



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 5, 2023 – 11:06 PM EST

PDB ID : 1UCY
Title : THROMBIN COMPLEXED WITH FIBRINOPEPTIDE A ALPHA (RESIDUES 7-19). THREE COMPLEXES, ONE WITH EPSILON-THROMBIN AND TWO WITH ALPHA-THROMBIN
Authors : Martin, P.; Edwards, B.
Deposited on : 1996-08-30
Resolution : 2.20 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 ⓘ 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 ⓘ](#)) 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 : 2.36
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) : 2.36

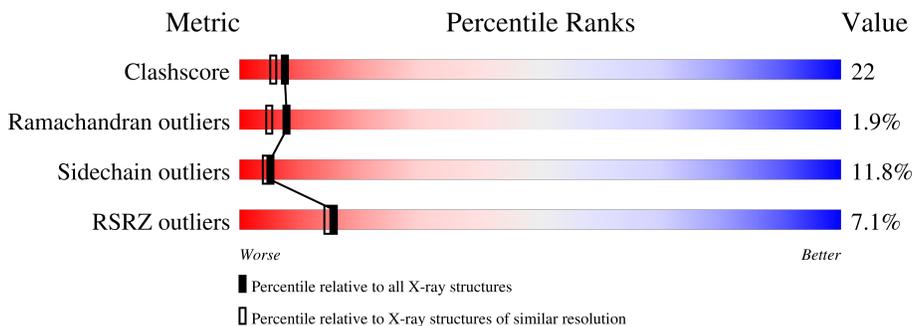
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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))
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 $\leq 5\%$. 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	J	49	
1	L	49	
1	M	49	
2	H	150	
3	E	109	
4	F	13	
4	G	13	

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Mol	Chain	Length	Quality of chain
4	I	13	
5	K	259	
5	N	259	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 8184 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called THROMBIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	L	36	290	181	48	60	1	0	0	0
1	J	36	290	181	48	60	1	0	0	0
1	M	36	290	181	48	60	1	0	0	0

- Molecule 2 is a protein called THROMBIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	150	1235	793	222	215	5	0	0	0

- Molecule 3 is a protein called THROMBIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	E	109	860	544	154	155	7	0	0	0

- Molecule 4 is a protein called FIBRINOPEPTIDE A-ALPHA.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	F	13	97	60	18	19	0	0	0
4	G	12	85	54	14	17	0	0	0
4	I	13	116	71	23	22	0	2	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	6	ACE	GLY	conflict	UNP P12803
F	16	OPR	ARG	conflict	UNP P12803
G	6	ACE	GLY	conflict	UNP P12803
G	16	OPR	ARG	conflict	UNP P12803
I	6	ACE	GLY	conflict	UNP P12803
I	16	OPR	ARG	conflict	UNP P12803

- Molecule 5 is a protein called THROMBIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	K	259	Total	C	N	O	S	0	0	0
			2094	1337	376	369	12			
5	N	259	Total	C	N	O	S	0	0	0
			2094	1337	376	369	12			

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	L	49	Total	O	0	0
			49	49		
6	H	99	Total	O	0	0
			99	99		
6	E	74	Total	O	0	0
			74	74		
6	F	8	Total	O	0	0
			8	8		
6	J	42	Total	O	0	0
			42	42		
6	K	226	Total	O	0	0
			226	226		
6	G	5	Total	O	0	0
			5	5		
6	M	17	Total	O	0	0
			17	17		
6	N	203	Total	O	0	0
			203	203		
6	I	10	Total	O	0	0
			10	10		

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.

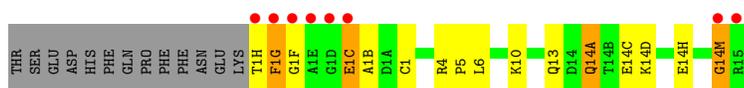
- Molecule 1: THROMBIN



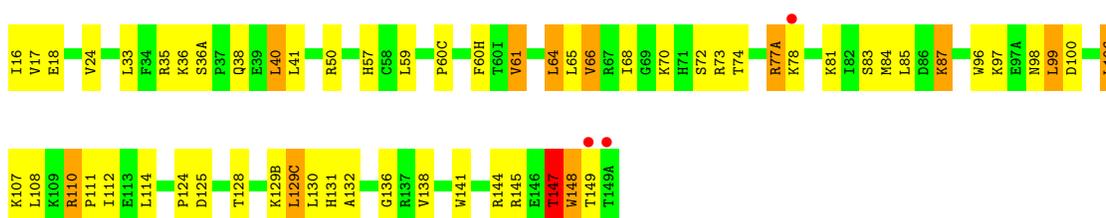
- Molecule 1: THROMBIN



- Molecule 1: THROMBIN

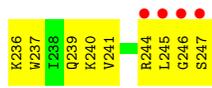


- Molecule 2: THROMBIN

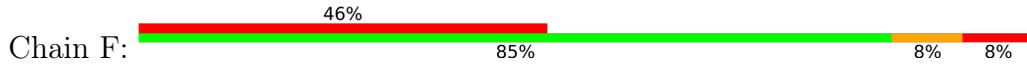


- Molecule 3: THROMBIN





• Molecule 4: FIBRINOPEPTIDE A-ALPHA



• Molecule 4: FIBRINOPEPTIDE A-ALPHA



• Molecule 4: FIBRINOPEPTIDE A-ALPHA

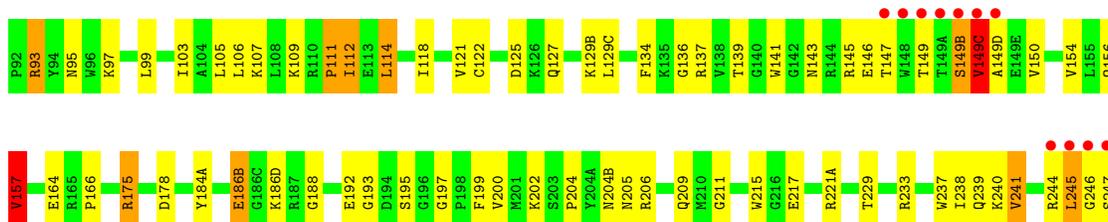


• Molecule 5: THROMBIN



• Molecule 5: THROMBIN





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	82.47Å 88.78Å 98.55Å 90.00° 106.21° 90.00°	Depositor
Resolution (Å)	7.00 – 2.20 41.38 – 2.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (7.00-2.20) 69.3 (41.38-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.75 (at 2.20Å)	Xtrriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.171 , (Not available) 0.176 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	25.3	Xtrriage
Anisotropy	0.166	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 120.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8184	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.62% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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.

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: ACE, OPR

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).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	J	0.61	0/294	0.80	0/390
1	L	0.59	0/294	0.81	0/390
1	M	0.47	0/294	0.83	1/390 (0.3%)
2	H	0.52	0/1267	0.84	2/1716 (0.1%)
3	E	0.50	0/881	0.78	1/1186 (0.1%)
4	F	0.56	0/80	0.83	0/103
4	G	0.44	0/68	0.77	0/89
4	I	0.66	0/99	1.06	0/125
5	K	0.57	0/2148	0.87	2/2905 (0.1%)
5	N	0.48	0/2148	0.77	2/2905 (0.1%)
All	All	0.53	0/7573	0.82	8/10199 (0.1%)

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
4	F	0	2
4	G	0	2
4	I	0	4
All	All	0	8

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	40	LEU	CA-CB-CG	6.89	131.14	115.30
1	M	14(M)	GLY	N-CA-C	6.36	129.01	113.10
5	N	157	VAL	CB-CA-C	-5.69	100.59	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	K	199	PHE	N-CA-C	-5.62	95.83	111.00
5	K	148	TRP	N-CA-C	5.21	125.07	111.00

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	F	16	OPR	Mainchain,Peptide
4	G	16	OPR	Mainchain,Peptide
4	I	16	OPR	Mainchain,Peptide

5.2 Too-close contacts

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	J	290	0	276	22	0
1	L	290	0	276	12	0
1	M	290	0	276	18	0
2	H	1235	0	1252	67	0
3	E	860	0	844	57	0
4	F	97	0	90	4	0
4	G	85	0	76	8	0
4	I	116	0	110	8	0
5	K	2094	0	2097	113	0
5	N	2094	0	2097	79	0
6	E	74	0	0	8	0
6	F	8	0	0	0	0
6	G	5	0	0	1	0
6	H	99	0	0	7	0
6	I	10	0	0	1	0
6	J	42	0	0	7	0
6	K	226	0	0	26	0
6	L	49	0	0	2	0
6	M	17	0	0	3	0
6	N	203	0	0	6	0
All	All	8184	0	7394	328	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 22.

The worst 5 of 328 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)
3:E:236:LYS:HZ2	3:E:239:GLN:HG3	1.24	1.03
3:E:149(C):VAL:HG21	3:E:153:SER:HA	1.45	0.99
1:L:15:ARG:HG3	2:H:131:HIS:HB3	1.45	0.97
5:K:99:LEU:HD11	4:G:15:VAL:HG12	1.47	0.94
4:I:19[B]:ARG:OXT	4:I:19[B]:ARG:HD3	1.68	0.93

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	Percentiles	
1	J	34/49 (69%)	27 (79%)	6 (18%)	1 (3%)	4	2
1	L	34/49 (69%)	26 (76%)	5 (15%)	3 (9%)	1	0
1	M	34/49 (69%)	29 (85%)	3 (9%)	2 (6%)	1	0
2	H	148/150 (99%)	136 (92%)	11 (7%)	1 (1%)	22	22
3	E	107/109 (98%)	94 (88%)	11 (10%)	2 (2%)	8	5
4	F	10/13 (77%)	8 (80%)	2 (20%)	0	100	100
4	G	9/13 (69%)	9 (100%)	0	0	100	100
4	I	11/13 (85%)	9 (82%)	2 (18%)	0	100	100
5	K	257/259 (99%)	231 (90%)	21 (8%)	5 (2%)	8	5
5	N	257/259 (99%)	227 (88%)	27 (10%)	3 (1%)	13	10
All	All	901/963 (94%)	796 (88%)	88 (10%)	17 (2%)	8	5

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	150	VAL
1	J	1(E)	ALA
5	K	148	TRP
5	K	149	THR
5	K	149(A)	THR

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	J	30/43 (70%)	25 (83%)	5 (17%)	2 1
1	L	30/43 (70%)	29 (97%)	1 (3%)	38 49
1	M	30/43 (70%)	26 (87%)	4 (13%)	4 3
2	H	134/134 (100%)	115 (86%)	19 (14%)	3 2
3	E	92/92 (100%)	83 (90%)	9 (10%)	8 7
4	F	7/7 (100%)	6 (86%)	1 (14%)	3 2
4	G	6/7 (86%)	5 (83%)	1 (17%)	2 1
4	I	9/7 (129%)	8 (89%)	1 (11%)	6 5
5	K	226/226 (100%)	197 (87%)	29 (13%)	4 3
5	N	226/226 (100%)	203 (90%)	23 (10%)	7 6
All	All	790/828 (95%)	697 (88%)	93 (12%)	5 4

5 of 93 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	K	180	MET
5	N	33	LEU
5	K	186(D)	LYS
1	M	1(G)	PHE
5	N	48	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
5	N	204(B)	ASN
5	N	239	GLN
3	E	204(B)	ASN
5	K	204(B)	ASN
1	M	13	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

3 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).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	OPR	G	16	4	13,14,15	0.87	0	12,16,18	0.68	0
4	OPR	I	16	4	13,14,15	0.81	1 (7%)	12,16,18	1.12	1 (8%)
4	OPR	F	16	4	13,14,15	0.50	0	12,16,18	1.40	1 (8%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	OPR	G	16	4	-	1/13/15/16	-
4	OPR	I	16	4	-	1/13/15/16	-
4	OPR	F	16	4	-	1/13/15/16	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	16	OPR	O1-C3	2.06	1.25	1.21

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	16	OPR	C3-CA-N	4.35	118.54	110.01
4	I	16	OPR	C3-CA-N	3.35	116.56	110.01

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	I	16	OPR	NE-CD-CG-CB
4	G	16	OPR	NE-CD-CG-CB
4	F	16	OPR	C3-CA-CB-CG

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	16	OPR	2	0
4	I	16	OPR	2	0
4	F	16	OPR	2	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	J	36/49 (73%)	0.68	6 (16%) 1 1	13, 30, 90, 100	0
1	L	36/49 (73%)	1.30	9 (25%) 0 0	16, 33, 101, 109	0
1	M	36/49 (73%)	1.59	8 (22%) 0 0	32, 50, 120, 126	0
2	H	150/150 (100%)	-0.56	3 (2%) 65 63	8, 25, 55, 90	0
3	E	109/109 (100%)	0.09	8 (7%) 15 14	8, 27, 92, 114	0
4	F	11/13 (84%)	2.17	6 (54%) 0 0	12, 29, 38, 43	11 (100%)
4	G	10/13 (76%)	0.91	1 (10%) 7 6	20, 35, 45, 54	10 (100%)
4	I	11/13 (84%)	-0.64	1 (9%) 9 8	11, 19, 35, 56	2 (18%)
5	K	259/259 (100%)	-0.37	10 (3%) 39 37	6, 19, 56, 106	0
5	N	259/259 (100%)	-0.13	13 (5%) 28 27	11, 31, 75, 120	0
All	All	917/963 (95%)	-0.05	65 (7%) 16 14	6, 26, 85, 126	23 (2%)

The worst 5 of 65 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	247	SER	20.1
1	M	1(F)	GLY	17.8
5	N	246	GLY	14.8
1	M	1(G)	PHE	14.7
1	J	1(F)	GLY	12.5

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th 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(\AA^2)	Q<0.9
4	OPR	G	16	15/16	0.95	0.18	6,19,50,52	15
4	OPR	F	16	15/16	0.96	0.26	8,13,27,27	15
4	OPR	I	16	15/16	0.98	0.10	4,19,31,33	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.