С	1457	LEU	CB-CG-CD1	-11.35	91.70	111.00
1	Е	1392	LEU	CA-CB-CG	6.59	130.45	115.30
1	А	1261	ASP	CB-CG-OD1	5.33	123.10	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
1	А	1244	VAL	Peptide
1	В	1244	VAL	Peptide
1	D	990	SER	Peptide

#### 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	4095	0	4125	49	0
1	В	4188	0	4203	49	1
1	С	4208	0	4237	72	0
1	D	4140	0	4157	70	0
1	Е	4085	0	4092	32	0
2	А	2	0	0	0	0
2	В	2	0	0	0	0
2	С	2	0	0	0	0
2	D	2	0	0	0	0
2	Ε	2	0	0	0	0
3	А	298	0	0	7	0
3	В	268	0	0	10	0
3	С	180	0	0	12	0
3	D	168	0	0	4	0
3	Ε	181	0	0	5	0
All	All	21821	0	20814	268	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 6.

All (268) 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:D:1344:ARG:HD2	1:D:1368:HIS:HE1	1.46	0.81
1:C:1164:ARG:NH2	3:C:1704:HOH:O	2.15	0.80
1:D:1204:LEU:HD23	1:D:1217:VAL:HG11	1.64	0.79
1:D:1433:LYS:HD3	1:D:1446:SER:HA	1.68	0.74
1:D:1071:GLN:NE2	3:D:1701:HOH:O	2.20	0.73
1:E:1253:ARG:HH22	1:E:1269:LYS:HE3	1.53	0.73



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:C:1136:ALA:HB1	1:C:1141:GLU:HB3	1.70	0.72
1:A:1023:ARG:NH1	3:A:1707:HOH:O	2.23	0.70
1:D:1019:ILE:HD11	1:D:1055:PHE:H	1.55	0.70
1:A:1459:GLU:OE2	3:A:1701:HOH:O	2.09	0.69
1:A:1417:MET:HE3	1:A:1419:ARG:HD3	1.75	0.69
1:B:1099:ILE:HG23	1:B:1100:HIS:HD2	1.58	0.69
1:C:1237:GLU:HG3	1:C:1306:ILE:HG21	1.74	0.69
1:C:1222:GLU:OE2	3:C:1701:HOH:O	2.11	0.68
1:C:991:CYS:N	3:C:1709:HOH:O	2.25	0.68
1:D:1376:ASP:HB2	1:D:1419:ARG:HE	1.58	0.68
1:B:1087:ASP:OD1	3:B:1701:HOH:O	2.11	0.68
1:E:1151:GLU:O	3:E:1701:HOH:O	2.11	0.68
1:C:982:ASP:OD2	3:C:1702:HOH:O	2.12	0.67
1:C:1034:LYS:HB2	1:C:1135:MET:HB3	1.77	0.67
1:B:1164:ARG:NH1	1:B:1459:GLU:OE2	2.28	0.66
1:D:1248:LYS:H	1:D:1248:LYS:HD3	1.59	0.65
1:A:1007:CYS:HB3	1:A:1008:PRO:HD3	1.79	0.65
1:B:1046:GLN:NE2	3:B:1706:HOH:O	2.30	0.65
1:B:1238:GLN:HB3	1:B:1257:SER:HB2	1.79	0.65
1:C:1210:SER:OG	1:C:1211:ARG:NH1	2.28	0.65
1:E:1269:LYS:NZ	3:E:1705:HOH:O	2.28	0.65
1:A:1111:ARG:HD2	1:A:1131:TYR:CD2	2.32	0.64
1:A:1111:ARG:HD2	1:A:1131:TYR:HD2	1.62	0.64
1:B:1099:ILE:HG23	1:B:1100:HIS:CD2	2.32	0.64
1:D:1280:ALA:HB2	1:D:1328:ILE:HG23	1.78	0.64
1:E:1075:ASN:ND2	3:E:1709:HOH:O	2.31	0.64
1:A:1095:GLU:HG2	1:A:1106:ILE:HG13	1.80	0.64
1:B:1062:CYS:HB3	1:B:1073:VAL:HG22	1.80	0.63
1:C:957:GLY:N	3:C:1712:HOH:O	2.31	0.63
1:C:1344:ARG:HG2	1:C:1368:HIS:NE2	2.13	0.63
1:D:1248:LYS:HD3	1:D:1248:LYS:N	2.14	0.63
1:D:1116:GLN:HG2	1:D:1118:LEU:HD23	1.79	0.62
1:D:1021:PRO:HB3	1:D:1155:LEU:HD11	1.81	0.62
1:E:1255:VAL:HG23	1:E:1265:LEU:HD22	1.81	0.62
1:A:1064:VAL:HG12	1:A:1071:GLN:HG2	1.80	0.62
1:C:1326:GLN:OE1	1:C:1389:GLU:HB2	2.01	0.61
1:D:1475:ASP:OD1	1:D:1477:ILE:HG22	2.00	0.61
1:A:1037:ARG:HB2	1:A:1037:ARG:NH1	2.14	0.61
1:B:1035:THR:HG22	1:B:1133:LEU:O	2.01	0.61
1:C:1019:ILE:HG13	1:C:1028:ALA:HB2	1.83	0.61
1:B:1105:ASP:HB3	1:B:1135:MET:HE2	1.80	0.61



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:A:1439:GLU:OE2	3:A:1702:HOH:O	2.16	0.60
1:D:988:CYS:SG	1:D:991:CYS:HB3	2.40	0.60
1:D:1099:ILE:HG13	1:D:1100:HIS:CD2	2.36	0.60
1:C:1251:HIS:HB3	1:C:1274:LYS:HD2	1.83	0.60
1:D:1162:ALA:N	3:D:1704:HOH:O	2.34	0.60
1:C:991:CYS:SG	1:C:993:TYR:HB2	2.42	0.60
1:D:958:HIS:ND1	1:D:1007:CYS:HB2	2.17	0.60
1:D:1059:LEU:HD11	1:D:1134:PHE:CE1	2.37	0.59
1:D:1046:GLN:OE1	1:D:1078:ARG:NH1	2.33	0.59
1:D:1286:PRO:HG2	1:D:1349:VAL:HG21	1.85	0.59
1:D:1367:GLN:OE1	1:D:1369:ILE:HG12	2.03	0.59
1:A:1019:ILE:HD13	1:A:1055:PHE:H	1.67	0.59
1:B:1147:VAL:O	1:B:1151:GLU:HG3	2.02	0.59
1:C:1077:ILE:O	1:C:1430:THR:HB	2.02	0.59
1:E:1136:ALA:HB1	1:E:1141:GLU:HG2	1.85	0.58
1:B:1019:ILE:HD13	1:B:1055:PHE:H	1.68	0.58
1:A:1402:GLU:OE2	1:A:1421:SER:OG	2.20	0.58
1:D:1222:GLU:OE2	1:D:1226:ARG:NH2	2.35	0.58
1:B:1253:ARG:HH11	1:B:1269:LYS:HB2	1.68	0.58
1:D:1136:ALA:HB1	1:D:1141:GLU:HG3	1.86	0.57
1:A:1116:GLN:HG3	1:A:1129:LYS:HG3	1.86	0.57
1:A:1433:LYS:HE2	1:A:1447:GLU:OE2	2.04	0.57
1:B:1380:GLN:NE2	3:B:1711:HOH:O	2.38	0.56
1:A:1111:ARG:HG3	1:A:1133:LEU:HD23	1.87	0.56
1:B:1019:ILE:HG13	1:B:1028:ALA:HB2	1.88	0.56
1:C:970:LYS:HE3	1:C:1030:GLU:OE2	2.06	0.56
1:D:1172:VAL:HB	1:D:1489:PHE:HD1	1.69	0.56
1:B:1095:GLU:OE2	1:B:1103:LYS:HG3	2.06	0.55
1:A:1019:ILE:HG13	1:A:1028:ALA:HB2	1.88	0.55
1:C:1034:LYS:HG2	1:C:1047:THR:HG22	1.88	0.55
1:B:988:CYS:O	1:B:989:GLN:HB3	2.07	0.55
1:D:991:CYS:SG	1:D:993:TYR:HB2	2.47	0.55
1:C:1222:GLU:OE1	1:C:1226:ARG:NH2	2.40	0.54
1:C:1178:LEU:HD23	1:C:1181:ILE:HB	1.88	0.54
1:E:1253:ARG:CZ	1:E:1269:LYS:HG2	2.38	0.54
1:C:1055:PHE:O	1:C:1083:MET:HG3	2.07	0.54
1:D:1150:SER:O	1:D:1154:THR:HG23	2.07	0.54
1:E:1380:GLN:NE2	3:E:1702:HOH:O	2.25	0.54
1:D:1204:LEU:O	1:D:1217:VAL:HG12	2.08	0.54
1:C:1168:LEU:HD12	1:C:1495:VAL:HG12	1.89	0.54
1:A:1339:PHE:CE1	1:A:1344:ARG:HD2	2.43	0.53



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:B:1105:ASP:OD1	3:B:1702:HOH:O	2.19	0.53
1:C:1309:SER:O	1:C:1312:ARG:HD2	2.09	0.53
1:C:1111:ARG:HD2	1:C:1131:TYR:CD2	2.42	0.52
1:C:1280:ALA:HB2	1:C:1328:ILE:HG23	1.91	0.52
1:A:1021:PRO:HG2	1:B:1124:TYR:CE2	2.44	0.52
1:A:1039:GLY:HA3	1:A:1043:LYS:NZ	2.25	0.52
1:B:1025:VAL:HA	1:B:1054:ASP:OD1	2.10	0.52
1:C:1011:GLU:OE1	1:C:1014:ARG:NH1	2.42	0.52
1:A:1368:HIS:O	1:A:1369:ILE:HD13	2.09	0.52
1:E:959:ASN:O	1:E:988:CYS:HA	2.09	0.52
1:C:1470:LYS:NZ	3:C:1703:HOH:O	2.14	0.52
1:C:1248:LYS:H	1:C:1248:LYS:HD3	1.74	0.52
1:E:1344:ARG:HD2	1:E:1368:HIS:NE2	2.25	0.52
1:B:1498:ASP:OD1	1:B:1498:ASP:N	2.41	0.52
1:C:1138:THR:OG1	1:C:1139:GLU:N	2.39	0.52
1:D:1034:LYS:HB2	1:D:1135:MET:HB3	1.90	0.51
1:B:1086:PRO:O	1:D:1102:GLN:HG2	2.10	0.51
1:D:1042:ARG:HG3	1:D:1100:HIS:ND1	2.26	0.51
1:D:1042:ARG:CZ	1:D:1100:HIS:HE1	2.23	0.51
1:D:1001:GLU:OE1	1:D:1002:ARG:HG3	2.10	0.51
1:B:1316:TRP:O	1:B:1317:LYS:HD2	2.11	0.51
1:C:1423:LEU:HB2	1:C:1424:PRO:HD3	1.93	0.51
1:E:996:HIS:HB2	1:E:999:CYS:HB2	1.92	0.50
1:D:1222:GLU:OE1	1:D:1266:LYS:HD2	2.12	0.50
1:D:1278:LEU:HB2	1:D:1296:ALA:HB3	1.94	0.50
1:B:1178:LEU:HD23	1:B:1181:ILE:HB	1.94	0.50
1:B:1377:THR:HA	1:B:1380:GLN:OE1	2.12	0.49
1:A:1197:ILE:HD12	1:A:1207:ILE:HD12	1.95	0.49
1:C:1139:GLU:HG2	1:C:1143:ARG:HE	1.77	0.49
1:E:971:CYS:HB2	1:E:996:HIS:CE1	2.47	0.49
1:B:1166:ALA:O	1:B:1495:VAL:HG22	2.13	0.49
1:C:1379:LEU:HD22	1:C:1412:LEU:HD21	1.94	0.49
1:D:1346:TRP:HA	1:D:1367:GLN:O	2.13	0.49
1:C:1321:MET:HG3	1:C:1325:PRO:HG3	1.95	0.49
1:C:1457:LEU:HD11	3:C:1826:HOH:O	2.12	0.49
1:A:1021:PRO:HG2	1:B:1124:TYR:HE2	1.77	0.49
1:E:974:CYS:O	1:E:975:THR:OG1	2.30	0.48
1:C:990:SER:HB2	3:C:1709:HOH:O	2.13	0.48
1:D:1335:LEU:O	1:D:1345:SER:HA	2.13	0.48
1:D:1344:ARG:HH11	1:D:1368:HIS:CE1	2.31	0.48
1:C:1129:LYS:HB2	1:C:1131:TYR:HE1	1.78	0.48



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:D:1210:SER:HB3	1:D:1503:GLU:OE2	2.13	0.48
1:D:1238:GLN:NE2	3:D:1713:HOH:O	2.46	0.48
3:B:1701:HOH:O	1:D:1103:LYS:HG2	2.13	0.47
1:C:1019:ILE:HD13	1:C:1055:PHE:H	1.79	0.47
1:A:1403:TYR:OH	1:A:1416:GLU:OE2	2.26	0.47
1:E:1057:LEU:HB2	1:E:1081:LEU:HB2	1.96	0.47
1:E:1160:LYS:NZ	3:E:1718:HOH:O	2.46	0.47
1:E:1385:GLN:HB3	1:E:1388:TYR:CD1	2.49	0.47
1:D:1059:LEU:HD11	1:D:1134:PHE:HE1	1.76	0.47
1:E:1088:PHE:HA	1:E:1113:THR:O	2.15	0.47
1:A:970:LYS:NZ	3:A:1716:HOH:O	2.47	0.47
1:A:957:GLY:N	3:A:1728:HOH:O	2.48	0.47
1:B:1143:ARG:HG3	3:B:1918:HOH:O	2.15	0.47
1:A:1253:ARG:NH1	3:A:1726:HOH:O	2.47	0.47
1:E:1025:VAL:HA	1:E:1054:ASP:OD1	2.15	0.47
1:A:1250:ARG:O	1:A:1274:LYS:HA	2.14	0.47
1:A:1021:PRO:HG3	1:A:1155:LEU:HD21	1.97	0.47
1:A:1160:LYS:HD2	1:A:1160:LYS:HA	1.65	0.47
1:C:968:PRO:HG3	1:C:1060:TYR:CE2	2.49	0.46
1:B:1253:ARG:NH1	1:B:1269:LYS:HB2	2.30	0.46
1:B:1277:HIS:ND1	3:B:1709:HOH:O	2.36	0.46
1:C:1389:GLU:HG3	1:C:1391:LYS:HE2	1.98	0.46
1:C:970:LYS:HE2	1:C:1017:LEU:HD21	1.96	0.46
1:C:1111:ARG:HG3	1:C:1133:LEU:HD23	1.98	0.46
1:C:1065:ASP:OD2	1:C:1069:LYS:HB3	2.15	0.46
1:C:1417:MET:HE3	3:C:1856:HOH:O	2.15	0.46
1:E:1478:LEU:HD23	1:E:1491:LEU:HD23	1.98	0.46
1:D:1204:LEU:HB3	1:D:1217:VAL:CG1	2.46	0.46
1:B:1317:LYS:NZ	3:B:1719:HOH:O	2.44	0.46
1:C:1142:LYS:O	1:C:1146:VAL:HG23	2.16	0.46
1:C:1240:LEU:HD11	1:C:1260:LEU:HD21	1.98	0.46
1:D:1328:ILE:CD1	1:D:1337:VAL:HG22	2.46	0.46
1:D:1303:ILE:HD11	1:D:1319:LEU:HD12	1.98	0.45
1:B:1335:LEU:O	1:B:1345:SER:HA	2.17	0.45
1:E:1095:GLU:OE2	1:E:1103:LYS:HG3	2.16	0.45
1:B:1010:PRO:HG2	1:B:1013:GLU:OE1	2.16	0.45
1:D:1344:ARG:HD2	1:D:1368:HIS:CE1	2.37	0.45
1:D:1439:GLU:HA	1:D:1440:PRO:HA	1.85	0.45
1:E:1136:ALA:HB1	1:E:1141:GLU:CG	2.45	0.45
1:B:1050:VAL:HG22	1:B:1059:LEU:HD13	1.98	0.45
1:B:1119:ASN:ND2	3:B:1724:HOH:O	2.48	0.45



<u> </u>	<b>A t</b> and <b>D</b>	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:B:1127:SER:HB2	1:B:1484:ASN:OD1	2.17	0.45
1:C:1034:LYS:HE3	1:C:1047:THR:HG23	1.97	0.45
1:D:958:HIS:CE1	1:D:1007:CYS:HB2	2.50	0.45
1:E:1231:VAL:HG23	1:E:1242:MET:HG2	1.99	0.45
1:A:1043:LYS:HB3	1:A:1043:LYS:HE2	1.58	0.45
1:B:1493:GLN:NE2	1:B:1500:ASP:HA	2.32	0.45
1:D:1204:LEU:HB3	1:D:1217:VAL:HG11	1.98	0.45
1:E:1160:LYS:HA	1:E:1160:LYS:HD2	1.75	0.45
1:C:977:ILE:HG13	1:C:1051:VAL:HG11	1.99	0.44
1:C:1246:PRO:HG2	1:C:1248:LYS:HE2	1.99	0.44
1:D:1025:VAL:HA	1:D:1054:ASP:OD1	2.17	0.44
1:E:1178:LEU:HD23	1:E:1181:ILE:HB	1.97	0.44
1:A:1391:LYS:HG3	1:A:1435:PHE:CE1	2.52	0.44
1:C:1111:ARG:HD2	1:C:1131:TYR:HD2	1.81	0.44
1:C:1088:PHE:HA	1:C:1113:THR:O	2.17	0.44
1:C:1037:ARG:NH1	1:C:1046:GLN:OE1	2.51	0.44
1:D:1023:ARG:HD2	1:D:1023:ARG:HA	1.82	0.44
1:A:988:CYS:O	1:A:989:GLN:HB3	2.17	0.44
1:C:1082:ASP:OD1	1:C:1084:ARG:NH1	2.51	0.44
1:C:1183:VAL:HB	1:C:1200:SER:OG	2.18	0.44
1:B:1010:PRO:O	1:B:1012:GLU:N	2.47	0.44
1:C:1351:VAL:HG21	1:C:1366:LEU:HD22	1.99	0.44
1:C:1174:ASP:OD2	1:C:1176:THR:N	2.50	0.43
1:D:1433:LYS:HD2	1:D:1433:LYS:N	2.33	0.43
1:C:1119:ASN:ND2	1:C:1119:ASN:O	2.50	0.43
1:C:1147:VAL:O	1:C:1151:GLU:HG3	2.18	0.43
1:D:1146:VAL:O	1:D:1150:SER:OG	2.22	0.43
1:A:988:CYS:SG	1:A:990:SER:HB2	2.58	0.43
1:C:1118:LEU:HD11	1:C:1168:LEU:HD22	2.00	0.43
1:D:1242:MET:O	1:D:1252:VAL:HA	2.18	0.43
1:B:1417:MET:CE	1:C:1341:HIS:CE1	3.02	0.43
1:D:1034:LYS:HB2	1:D:1034:LYS:HE2	1.75	0.43
1:A:1062:CYS:HB3	1:A:1073:VAL:HG22	1.99	0.43
1:D:1165:LYS:NZ	3:D:1727:HOH:O	2.52	0.43
1:A:1037:ARG:HB2	1:A:1037:ARG:CZ	2.49	0.43
1:C:1213:LEU:HD23	1:C:1213:LEU:HA	1.81	0.43
1:B:1019:ILE:HG12	1:B:1026:GLY:O	2.19	0.43
1:B:1055:PHE:O	1:B:1083:MET:HG3	2.18	0.43
1:A:1030:GLU:HG2	1:A:1051:VAL:HG22	2.00	0.42
1:A:1335:LEU:O	1:A:1345:SER:HA	2.19	0.42
1:C:967:THR:HG22	1:C:1073:VAL:O	2.18	0.42



	<b>A</b> + <b>O</b>	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:D:1317:LYS:HD3	1:D:1318:ASP:N	2.34	0.42
1:A:1222:GLU:OE1	1:A:1226:ARG:NH2	2.53	0.42
1:E:966:LYS:HD2	1:E:966:LYS:HA	1.79	0.42
1:B:987:PHE:CE2	1:B:989:GLN:HA	2.53	0.42
1:C:1317:LYS:HE2	3:C:1793:HOH:O	2.20	0.42
1:A:1057:LEU:HD11	1:A:1149:LEU:HD22	2.01	0.42
1:E:1190:ILE:HG21	1:E:1194:LYS:HE2	2.00	0.42
1:E:1381:PHE:O	1:E:1385:GLN:HG2	2.19	0.42
1:A:1009:VAL:HG12	1:A:1010:PRO:HD2	2.02	0.42
1:B:1086:PRO:HG3	1:B:1165:LYS:HE2	2.01	0.42
1:C:1036:PRO:HD3	1:C:1045:TRP:CZ3	2.54	0.42
1:D:1194:LYS:HG2	1:D:1208:GLU:HG2	2.02	0.42
1:A:1424:PRO:HG2	3:A:1984:HOH:O	2.20	0.42
1:B:1088:PHE:HA	1:B:1113:THR:O	2.20	0.42
1:C:1116:GLN:HB2	1:C:1129:LYS:HG2	2.01	0.42
1:D:1142:LYS:HE2	1:D:1142:LYS:HB3	1.86	0.42
1:D:1346:TRP:NE1	1:D:1368:HIS:HB2	2.35	0.42
1:D:1379:LEU:HD21	1:D:1420:ARG:HB2	2.01	0.42
1:B:1280:ALA:HB2	1:B:1328:ILE:HG23	2.01	0.41
1:B:1314:LYS:HD2	1:B:1315:LYS:O	2.20	0.41
1:E:1084:ARG:HG3	1:E:1156:LEU:HD21	2.02	0.41
1:D:1099:ILE:HG13	1:D:1100:HIS:HD2	1.83	0.41
1:D:1168:LEU:HG	1:D:1495:VAL:HG12	2.02	0.41
1:D:1294:ALA:HB2	1:D:1330:ILE:HD11	2.01	0.41
1:B:1124:TYR:CG	1:B:1125:SER:N	2.88	0.41
1:C:1097:ASP:OD2	1:C:1111:ARG:NH1	2.53	0.41
1:D:1103:LYS:HA	1:D:1103:LYS:HD3	1.78	0.41
1:D:1241:MET:HG3	1:D:1254:ILE:HG13	2.02	0.41
1:A:1168:LEU:HG	1:A:1495:VAL:HG12	2.02	0.41
1:B:1448:ASN:ND2	3:B:1728:HOH:O	2.53	0.41
1:A:1111:ARG:CD	1:A:1131:TYR:HD2	2.30	0.41
1:C:1274:LYS:HD3	3:C:1827:HOH:O	2.20	0.41
1:D:1381:PHE:O	1:D:1384:GLN:HG2	2.20	0.41
1:E:1251:HIS:NE2	1:E:1253:ARG:HD2	2.35	0.41
1:C:1087:ASP:HB2	1:C:1114:THR:O	2.20	0.41
1:C:1185:GLN:NE2	1:C:1200:SER:HB3	2.35	0.41
1:D:1369:ILE:HD13	1:D:1369:ILE:HA	1.87	0.41
1:A:1137:GLU:HG3	1:A:1141:GLU:HG3	2.01	0.41
1:A:1417:MET:CE	1:A:1419:ARG:HD3	2.48	0.41
1:C:1344:ARG:CG	1:C:1368:HIS:NE2	2.83	0.41
1:A:1019:ILE:CD1	1:A:1055:PHE:H	2.31	0.41



Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap (Å)
1:A:1240:LEU:O	1:A:1254:ILE:HA	2.20	0.41
1:C:1069:LYS:HA	1:C:1069:LYS:HD3	1.94	0.41
1:C:1104:GLY:O	1:C:1107:PRO:HD2	2.20	0.41
1:C:1129:LYS:HB2	1:C:1129:LYS:HE3	1.81	0.41
1:A:1106:ILE:HB	1:A:1107:PRO:HD3	2.03	0.41
1:A:1197:ILE:HD12	1:A:1207:ILE:CD1	2.50	0.41
1:B:976:SER:OG	1:B:1054:ASP:OD1	2.39	0.41
1:C:1310:GLU:O	3:C:1705:HOH:O	2.22	0.41
1:E:1309:SER:O	1:E:1312:ARG:HD2	2.20	0.41
1:E:1106:ILE:HD13	1:E:1109:ILE:HD12	2.04	0.40
1:B:1312:ARG:HA	1:B:1312:ARG:HD2	1.91	0.40
1:D:1274:LYS:HD3	1:D:1274:LYS:HA	1.95	0.40
1:E:1059:LEU:HD12	1:E:1079:LEU:HD23	2.04	0.40
1:D:1377:THR:HA	1:D:1380:GLN:HG3	2.02	0.40
1:D:1419:ARG:N	1:D:1419:ARG:HD2	2.36	0.40
1:D:1376:ASP:HA	1:D:1419:ARG:HH21	1.87	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:B:957:GLY:O	1:B:1308:ARG:NH2[1_655]	2.08	0.12

### 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	509/582~(88%)	489 (96%)	20 (4%)	0	100	100
1	В	522/582~(90%)	500 (96%)	22 (4%)	0	100	100
1	С	524/582~(90%)	511 (98%)	13 (2%)	0	100	100
1	D	517/582~(89%)	501 (97%)	16 (3%)	0	100	100



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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentile	$\mathbf{S}$
1	Ε	507/582~(87%)	484 (96%)	23~(4%)	0	100 100	
All	All	2579/2910~(89%)	2485 (96%)	94 (4%)	0	100 100	

There are no Ramachandran outliers to report.

#### 5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	А	459/511~(90%)	445 (97%)	14 (3%)	40 38
1	В	469/511~(92%)	450 (96%)	19 (4%)	30 27
1	С	471/511~(92%)	446 (95%)	25~(5%)	22 18
1	D	464/511~(91%)	436~(94%)	28~(6%)	19 14
1	Е	459/511~(90%)	442 (96%)	17 (4%)	34 31
All	All	2322/2555~(91%)	2219 (96%)	103 (4%)	28 24

All (103) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	989	GLN
1	А	1009	VAL
1	А	1063	THR
1	А	1064	VAL
1	А	1128	SER
1	А	1142	LYS
1	А	1164	ARG
1	А	1165	LYS
1	А	1187	CYS
1	А	1305	GLN
1	А	1366	LEU
1	А	1395	ASN
1	А	1399	SER
1	А	1485	ASP



Mol	Chain	Res	Type
1	В	1004	SER
1	В	1009	VAL
1	B	1012	GLU
1	B	1017	LEU
1	B	1041	VAL
1	В	1072	ASP
1	В	1094	SER
1	В	1103	LYS
1	В	1164	ARG
1	В	1175	VAL
1	В	1187	CYS
1	В	1191	ASP
1	В	1194	LYS
1	B	1200	SER
1	B	1213	LEU
1	В	1241	MET
1	В	1248	LYS
1	В	1314	LYS
1	В	1498	ASP
1	С	976	SER
1	C	1001	GLU
1	C	1004	SER
1	С	1029	TYR
1	C	1033	VAL
1	С	1064	VAL
1	C	1138	THR
1	C	1142	LYS
1	С	1143	ARG
1	С	1187	CYS
1	С	1201	ASP
1	С	1265	LEU
1	С	1308	ARG
1	С	1317	LYS
1	С	1340	SER
1	С	1341	HIS
1	С	1342	SER
1	С	1345	SER
1	С	1351	VAL
1	C	1368	HIS
1	С	1371	LEU
1	C	1374	MET
1	C	1395	ASN
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Mol	Chain	Res	Type
1	С	1399	SER
1	С	1498	ASP
1	D	979	ILE
1	D	989	GLN
1	D	990	SER
1	D	998	SER
1	D	1009	VAL
1	D	1019	ILE
1	D	1032	LEU
1	D	1034	LYS
1	D	1122	SER
1	D	1126	SER
1	D	1127	SER
1	D	1140	GLU
1	D	1142	LYS
1	D	1154	THR
1	D	1165	LYS
1	D	1176	THR
1	D	1187	CYS
1	D	1201	ASP
1	D	1248	LYS
1	D	1340	SER
1	D	1367	GLN
1	D	1368	HIS
1	D	1374	MET
1	D	1378	SER
1	D	1395	ASN
1	D	1399	SER
1	D	1477	ILE
1	D	1485	ASP
1	Е	1042	ARG
1	Е	1094	SER
1	Е	1178	LEU
1	E	1181	ILE
1	E	1187	CYS
1	E	1200	SER
1	E	1201	ASP
1	E	1212	GLN
1	E	1213	LEU
1	Е	1248	LYS
1	E	1368	HIS
1	Е	1375	GLU



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Mol	Chain	Res	Type
1	Е	1386	THR
1	Е	1395	ASN
1	Е	1399	SER
1	Е	1431	GLN
1	Е	1485	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	$\mathbf{Res}$	Type
1	А	1383	ASN
1	В	1100	HIS
1	В	1499	GLN
1	С	1284	ASN
1	D	1100	HIS
1	D	1185	GLN
1	D	1368	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)

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 10 ligands modelled in this entry, 10 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)

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	< <b>RSRZ</b> >	#RSRZ>2	$OWAB(Å^2)$	Q<0.9
1	А	519/582~(89%)	0.31	13 (2%) 57 64	24, 38, 79, 121	0
1	В	530/582~(91%)	0.42	21 (3%) 38 46	26, 41, 81, 141	0
1	С	534/582~(91%)	0.70	57 (10%) 6 7	27, 51, 108, 143	0
1	D	525/582~(90%)	0.46	35 (6%) 17 22	30, 53, 88, 133	0
1	Е	517/582~(88%)	0.49	39 (7%) 14 18	27, 50, 90, 120	0
All	All	2625/2910 (90%)	0.48	165 (6%) 20 25	24, 46, 94, 143	0

All (165) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1016	PRO	7.2
1	D	1022	THR	7.1
1	D	1017	LEU	6.6
1	С	1017	LEU	6.5
1	В	1016	PRO	6.3
1	В	1014	ARG	6.1
1	Ε	1374	MET	6.0
1	В	1022	THR	6.0
1	В	1017	LEU	5.9
1	С	1363	GLY	5.7
1	С	1093	VAL	5.7
1	D	1351	VAL	5.5
1	Е	1022	THR	5.5
1	С	1068	ASN	5.3
1	Е	1286	PRO	5.3
1	С	1098	VAL	5.2
1	С	1362	SER	5.0
1	Е	1064	VAL	4.9
1	С	1012	GLU	4.9
1	D	1039	GLY	4.7



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Type RSRZ

1	C	1096	ALA	4.6
1	В	1021	PRO	4.6
1	С	1095	GLU	4.5
1	С	1064	VAL	4.5
1	С	1016	PRO	4.4
1	D	1020	ASP	4.4
1	А	1351	VAL	4.3
1	С	1509	ALA	4.3
1	С	1366	LEU	4.3
1	С	1110	PHE	4.3
1	D	1384	GLN	4.2
1	А	1038	ALA	4.2
1	В	1015	ARG	4.2
1	С	1508	LEU	4.2
1	А	1023	ARG	4.2
1	С	1022	THR	4.1
1	С	1158	ARG	4.0
1	С	1161	LEU	4.0
1	В	1213	LEU	4.0
1	D	1024	GLY	4.0
1	С	1071	GLN	3.9
1	В	1023	ARG	3.9
1	С	1364	ALA	3.9
1	D	1023	ARG	3.8
1	С	1107	PRO	3.8
1	А	1020	ASP	3.8
1	С	1131	TYR	3.8
1	Ε	1023	ARG	3.7
1	А	1064	VAL	3.7
1	С	1018	GLY	3.7
1	В	1020	ASP	3.7
1	С	1020	ASP	3.7
1	D	1211	ARG	3.7
1	С	1498	ASP	3.6
1	С	1038	ALA	3.6
1	Е	1213	LEU	3.6
1	D	1071	GLN	3.6
1	D	1018	GLY	3.6
1	D	1019	ILE	3.5
1	С	1090	VAL	3.5
1	Е	1039	GLY	3.5
1	С	1097	ASP	3.4



7Z6E	
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Mol	Chain	Res	Type	RSRZ	
1	D	1021	PRO	3.4	
1	С	1094	SER	3.4	
1	С	1365	VAL	3.4	
1	Е	1284	ASN	3.4	
1	С	1021	PRO	3.3	
1	В	1124	TYR	3.3	
1	Е	1005	GLN	3.2	
1	А	1021	PRO	3.2	
1	С	1157	ARG	3.2	
1	С	1351	VAL	3.1	
1	А	1039	GLY	3.1	
1	Е	1020	ASP	3.1	
1	А	1063	THR	3.1	
1	Е	1377	THR	3.0	
1	Е	1386	THR	3.0	
1	D	1367	GLN	3.0	
1	Е	1004	SER	3.0	
1	Е	1099	ILE	2.9	
1	В	1012	GLU	2.9	
1	С	1015	ARG	2.9	
1	Е	1211	ARG	2.9	
1	Е	1124	TYR	2.9	
1	D	1201	ASP	2.9	
1	С	1127	SER	2.9	
1	Е	1125	SER	2.9	
1	D	957	GLY	2.8	
1	Е	1369	ILE	2.7	
1	Е	1208	GLU	2.7	
1	Е	1003	VAL	2.7	
1	D	1385	GLN	2.7	
1	В	1002	ARG	2.7	
1	С	1104	GLY	2.7	
1	Ε	1285	ASN	2.7	
1	E	1062	CYS	2.6	
1	А	957	GLY	2.6	
1	С	1042	ARG	2.6	
1	В	1025	VAL	2.6	
1	D	1213	LEU	2.6	
1	С	1367	GLN	2.6	
1	В	1126	SER	2.6	
1	Е	1398	GLY	2.6	
1	D	1025	VAL	2.6	



Mol	Chain	Res	Type	RSRZ
1	Е	1042	ARG	2.6
1	С	1109	ILE	2.6
1	Е	957	GLY	2.6
1	D	1210	SER	2.5
1	В	1013	GLU	2.5
1	С	1141	GLU	2.5
1	Е	1499	GLN	2.5
1	В	1210	SER	2.5
1	D	1042	ARG	2.5
1	А	1043	LYS	2.5
1	В	1005	GLN	2.5
1	С	1037	ARG	2.5
1	В	1072	ASP	2.4
1	D	1224	LYS	2.4
1	D	1029	TYR	2.4
1	D	1205	TYR	2.4
1	D	1073	VAL	2.4
1	Е	1009	VAL	2.4
1	Е	1021	PRO	2.4
1	С	1044	GLY	2.4
1	D	1507	ASN	2.4
1	В	1004	SER	2.4
1	С	1212	GLN	2.4
1	В	1011	GLU	2.4
1	С	1442	LEU	2.3
1	D	1319	LEU	2.3
1	А	1071	GLN	2.3
1	Е	1283	THR	2.3
1	С	1140	GLU	2.3
1	С	1103	LYS	2.3
1	Е	1037	ARG	2.3
1	В	1018	GLY	2.3
1	D	1101	ALA	2.3
1	С	1011	GLU	2.3
1	С	1041	VAL	2.3
1	С	1210	SER	2.3
1	Е	1040	GLY	2.3
1	Е	1385	GLN	2.3
1	Е	1503	GLU	2.2
1	С	1014	ARG	2.2
1	С	1046	GLN	2.2
1	А	1508	LEU	2.2



Mol	Chain	Res	Type	RSRZ
1	D	1072	ASP	2.2
1	Е	1484	ASN	2.2
1	С	1045	TRP	2.1
1	D	1508	LEU	2.1
1	С	1069	LYS	2.1
1	D	1225	GLN	2.1
1	D	1215	ILE	2.1
1	С	1133	LEU	2.1
1	Е	1070	MET	2.1
1	С	1154	THR	2.1
1	Е	1063	THR	2.1
1	Е	1316	TRP	2.1
1	D	1264	ASP	2.1
1	Е	1071	GLN	2.1
1	А	1162	ALA	2.0
1	С	1147	VAL	2.0
1	D	1202	HIS	2.0
1	С	1108	LYS	2.0
1	Е	1388	TYR	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	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	Q<0.9
2	ZN	А	1601	1/1	0.97	0.09	40,40,40,40	0
2	ZN	Е	1602	1/1	0.98	0.11	$50,\!50,\!50,\!50$	0
2	ZN	В	1601	1/1	0.99	0.11	53,53,53,53	0
2	ZN	В	1602	1/1	0.99	0.10	42,42,42,42	0



Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
2	ZN	С	1601	1/1	0.99	0.07	48,48,48,48	0
2	ZN	С	1602	1/1	0.99	0.13	44,44,44,44	0
2	ZN	D	1601	1/1	0.99	0.08	41,41,41,41	0
2	ZN	D	1602	1/1	0.99	0.07	57,57,57,57	0
2	ZN	Е	1601	1/1	0.99	0.07	$50,\!50,\!50,\!50$	0
2	ZN	А	1602	1/1	0.99	0.14	40,40,40,40	0

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









































## 6.5 Other polymers (i)

There are no such residues in this entry.

