



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 12:23 AM GMT

PDB ID : 2A45  
Title : Crystal structure of the complex between thrombin and the central "E" region of fibrin  
Authors : Pechik, I.; Madrazo, J.; Gilliland, G.L.; Medved, L.  
Deposited on : 2005-06-27  
Resolution : 3.65 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

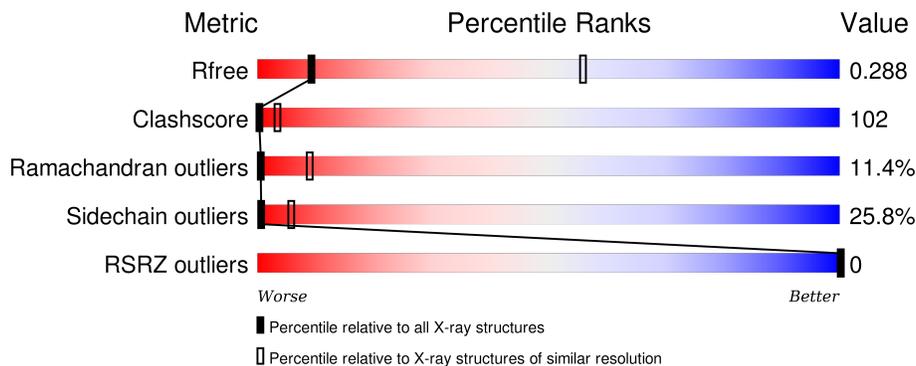
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.65 Å.

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



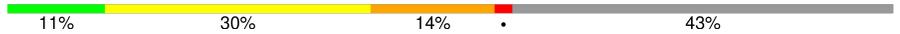
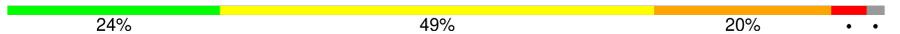
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1010 (3.82-3.50)
Clashscore	102246	1125 (3.82-3.50)
Ramachandran outliers	100387	1079 (3.82-3.50)
Sidechain outliers	100360	1078 (3.82-3.50)
RSRZ outliers	91569	1017 (3.82-3.50)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	A	36	
1	D	36	
2	B	259	
2	E	259	
3	G	57	

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Mol	Chain	Length	Quality of chain
3	J	57	
4	H	91	
4	K	91	
5	I	45	
5	L	45	

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
6	0G6	B	1	-	-	X	-

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 6904 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 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	32	259	159	44	55	1	0	0	0
1	D	32	259	159	44	55	1	0	0	0

- Molecule 2 is a protein called Thrombin heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	258	2069	1320	364	371	14	0	0	0
2	E	258	2069	1320	364	371	14	0	0	0

- Molecule 3 is a protein called Fibrinogen alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	G	48	384	235	67	77	5	17	0	0
3	J	48	384	235	67	77	5	17	0	0

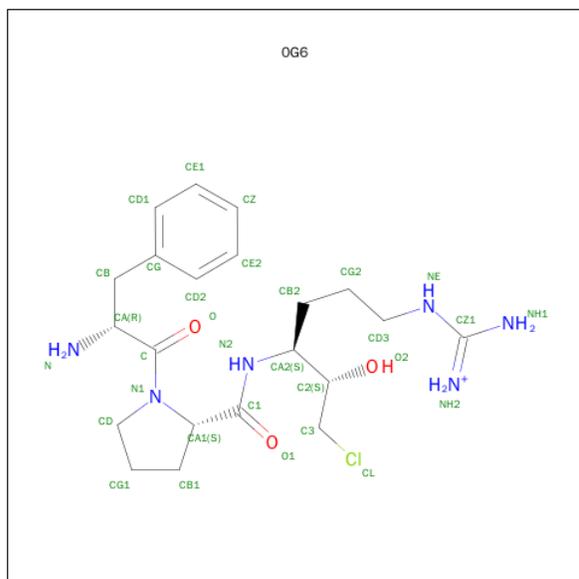
- Molecule 4 is a protein called Fibrinogen beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	H	52	382	230	72	77	3	0	0	0
4	K	52	382	230	72	77	3	0	0	0

- Molecule 5 is a protein called Fibrinogen gamma chain.

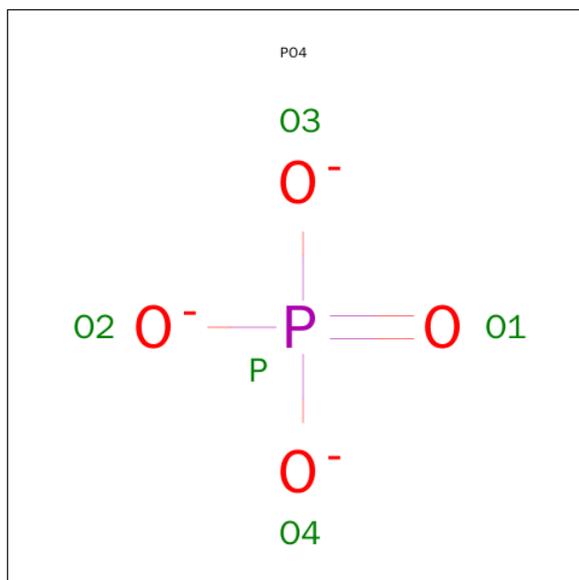
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	I	40	Total 308	C 189	N 47	O 68	S 4	0	0	0
5	L	44	Total 338	C 207	N 54	O 73	S 4	0	0	0

- Molecule 6 is D-PHENYLALANYL-N-[(2S,3S)-6-{{[AMINO(IMINIO)METHYL]AMINO}-1-CHLORO-2-HYDROXYHEXAN-3-YL]-L-PROLINAMIDE (three-letter code: 0G6) (formula: C<sub>21</sub>H<sub>34</sub>ClN<sub>6</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
6	B	1	Total 30	C 21	N 6	O 3	0	0
6	E	1	Total 30	C 21	N 6	O 3	0	0

- Molecule 7 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	O	P	0	0
			5	4	1		
7	E	1	Total	O	P	0	0
			5	4	1		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 light chain

Chain A: 



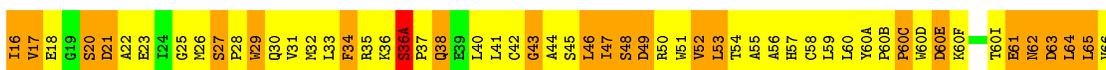
- Molecule 1: Thrombin light chain

Chain D: 



- Molecule 2: Thrombin heavy chain

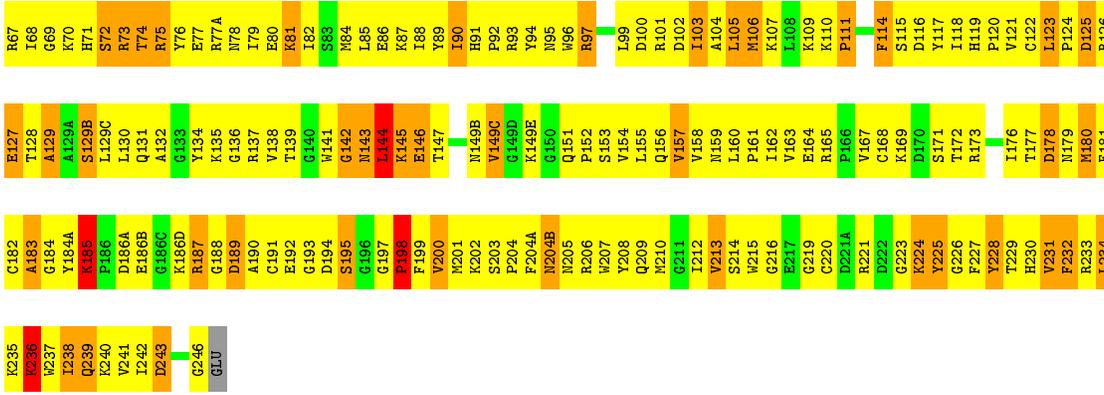
Chain B: 



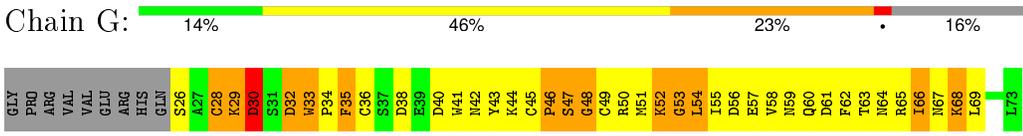
- Molecule 2: Thrombin heavy chain

Chain E: 





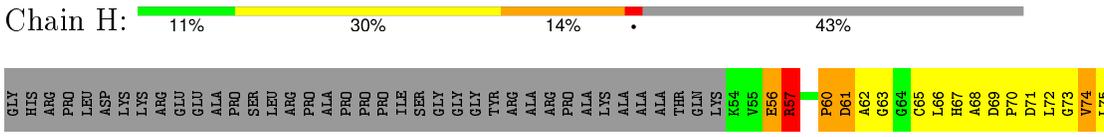
• Molecule 3: Fibrinogen alpha chain



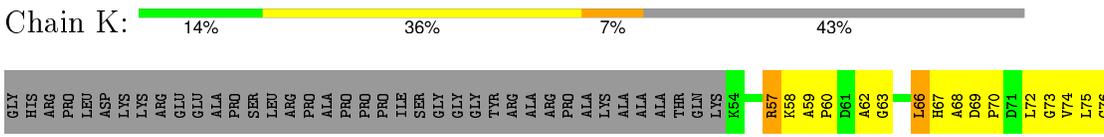
• Molecule 3: Fibrinogen alpha chain



• Molecule 4: Fibrinogen beta chain



• Molecule 4: Fibrinogen beta chain



• Molecule 5: Fibrinogen gamma chain





- Molecule 5: Fibrinogen gamma chain

Chain L: 24% 49% 20% . .



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	76.26Å 76.26Å 192.45Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.70 – 3.65 31.23 – 3.28	Depositor EDS
% Data completeness (in resolution range)	93.4 (19.70-3.65) 97.5 (31.23-3.28)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.00 (at 3.24Å)	Xtriage
Refinement program	SHELX-97	Depositor
R, $R_{free}$	0.221 , 0.290 0.217 , 0.288	Depositor DCC
$R_{free}$ test set	1241 reflections (9.90%)	DCC
Wilson B-factor (Å <sup>2</sup> )	60.4	Xtriage
Anisotropy	0.236	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.23 , 21.2	EDS
Estimated twinning fraction	0.088 for -h,-k,l 0.347 for h,-h-k,-l 0.089 for -k,-h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.39$ , $\langle L^2 \rangle = 0.22$	Xtriage
Outliers	0 of 37273 reflections	Xtriage
$F_o, F_c$ correlation	0.85	EDS
Total number of atoms	6904	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.53% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 0G6, PO4

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	A	0.61	0/261	0.85	0/345
1	D	0.65	0/261	0.86	0/345
2	B	0.63	1/2124 (0.0%)	0.86	1/2876 (0.0%)
2	E	0.64	0/2124	0.86	0/2876
3	G	0.63	0/392	0.94	2/527 (0.4%)
3	J	0.65	0/392	0.95	2/527 (0.4%)
4	H	0.69	0/386	0.86	0/524
4	K	0.61	0/386	0.85	0/524
5	I	0.74	0/312	0.81	0/423
5	L	0.67	0/342	0.89	0/464
All	All	0.65	1/6980 (0.0%)	0.87	5/9431 (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
5	L	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	36(A)	SER	CB-OG	6.55	1.50	1.42

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	28	CYS	CA-CB-SG	-7.49	100.52	114.00
3	G	28	CYS	CA-CB-SG	-7.26	100.93	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	28	CYS	N-CA-C	7.24	130.55	111.00
3	G	28	CYS	N-CA-C	6.64	128.93	111.00
2	B	43	GLY	N-CA-C	-5.68	98.89	113.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	L	32	TYR	Sidechain

## 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	A	259	0	254	57	0
1	D	259	0	254	50	0
2	B	2069	0	2024	498	0
2	E	2069	0	2024	444	0
3	G	384	0	348	76	0
3	J	384	0	348	88	0
4	H	382	0	362	79	0
4	K	382	0	362	67	0
5	I	308	0	273	67	0
5	L	338	0	307	66	0
6	B	30	0	30	32	0
6	E	30	0	30	19	0
7	B	5	0	0	0	0
7	E	5	0	0	0	0
All	All	6904	0	6616	1379	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 102.

The worst 5 of 1379 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:12:LEU:HD23	1:A:13:GLU:H	1.09	1.17
4:K:98:ASP:HA	4:K:101:ASN:HD21	1.09	1.16
2:E:99:LEU:HD11	6:E:1:0G6:HB21	1.20	1.13
2:E:60(A):TYR:H	2:E:60(F):LYS:HB3	1.07	1.12
2:E:138:VAL:HG22	2:E:199:PHE:HA	1.26	1.10

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	A	30/36 (83%)	16 (53%)	7 (23%)	7 (23%)	0	1
1	D	30/36 (83%)	16 (53%)	6 (20%)	8 (27%)	0	0
2	B	256/259 (99%)	179 (70%)	57 (22%)	20 (8%)	1	19
2	E	256/259 (99%)	174 (68%)	55 (22%)	27 (10%)	1	11
3	G	46/57 (81%)	27 (59%)	14 (30%)	5 (11%)	0	10
3	J	46/57 (81%)	28 (61%)	13 (28%)	5 (11%)	0	10
4	H	50/91 (55%)	36 (72%)	7 (14%)	7 (14%)	0	6
4	K	50/91 (55%)	36 (72%)	11 (22%)	3 (6%)	2	26
5	I	38/45 (84%)	22 (58%)	10 (26%)	6 (16%)	0	5
5	L	42/45 (93%)	29 (69%)	5 (12%)	8 (19%)	0	3
All	All	844/976 (86%)	563 (67%)	185 (22%)	96 (11%)	0	9

5 of 96 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1(C)	GLU
1	A	2	GLY
2	B	60(E)	ASP

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Mol	Chain	Res	Type
2	B	127	GLU
2	B	129	ALA

### 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	A	28/31 (90%)	22 (79%)	6 (21%)	1	9
1	D	28/31 (90%)	22 (79%)	6 (21%)	1	9
2	B	221/225 (98%)	156 (71%)	65 (29%)	0	4
2	E	221/225 (98%)	168 (76%)	53 (24%)	1	7
3	G	44/53 (83%)	31 (70%)	13 (30%)	0	4
3	J	44/53 (83%)	32 (73%)	12 (27%)	0	4
4	H	41/72 (57%)	29 (71%)	12 (29%)	0	4
4	K	41/72 (57%)	35 (85%)	6 (15%)	4	27
5	I	36/41 (88%)	24 (67%)	12 (33%)	0	2
5	L	39/41 (95%)	32 (82%)	7 (18%)	2	16
All	All	743/844 (88%)	551 (74%)	192 (26%)	0	6

5 of 192 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	41	LEU
2	E	114	PHE
3	J	69	LEU
2	E	47	ILE
2	E	73	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
2	E	151	GLN

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Mol	Chain	Res	Type
3	G	67	ASN
4	K	101	ASN
2	E	204(B)	ASN
2	B	149(B)	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 carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

4 ligands 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
6	OG6	B	1	2	27,31,32	2.05	1 (3%)	35,41,42	1.29	4 (11%)
7	PO4	B	248	-	4,4,4	0.89	0	6,6,6	0.27	0
6	OG6	E	1	2	27,31,32	1.93	2 (7%)	35,41,42	0.69	0
7	PO4	E	2	-	4,4,4	0.89	0	6,6,6	0.27	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	0G6	B	1	2	-	0/29/41/43	0/2/2/2
7	PO4	B	248	-	-	0/0/0/0	0/0/0/0
6	0G6	E	1	2	-	0/29/41/43	0/2/2/2
7	PO4	E	2	-	-	0/0/0/0	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	1	0G6	O2-C2	-9.50	1.22	1.43
6	E	1	0G6	O2-C2	-9.30	1.22	1.43
6	E	1	0G6	C3-C2	3.10	1.59	1.51

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	1	0G6	C2-CA2-N2	-4.00	102.62	110.11
6	B	1	0G6	CE2-CD2-CG	2.24	124.21	120.65
6	B	1	0G6	O2-C2-CA2	2.25	113.64	108.58
6	B	1	0G6	CB2-CG2-CD3	2.74	120.57	112.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 51 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	1	0G6	32	0
6	E	1	0G6	19	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	32/36 (88%)	-1.02	0 100 100	28, 28, 28, 28	0
1	D	32/36 (88%)	-1.06	0 100 100	28, 28, 28, 28	0
2	B	258/259 (99%)	-0.97	0 100 100	28, 28, 28, 28	0
2	E	258/259 (99%)	-0.96	0 100 100	28, 28, 28, 28	0
3	G	45/57 (78%)	-1.00	0 100 100	28, 28, 28, 28	0
3	J	45/57 (78%)	-1.09	0 100 100	28, 28, 28, 28	0
4	H	52/91 (57%)	-0.97	0 100 100	28, 28, 28, 28	0
4	K	52/91 (57%)	-1.02	0 100 100	28, 28, 28, 28	0
5	I	40/45 (88%)	-1.06	0 100 100	28, 28, 28, 28	0
5	L	44/45 (97%)	-1.06	0 100 100	28, 28, 28, 28	0
All	All	858/976 (87%)	-0.99	0 100 100	28, 28, 28, 28	0

There are no RSRZ outliers to report.

### 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 carbohydrates 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. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
6	OG6	E	1	30/31	0.97	0.15	0.40	27,27,27,27	0
7	PO4	E	2	5/5	0.98	0.16	0.38	27,27,27,27	0
6	OG6	B	1	30/31	0.97	0.14	0.01	27,27,27,27	0
7	PO4	B	248	5/5	0.99	0.11	-	27,27,27,27	0

## 6.5 Other polymers

There are no such residues in this entry.