

Full wwPDB X-ray Structure Validation Report (i)

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PDB ID	:	6IVR
Title	:	Crystal structure of a membrane protein W16A
Authors	:	Kittredge, A.; Fukuda, F.; Zhang, Y.; Yang, T.
Deposited on	:	2018-12-04
Resolution	:	2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org* A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.27
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)	:	2.27

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 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569(2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	297	3% 68%	21%	• 10%
1	В	297	64%	26%	• 9%
1	С	297	4% 67%	21%	• 9%
1	D	297	5%	26%	10%
1	Е	297	^{2%} 70 %	21%	• 9%



The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CL	А	305	-	-	Х	-



2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 10827 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	Λ	268	Total	С	Ν	0	\mathbf{S}	0	0	0
1	Л	200	2135	1383	361	382	9	0	0	0
1	В	270	Total	С	Ν	0	S	0	0	0
1	D	210	2148	1391	364	384	9	0	0	0
1	С	260	Total	С	Ν	0	S	0	0	0
1	U	209	2146	1391	364	382	9			
1	Л	268	Total	С	Ν	0	S	0	0	0
1	D	208	2135	1383	361	382	9	0	0	0
1	F	271	Total	С	Ν	0	S	0	0	0
1		271	2162	1401	365	387	9	0	0	0

• Molecule 1 is a protein called Ibestrophin.

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	-2	SER	-	expression tag	UNP W9BH30
А	-1	ASN	-	expression tag	UNP W9BH30
А	0	ALA	-	expression tag	UNP W9BH30
А	16	ALA	TRP	engineered mutation	UNP W9BH30
В	-2	SER	-	expression tag	UNP W9BH30
В	-1	ASN	-	expression tag	UNP W9BH30
В	0	ALA	-	expression tag	UNP W9BH30
В	16	ALA	TRP	engineered mutation	UNP W9BH30
С	-2	SER	-	expression tag	UNP W9BH30
С	-1	ASN	-	expression tag	UNP W9BH30
С	0	ALA	-	expression tag	UNP W9BH30
С	16	ALA	TRP	engineered mutation	UNP W9BH30
D	-2	SER	-	expression tag	UNP W9BH30
D	-1	ASN	-	expression tag	UNP W9BH30
D	0	ALA	-	expression tag	UNP W9BH30
D	16	ALA	TRP	engineered mutation	UNP W9BH30
E	-2	SER	-	expression tag	UNP W9BH30
E	-1	ASN	-	expression tag	UNP W9BH30
E	0	ALA	_	expression tag	UNP W9BH30



Chain	Residue	Modelled	Actual	Comment	Reference
Ε	16	ALA	TRP	engineered mutation	UNP W9BH30

• Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	3	Total Zn 3 3	0	0
2	В	4	Total Zn 4 4	0	0
2	С	3	Total Zn 3 3	0	0
2	D	3	Total Zn 3 3	0	0
2	Е	2	Total Zn 2 2	0	0

• Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	А	1	Total 4	$\begin{array}{c} \mathrm{C} \\ \mathrm{2} \end{array}$	O 2	0	0

• Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	5	Total Cl 5 5	0	0
4	В	1	Total Cl 1 1	0	0
4	С	1	Total Cl 1 1	0	0
4	D	1	Total Cl 1 1	0	0
4	Е	3	Total Cl 3 3	0	0



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

• Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	А	15	Total O 15 15	0	0
6	В	13	Total O 13 13	0	0
6	С	11	Total O 11 11	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	D	16	Total O 16 16	0	0
6	Е	8	Total O 8 8	0	0



3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.



• Molecule 1: Ibestrophin





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	113.91Å 159.57Å 161.72Å	Deperitor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
$\mathbf{P}_{\text{assolution}}(\hat{\mathbf{A}})$	48.73 - 2.80	Depositor
Resolution (A)	48.73 - 2.80	EDS
% Data completeness	99.8 (48.73-2.80)	Depositor
(in resolution range)	99.8 (48.73-2.80)	EDS
R _{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.69 (at 2.81 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
P. P.	0.217 , 0.248	Depositor
n, n_{free}	0.217 , 0.248	DCC
R_{free} test set	3668 reflections $(5.02%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	74.7	Xtriage
Anisotropy	0.113	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.29 , 49.5	EDS
L-test for twinning ²	$< L > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	10827	wwPDB-VP
Average B, all atoms $(Å^2)$	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.30% 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: CL, EDO, ZN, ACY

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	
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.51	0/2181	0.66	0/2968
1	В	0.51	0/2196	0.64	0/2991
1	С	0.44	0/2194	0.58	0/2987
1	D	0.43	0/2181	0.57	0/2968
1	Е	0.47	0/2211	0.64	0/3011
All	All	0.47	0/10963	0.62	0/14925

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	Е	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	А	47	GLN	Peptide
1	Е	205	THR	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	2135	0	2181	67	0
1	В	2148	0	2184	80	0
1	С	2146	0	2190	60	0
1	D	2135	0	2181	61	0
1	Е	2162	0	2201	58	0
2	А	3	0	0	0	0
2	В	4	0	0	0	0
2	С	3	0	0	0	0
2	D	3	0	0	0	0
2	Е	2	0	0	0	0
3	А	4	0	6	0	0
4	А	5	0	0	3	0
4	В	1	0	0	0	0
4	С	1	0	0	0	0
4	D	1	0	0	0	0
4	Е	3	0	0	1	0
5	В	4	0	3	0	0
5	С	4	0	3	1	0
6	А	15	0	0	0	0
6	В	13	0	0	1	0
6	С	11	0	0	1	0
6	D	16	0	0	1	0
6	Е	8	0	0	1	0
All	All	10827	0	10949	283	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 13.

All (283) 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:A:68:LEU:HD23	1:A:215:LEU:HD13	1.34	1.04
1:C:211:TYR:CE1	1:E:255:LEU:HD21	1.92	1.02
1:D:210:ALA:O	1:D:214:ILE:HG13	1.62	0.99
1:B:71:ARG:NH2	1:B:212:THR:HG22	1.78	0.97



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:71:ARG:HH22	1:B:212:THR:HG22	1.32	0.94
1:C:211:TYR:HE1	1:E:255:LEU:HD21	1.31	0.93
1:B:210:ALA:HA	1:B:213:LEU:HD12	1.51	0.92
1:B:210:ALA:CA	1:B:213:LEU:HD12	2.00	0.91
1:B:210:ALA:N	1:B:213:LEU:HD12	1.85	0.90
1:B:210:ALA:HA	1:B:213:LEU:CD1	2.03	0.89
1:B:209:PHE:HD2	1:B:213:LEU:HG	1.37	0.87
1:E:207:VAL:HG23	1:E:208:PRO:HD3	1.57	0.86
1:B:35:SER:OG	1:B:239:PRO:HA	1.73	0.86
1:C:51:HIS:O	1:C:52:LEU:HD12	1.74	0.85
1:B:209:PHE:C	1:B:213:LEU:HD12	1.98	0.84
1:A:188:LYS:HE3	4:A:305:CL:CL	2.13	0.84
1:E:207:VAL:N	1:E:208:PRO:HD2	1.95	0.82
1:A:45:TYR:O	1:A:49:GLY:N	2.12	0.82
1:E:234:LEU:HB2	1:E:238:THR:HG22	1.60	0.80
1:E:71:ARG:NH2	1:E:253:ASP:OD1	2.16	0.78
1:C:194:HIS:HA	1:E:91:ILE:HD13	1.66	0.78
1:C:23:LYS:HG2	1:C:24:ILE:HD12	1.66	0.77
1:A:230:LEU:HB3	1:A:234:LEU:HD12	1.67	0.77
1:B:135:THR:HG23	1:B:151:LEU:HD11	1.66	0.76
1:C:51:HIS:C	1:C:52:LEU:HD12	2.05	0.76
1:B:39:ILE:HD12	1:B:39:ILE:O	1.85	0.76
1:E:231:VAL:HA	1:E:238:THR:HG21	1.68	0.75
1:A:226:LEU:HG	1:A:230:LEU:HD11	1.70	0.74
1:B:209:PHE:CD2	1:B:213:LEU:HG	2.20	0.74
1:A:24:ILE:HA	1:A:27:ARG:HH22	1.52	0.74
1:A:210:ALA:O	1:A:214:ILE:HG13	1.87	0.74
1:C:78:ARG:NH2	1:C:260:GLU:O	2.22	0.72
1:B:214:ILE:HD13	1:D:247:TYR:OH	1.90	0.71
1:A:50:ILE:HB	1:B:237:MET:HG2	1.72	0.70
1:A:24:ILE:HA	1:A:27:ARG:NH2	2.06	0.70
1:A:100:LEU:HD11	1:A:114:ILE:HD12	1.73	0.70
1:C:211:TYR:CD1	1:E:255:LEU:HD21	2.26	0.69
1:A:68:LEU:CD2	1:A:215:LEU:HD13	2.19	0.69
1:C:214:ILE:HG12	1:E:251:SER:HB3	1.75	0.68
1:B:32:VAL:O	1:B:36:ILE:HG13	1.93	0.68
1:C:33:LEU:HD22	1:C:36:ILE:HD11	1.75	0.67
1:B:208:PRO:HG2	1:D:259:LEU:HD21	1.75	0.67
1:C:212:THR:O	1:C:216:GLN:N	2.28	0.67
1:C:81:GLU:HG2	1:C:202:LEU:HD11	1.75	0.67
1:B:214:ILE:HG23	1:B:217:ARG:NE	2.10	0.66



	lo uo pugom	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:38:ALA:HB2	1:B:228:PHE:CD1	2.31	0.66
1:D:78:ARG:HD3	1:D:207:VAL:HG23	1.78	0.66
1:D:231:VAL:HA	1:D:238:THR:HG21	1.78	0.66
1:B:214:ILE:O	1:B:218:THR:HG23	1.96	0.66
1:E:207:VAL:HG23	1:E:208:PRO:CD	2.27	0.65
1:B:35:SER:OG	1:B:239:PRO:CA	2.42	0.65
1:B:168:ILE:HA	1:B:171:LEU:HD12	1.78	0.65
1:A:194:HIS:HA	1:B:91:ILE:HD13	1.78	0.65
1:E:130:ARG:NH2	1:E:269:ASP:HA	2.11	0.65
1:A:213:LEU:C	1:A:213:LEU:HD23	2.16	0.64
1:B:71:ARG:NH2	1:B:212:THR:CG2	2.57	0.64
1:D:213:LEU:O	1:D:217:ARG:HG3	1.96	0.64
1:A:214:ILE:HD13	1:B:251:SER:HB2	1.80	0.64
1:D:37:ILE:O	1:D:41:SER:HB3	1.98	0.64
1:C:251:SER:HB3	1:D:214:ILE:HD13	1.78	0.64
5:C:304:ACY:H3	1:E:281:ARG:HD3	1.80	0.63
1:E:91:ILE:O	1:E:95:THR:HG23	1.97	0.63
1:D:235:HIS:O	1:D:238:THR:HG23	1.99	0.63
1:C:213:LEU:HD23	1:C:217:ARG:HH21	1.64	0.63
1:D:230:LEU:HB3	1:D:234:LEU:HD12	1.79	0.63
1:B:127:HIS:HD1	1:B:132:THR:HG1	1.47	0.63
1:C:210:ALA:HB3	1:E:255:LEU:HD13	1.81	0.63
1:E:85:LEU:HD22	1:E:195:VAL:HA	1.81	0.63
1:B:285:ASP:HB3	6:B:408:HOH:O	1.98	0.62
1:E:207:VAL:N	1:E:208:PRO:CD	2.63	0.61
1:D:101:ARG:HH12	1:D:108:HIS:CD2	2.19	0.61
1:A:218:THR:HG21	1:B:248:THR:HG22	1.82	0.61
1:C:210:ALA:HB3	1:E:255:LEU:CD1	2.31	0.61
1:D:100:LEU:HD11	1:D:114:ILE:HD12	1.83	0.60
1:D:96:LEU:HD12	1:D:188:LYS:HB2	1.83	0.60
1:E:50:ILE:HG13	1:E:50:ILE:O	2.00	0.60
1:C:68:LEU:HD23	1:C:215:LEU:HD13	1.84	0.60
1:D:234:LEU:HB2	1:D:238:THR:HG22	1.83	0.59
1:A:49:GLY:HA3	1:B:236:TYR:CE2	2.37	0.59
1:B:209:PHE:O	1:B:213:LEU:N	2.34	0.59
1:E:60:LEU:HD23	1:E:222:PHE:HD1	1.66	0.59
1:A:230:LEU:HB3	1:A:234:LEU:CD1	2.33	0.59
1:A:71:ARG:HH11	1:A:212:THR:HG22	1.66	0.59
1:B:113:ARG:O	1:B:116:SER:OG	2.21	0.59
1:A:91:ILE:O	1:A:95:THR:HG23	2.03	0.58
1:C:91:ILE:O	1:C:95:THR:HG23	2.04	0.58



	i agem	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:35:SER:HB2	1:A:238:THR:HG22	1.86	0.58
1:D:96:LEU:HD22	1:D:118:LEU:HD11	1.85	0.58
1:B:271:PRO:O	1:B:275:MET:HG3	2.05	0.57
1:D:71:ARG:NH2	1:D:253:ASP:OD1	2.37	0.57
1:C:83:ARG:NH2	1:D:205:THR:OG1	2.37	0.56
1:B:210:ALA:HA	1:B:213:LEU:HD13	1.84	0.56
1:B:41:SER:HA	1:B:44:TRP:HD1	1.70	0.56
1:E:235:HIS:O	1:E:238:THR:HG23	2.06	0.56
1:B:27:ARG:CG	1:B:27:ARG:HH21	2.19	0.56
1:B:38:ALA:HB2	1:B:228:PHE:HD1	1.70	0.56
1:C:213:LEU:O	1:C:217:ARG:HB3	2.05	0.56
1:D:89:VAL:HG23	1:D:195:VAL:HG11	1.87	0.56
1:E:130:ARG:NH2	1:E:272:LEU:HB2	2.21	0.56
1:A:60:LEU:HD13	1:B:245:ILE:HG12	1.88	0.55
1:A:271:PRO:O	1:A:275:MET:HG3	2.07	0.55
1:B:27:ARG:HH21	1:B:27:ARG:HG3	1.72	0.54
1:E:31:ASN:ND2	1:E:223:CYS:O	2.39	0.54
1:E:217:ARG:HA	1:E:220:TYR:HB2	1.89	0.54
1:D:204:THR:O	1:D:206:PRO:HD3	2.08	0.53
1:A:58:SER:HA	1:E:59:LEU:HD13	1.91	0.53
1:A:45:TYR:CG	1:A:50:ILE:HD11	2.43	0.53
1:C:240:PHE:O	1:C:243:VAL:HG12	2.09	0.53
1:A:68:LEU:HD23	1:A:215:LEU:CD1	2.24	0.53
1:D:270:LEU:HD22	1:D:275:MET:HE1	1.90	0.53
1:C:44:TRP:O	1:C:48:LEU:HG	2.09	0.53
1:A:237:MET:O	1:A:237:MET:HG3	2.09	0.52
1:D:42:TYR:HA	1:D:45:TYR:CD1	2.44	0.52
1:E:52:LEU:HB3	1:E:229:ALA:HA	1.92	0.52
1:A:49:GLY:HA3	1:B:236:TYR:CD2	2.45	0.52
1:A:45:TYR:CD1	1:A:50:ILE:HD11	2.44	0.52
1:A:256:ALA:O	1:A:260:GLU:HG2	2.10	0.51
1:A:44:TRP:O	1:A:48:LEU:HB2	2.11	0.51
1:B:236:TYR:O	1:B:239:PRO:HD2	2.09	0.51
1:C:71:ARG:NH2	1:C:253:ASP:OD1	2.43	0.51
1:C:35:SER:OG	1:C:239:PRO:HB3	2.11	0.51
1:A:153:SER:OG	1:B:285:ASP:OD2	2.17	0.51
1:A:271:PRO:HG2	1:A:275:MET:HE2	1.91	0.51
1:C:91:ILE:HD13	1:D:194:HIS:HA	1.92	0.51
1:D:213:LEU:HD23	1:D:213:LEU:C	2.31	0.51
1:D:117:TYR:OH	1:D:146:ARG:HD3	2.11	0.51
1:D:146:ARG:NH2	1:D:149:GLU:OE1	2.44	0.51



	A + O	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:D:71:ARG:HD2	1:D:71:ARG:C	2.31	0.50
1:B:214:ILE:HA	1:B:217:ARG:CG	2.41	0.50
1:B:201:ARG:HG3	1:D:83:ARG:HG3	1.94	0.50
1:B:209:PHE:O	1:B:213:LEU:HD12	2.10	0.50
1:E:213:LEU:O	1:E:217:ARG:HG2	2.10	0.50
1:A:26:PHE:CD2	1:A:27:ARG:HG3	2.47	0.50
1:C:255:LEU:HD13	1:D:210:ALA:HB3	1.93	0.50
1:C:127:HIS:ND1	1:C:132:THR:OG1	2.45	0.49
1:A:57:PHE:HD2	1:A:226:LEU:HD12	1.76	0.49
1:A:245:ILE:HG12	1:E:60:LEU:HD13	1.94	0.49
1:C:107:GLU:OE2	1:C:176:LYS:HE2	2.11	0.49
1:E:29:LEU:HA	1:E:32:VAL:HG22	1.95	0.49
1:A:76:TYR:CE1	1:E:207:VAL:HG21	2.47	0.49
1:A:230:LEU:CB	1:A:234:LEU:HD12	2.38	0.49
1:B:208:PRO:O	1:B:211:TYR:HB2	2.13	0.49
1:A:244:PHE:CE1	1:E:221:LEU:HD23	2.48	0.49
1:B:27:ARG:CG	1:B:27:ARG:NH2	2.73	0.49
1:C:210:ALA:CB	1:E:255:LEU:HD13	2.42	0.49
1:B:91:ILE:O	1:B:95:THR:HG23	2.13	0.48
1:B:209:PHE:O	1:B:212:THR:OG1	2.27	0.48
1:D:238:THR:N	1:D:239:PRO:HD2	2.28	0.48
1:B:29:LEU:N	1:B:29:LEU:CD2	2.75	0.48
1:D:91:ILE:O	1:D:95:THR:HG23	2.13	0.48
1:D:212:THR:O	1:D:216:GLN:HB2	2.14	0.48
1:A:50:ILE:HD12	1:A:50:ILE:O	2.14	0.48
1:B:207:VAL:HG21	1:B:260:GLU:OE2	2.13	0.48
1:A:188:LYS:CE	4:A:305:CL:CL	2.95	0.48
1:C:256:ALA:O	1:C:260:GLU:HG2	2.13	0.48
1:D:145:GLU:HG2	1:D:146:ARG:HG2	1.96	0.47
1:A:26:PHE:HD2	1:A:27:ARG:HG3	1.78	0.47
1:B:35:SER:CB	1:B:239:PRO:HA	2.43	0.47
1:B:220:TYR:O	1:B:224:THR:HG23	2.15	0.47
1:A:49:GLY:HA3	1:B:236:TYR:HE2	1.80	0.47
1:A:91:ILE:HD13	1:E:194:HIS:HA	1.96	0.47
1:A:96:LEU:HD23	1:A:118:LEU:HD11	1.97	0.47
1:C:158:ASN:OD1	1:E:94:ARG:HD3	2.14	0.47
1:E:31:ASN:HB3	1:E:243:VAL:HG12	1.96	0.47
1:A:159:ARG:NH1	1:B:291:PRO:HD3	2.30	0.47
1:A:226:LEU:O	1:A:230:LEU:HD12	2.15	0.47
1:B:101:ARG:HG2	1:B:290:HIS:CE1	2.50	0.47
1:B:240:PHE:O	1:B:243:VAL:HG12	2.15	0.47



	ti a	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:31:ASN:ND2	1:D:223:CYS:O	2.46	0.47
1:E:34:MET:HA	1:E:37:ILE:HD12	1.96	0.47
1:B:212:THR:HG22	1:B:257:GLU:OE1	2.14	0.47
1:C:60:LEU:HD13	1:E:245:ILE:HG12	1.96	0.47
1:C:215:LEU:HD23	1:C:215:LEU:HA	1.65	0.47
1:D:177:LEU:HD13	1:D:182:TYR:HA	1.96	0.47
1:A:89:VAL:CG2	1:A:195:VAL:HG11	2.45	0.47
1:D:141:LEU:O	1:D:142:LEU:HD23	2.14	0.47
1:E:130:ARG:HH21	1:E:272:LEU:HB2	1.80	0.47
1:C:244:PHE:CZ	1:D:221:LEU:HD23	2.50	0.47
1:D:44:TRP:O	1:D:48:LEU:HG	2.14	0.47
1:E:130:ARG:NH2	1:E:272:LEU:HD12	2.29	0.46
1:B:214:ILE:HA	1:B:217:ARG:HG2	1.97	0.46
1:D:24:ILE:O	1:D:28:LEU:HD12	2.15	0.46
1:E:42:TYR:HA	1:E:45:TYR:CD2	2.50	0.46
1:B:44:TRP:O	1:B:48:LEU:HD12	2.15	0.46
1:C:40:ILE:HG13	1:C:41:SER:N	2.30	0.46
1:A:84:ASN:O	1:A:88:THR:HG23	2.15	0.46
1:A:260:GLU:OE1	1:A:260:GLU:HA	2.16	0.46
1:A:108:HIS:HB3	4:A:308:CL:CL	2.53	0.46
1:D:78:ARG:HD3	1:D:207:VAL:CG2	2.44	0.46
1:E:46:GLU:HA	1:E:49:GLY:H	1.81	0.46
1:B:155:MET:HG2	1:B:158:ASN:HB2	1.98	0.45
1:C:115:VAL:HG21	1:C:287:THR:HG21	1.97	0.45
1:A:78:ARG:NH1	1:A:206:PRO:HA	2.31	0.45
1:B:121:PHE:CD1	1:B:161:LEU:HD21	2.51	0.45
1:C:60:LEU:HD21	1:E:244:PHE:CE2	2.50	0.45
1:D:206:PRO:HD2	6:D:406:HOH:O	2.15	0.45
1:B:227:PRO:HA	1:B:230:LEU:HB2	1.98	0.45
1:D:89:VAL:CG2	1:D:195:VAL:HG11	2.46	0.45
1:E:130:ARG:NE	1:E:269:ASP:OD1	2.42	0.45
1:E:188:LYS:HD3	1:E:188:LYS:HA	1.76	0.45
1:B:127:HIS:CD2	1:B:134:PRO:HA	2.52	0.44
1:B:146:ARG:HA	1:B:146:ARG:HD3	1.74	0.44
1:D:200:GLU:O	1:D:204:THR:HG23	2.17	0.44
1:C:83:ARG:HG2	1:D:205:THR:HG21	1.99	0.44
1:A:218:THR:CG2	1:B:248:THR:HG22	2.47	0.44
1:E:51:HIS:HA	6:E:401:HOH:O	2.17	0.44
1:B:29:LEU:N	1:B:29:LEU:HD23	2.32	0.44
1:B:224:THR:O	1:B:227:PRO:HD2	2.17	0.44
1:C:190:ASP:OD1	4:E:303:CL:CL	2.72	0.44



	A h o	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:36:ILE:HD12	1:C:37:ILE:N	2.33	0.44
1:B:22:SER:HB2	1:B:25:ILE:HG22	2.00	0.44
1:C:226:LEU:N	1:C:227:PRO:HD2	2.33	0.44
1:E:208:PRO:HG2	1:E:208:PRO:O	2.17	0.44
1:C:42:TYR:HA	1:C:45:TYR:CD1	2.53	0.43
1:C:96:LEU:HD23	1:C:118:LEU:HD11	2.00	0.43
1:A:51:HIS:HD2	1:B:235:HIS:CD2	2.36	0.43
1:A:227:PRO:HA	1:A:230:LEU:HD12	1.99	0.43
1:C:214:ILE:O	1:C:218:THR:OG1	2.29	0.43
1:A:213:LEU:C	1:A:213:LEU:CD2	2.85	0.43
1:C:234:LEU:HD23	1:D:51:HIS:O	2.19	0.43
1:A:22:SER:C	1:A:24:ILE:H	2.21	0.43
1:A:22:SER:HA	1:A:24:ILE:HG22	2.00	0.43
1:C:42:TYR:HD1	1:C:45:TYR:CD2	2.36	0.43
1:D:129:LEU:HD21	1:D:199:CYS:HB3	1.98	0.43
1:D:254:SER:O	1:D:258:GLU:HG3	2.18	0.43
1:B:59:LEU:HD23	1:D:245:ILE:HD13	2.00	0.43
1:C:126:LYS:HE3	1:C:126:LYS:HB3	1.76	0.43
1:E:156:PRO:O	1:E:160:ILE:HG13	2.18	0.43
1:C:252:TRP:CH2	1:D:67:PHE:HB3	2.53	0.43
1:A:71:ARG:HD3	1:A:212:THR:HG22	2.00	0.43
1:A:85:LEU:HD22	1:A:195:VAL:HA	2.01	0.43
1:B:89:VAL:CG2	1:B:195:VAL:HG11	2.48	0.43
1:E:126:LYS:HD2	1:E:272:LEU:HB3	2.01	0.43
1:D:100:LEU:HD11	1:D:114:ILE:CD1	2.48	0.43
1:C:113:ARG:HG2	6:C:410:HOH:O	2.19	0.42
1:D:210:ALA:O	1:D:214:ILE:CG1	2.51	0.42
1:C:27:ARG:HD2	1:C:220:TYR:CZ	2.53	0.42
1:C:190:ASP:OD2	1:E:188:LYS:HE3	2.19	0.42
1:A:32:VAL:O	1:A:36:ILE:HG13	2.19	0.42
1:D:45:TYR:OH	1:D:228:PHE:HD1	2.03	0.42
1:C:60:LEU:HD23	1:C:222:PHE:HD2	1.85	0.42
1:A:130:ARG:NH2	1:A:264:GLY:O	2.52	0.42
1:B:24:ILE:HG22	1:B:28:LEU:HG	2.02	0.42
1:C:83:ARG:HA	1:C:83:ARG:HD2	1.87	0.42
1:C:234:LEU:HD13	1:C:241:VAL:HG21	2.02	0.42
1:D:215:LEU:HD12	1:D:215:LEU:HA	1.77	0.42
1:B:207:VAL:H	1:B:207:VAL:HG22	1.60	0.42
1:D:161:LEU:HD23	1:D:161:LEU:HA	1.90	0.42
1:A:81:GLU:OE1	1:A:202:LEU:HD21	2.20	0.42
1:A:270:LEU:HB3	1:A:275:MET:CE	2.50	0.42



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:B:210:ALA:CA	1:B:213:LEU:CD1	2.76	0.42
1:B:238:THR:N	1:B:239:PRO:HD2	2.35	0.42
1:E:238:THR:N	1:E:239:PRO:HD2	2.35	0.42
1:E:272:LEU:HA	1:E:272:LEU:HD23	1.73	0.42
1:B:287:THR:O	1:B:287:THR:CG2	2.68	0.42
1:D:231:VAL:CA	1:D:238:THR:HG21	2.48	0.41
1:B:214:ILE:HG21	1:D:247:TYR:OH	2.20	0.41
1:E:60:LEU:HD23	1:E:222:PHE:CD1	2.52	0.41
1:E:116:SER:HB3	1:E:142:LEU:HD23	2.01	0.41
1:A:86:TRP:CE2	1:A:272:LEU:HD22	2.55	0.41
1:D:30:LEU:O	1:D:34:MET:HG2	2.21	0.41
1:D:231:VAL:HA	1:D:238:THR:CG2	2.47	0.41
1:B:115:VAL:O	1:B:119:VAL:HG23	2.20	0.41
1:C:43:GLN:HB2	1:C:44:TRP:CD1	2.55	0.41
1:C:89:VAL:HG23	1:C:195:VAL:HG11	2.03	0.41
1:D:64:ILE:HD11	1:D:218:THR:HG22	2.03	0.41
1:E:113:ARG:O	1:E:116:SER:HB2	2.20	0.41
1:C:215:LEU:O	1:C:219:VAL:HG23	2.20	0.41
1:E:231:VAL:HA	1:E:238:THR:CG2	2.46	0.41
1:C:230:LEU:HB3	1:C:234:LEU:HD12	2.03	0.41
1:A:230:LEU:HD22	1:A:234:LEU:HD11	2.03	0.40
1:C:44:TRP:CD1	1:C:44:TRP:N	2.89	0.40
1:D:240:PHE:O	1:D:243:VAL:HG12	2.20	0.40
1:E:139:ARG:HD3	1:E:144:GLU:OE1	2.21	0.40
1:E:211:TYR:O	1:E:215:LEU:HD12	2.21	0.40
1:A:52:LEU:HD12	1:A:228:PHE:HB3	2.04	0.40
1:A:237:MET:O	1:A:237:MET:CG	2.69	0.40
1:B:54:VAL:O	1:B:57:PHE:N	2.54	0.40
1:B:72:ASN:HD22	1:B:256:ALA:HB2	1.86	0.40
1:C:52:LEU:HB3	1:C:229:ALA:HA	2.02	0.40
1:D:39:ILE:HD11	1:D:239:PRO:HD3	2.04	0.40
1:B:52:LEU:HD23	1:D:234:LEU:HD22	2.03	0.40
1:E:226:LEU:N	1:E:227:PRO:HD2	2.37	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	266/297~(90%)	258~(97%)	8 (3%)	0	100	100
1	В	268/297~(90%)	254 (95%)	14 (5%)	0	100	100
1	С	267/297~(90%)	254 (95%)	13 (5%)	0	100	100
1	D	266/297~(90%)	259~(97%)	7(3%)	0	100	100
1	Е	269/297~(91%)	258 (96%)	11 (4%)	0	100	100
All	All	1336/1485~(90%)	1283 (96%)	53 (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 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	Percentiles
1	А	233/259~(90%)	229~(98%)	4 (2%)	60 87
1	В	234/259~(90%)	224 (96%)	10 (4%)	29 62
1	С	234/259~(90%)	226~(97%)	8 (3%)	37 71
1	D	233/259~(90%)	228~(98%)	5 (2%)	53 84
1	Ε	236/259~(91%)	230~(98%)	6 (2%)	47 80
All	All	1170/1295~(90%)	1137 (97%)	33 (3%)	43 77

All (33) residues with a non-rotameric sidechain are listed below:



Mol	Chain	\mathbf{Res}	Type
1	А	22	SER
1	А	78	ARG
1	А	126	LYS
1	А	237	MET
1	В	27	ARG
1	В	29	LEU
1	В	58	SER
1	В	126	LYS
1	В	172	ARG
1	В	211	TYR
1	В	213	LEU
1	В	214	ILE
1	В	233	ASP
1	В	244	PHE
1	С	45	TYR
1	С	51	HIS
1	С	58	SER
1	С	83	ARG
1	С	126	LYS
1	С	190	ASP
1	С	211	TYR
1	С	244	PHE
1	D	83	ARG
1	D	109	ASP
1	D	126	LYS
1	D	242	SER
1	D	244	PHE
1	Е	26	PHE
1	Е	71	ARG
1	Е	73	SER
1	Е	140	ARG
1	Е	207	VAL
1	Е	268	ASN

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

Mol	Chain	Res	Type
1	А	99	GLN
1	А	187	ASN
1	С	268	ASN
1	D	108	HIS
1	D	170	GLN
1	Е	235	HIS



Continued from previous page...

Mol	Chain	Res	Type
1	Ε	268	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 29 ligands modelled in this entry, 26 are monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the 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	True	Chain	Dec	Tinle	B	ond len	gths	E	ond ang	gles
INIOI	туре	Chain	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
5	ACY	В	305	2	1,3,3	7.29	1 (100%)	0,3,3	-	-
3	EDO	А	304	-	3,3,3	0.50	0	2,2,2	0.31	0
5	ACY	С	304	2	1,3,3	17.24	1 (100%)	0,3,3	-	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	А	304	-	-	1/1/1/1	-



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
5	С	304	ACY	CH3-C	17.24	1.70	1.48
5	В	305	ACY	CH3-C	7.29	1.58	1.48

All (2) bond length outliers are listed below:

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	А	304	EDO	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	С	304	ACY	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<rsrz></rsrz>	#RSRZ>2	$OWAB(Å^2)$	Q < 0.9
1	А	268/297~(90%)	-0.21	8 (2%) 50 40	43, 66, 113, 131	0
1	В	270/297~(90%)	0.02	25 (9%) 8 4	47, 73, 113, 131	0
1	С	269/297~(90%)	-0.07	12 (4%) 33 23	46, 68, 126, 173	0
1	D	268/297~(90%)	-0.03	14 (5%) 27 18	48, 78, 115, 131	0
1	Ε	271/297~(91%)	-0.15	7 (2%) 56 46	45, 66, 113, 139	0
All	All	1346/1485~(90%)	-0.09	66 (4%) 29 20	43, 71, 117, 173	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Е	266	ALA	6.7
1	С	209	PHE	5.8
1	В	211	TYR	5.7
1	А	289	GLN	5.1
1	В	220	TYR	5.0
1	С	208	PRO	5.0
1	С	47	GLN	4.7
1	D	267	ALA	4.6
1	Е	265	THR	4.5
1	С	48	LEU	4.4
1	С	206	PRO	4.2
1	С	207	VAL	4.2
1	С	26	PHE	4.1
1	D	268	ASN	4.0
1	D	209	PHE	4.0
1	С	268	ASN	3.9
1	В	146	ARG	3.8
1	D	265	THR	3.7
1	А	29	LEU	3.7
1	D	236	TYR	3.7



6IVR

Mol	Chain	Res	Type	RSRZ
1	А	26	PHE	3.6
1	Ε	47	GLN	3.4
1	В	150	ILE	3.4
1	В	204	THR	3.3
1	А	24	ILE	3.2
1	В	209	PHE	3.2
1	Ε	204	THR	3.2
1	В	26	PHE	3.2
1	А	25	ILE	3.0
1	Ε	264	GLY	3.0
1	В	155	MET	3.0
1	В	289	GLN	2.9
1	В	144	GLU	2.8
1	В	213	LEU	2.8
1	А	48	LEU	2.7
1	В	24	ILE	2.7
1	А	288	GLY	2.6
1	А	28	LEU	2.6
1	В	210	ALA	2.6
1	D	204	THR	2.5
1	D	266	ALA	2.5
1	В	153	SER	2.5
1	В	207	VAL	2.5
1	D	205	THR	2.5
1	D	130	ARG	2.4
1	D	269	ASP	2.4
1	Е	48	LEU	2.4
1	D	264	GLY	2.3
1	В	217	ARG	2.3
1	D	40	ILE	2.3
1	В	152	ALA	2.3
1	В	145	GLU	2.3
1	В	154	SER	2.2
1	В	143	PRO	2.2
1	В	216	GLN	2.2
1	В	148	THR	2.2
1	В	149	GLU	2.1
1	С	44	TRP	2.1
1	С	211	TYR	2.1
1	С	145	GLU	2.1
1	D	43	GLN	2.1
1	С	146	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
1	В	287	THR	2.0
1	В	27	ARG	2.0
1	D	26	PHE	2.0
1	Е	26	PHE	2.0

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	$B-factors(Å^2)$	Q<0.9
5	ACY	С	304	4/4	0.86	0.30	48,50,56,58	0
2	ZN	D	303	1/1	0.91	0.11	130,130,130,130	0
3	EDO	А	304	4/4	0.93	0.21	65,65,69,78	0
4	CL	А	309	1/1	0.95	0.07	93,93,93,93	0
2	ZN	D	302	1/1	0.95	0.10	104,104,104,104	0
5	ACY	В	305	4/4	0.96	0.15	66,72,73,74	0
2	ZN	В	302	1/1	0.96	0.18	126,126,126,126	0
4	CL	А	305	1/1	0.98	0.13	67,67,67,67	0
4	CL	Е	305	1/1	0.98	0.11	64,64,64,64	0
2	ZN	А	303	1/1	0.99	0.09	74,74,74,74	0
2	ZN	Е	301	1/1	0.99	0.10	59,59,59,59	0
2	ZN	В	301	1/1	0.99	0.11	74,74,74,74	0
2	ZN	А	301	1/1	0.99	0.13	$65,\!65,\!65,\!65$	0
4	CL	А	306	1/1	0.99	0.17	88,88,88,88	0
2	ZN	С	302	1/1	0.99	0.17	75,75,75,75	0
4	CL	В	306	1/1	0.99	0.12	73,73,73,73	0
4	CL	Е	303	1/1	0.99	0.18	59,59,59,59	1
2	ZN	С	303	1/1	0.99	0.13	67,67,67,67	0
2	ZN	D	301	1/1	0.99	0.13	81,81,81,81	0



Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} extsf{-}\mathbf{factors}(\mathbf{\AA}^2)$	Q<0.9
2	ZN	А	302	1/1	0.99	0.06	71,71,71,71	0
2	ZN	Е	302	1/1	1.00	0.12	$57,\!57,\!57,\!57$	0
2	ZN	В	303	1/1	1.00	0.12	73,73,73,73	0
4	CL	С	305	1/1	1.00	0.13	$61,\!61,\!61,\!61$	0
4	CL	D	304	1/1	1.00	0.11	77,77,77,77	0
2	ZN	В	304	1/1	1.00	0.11	70,70,70,70	0
4	CL	Е	304	1/1	1.00	0.09	72,72,72,72	0
2	ZN	С	301	1/1	1.00	0.17	62,62,62,62	0
4	CL	А	307	1/1	1.00	0.07	80,80,80,80	0
4	CL	А	308	1/1	1.00	0.09	84,84,84,84	0

6.5 Other polymers (i)

There are no such residues in this entry.

