



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 01:41 PM 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 validation summary report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

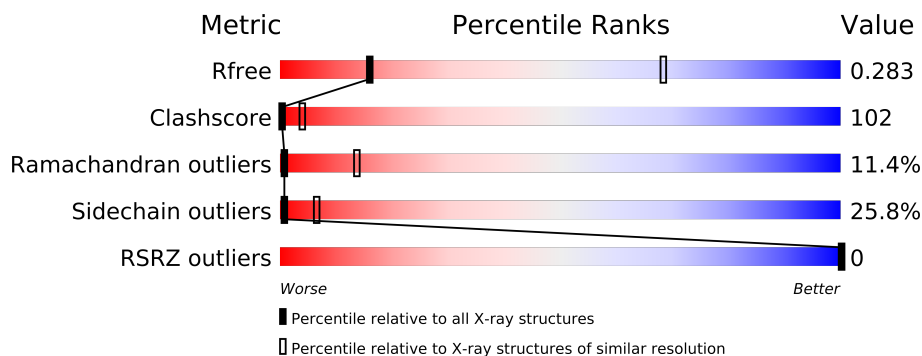
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	1021 (3.94-3.38)
Clashscore	79885	1025 (3.90-3.42)
Ramachandran outliers	78287	1195 (3.92-3.40)
Sidechain outliers	78261	1193 (3.92-3.40)
RSRZ outliers	66119	1021 (3.94-3.38)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	36	
1	D	36	
2	B	259	
2	E	259	
3	G	57	
3	J	57	
4	H	91	
4	K	91	
5	I	45	
5	L	45	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6904 atoms, of which 0 are hydrogen and 0 are deuterium.

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
1	A	32	Total	C	N	O	S	0	0	0
			259	159	44	55	1			
1	D	32	Total	C	N	O	S	0	0	0
			259	159	44	55	1			

- Molecule 2 is a protein called Thrombin heavy chain.

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

- Molecule 3 is a protein called Fibrinogen alpha chain.

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

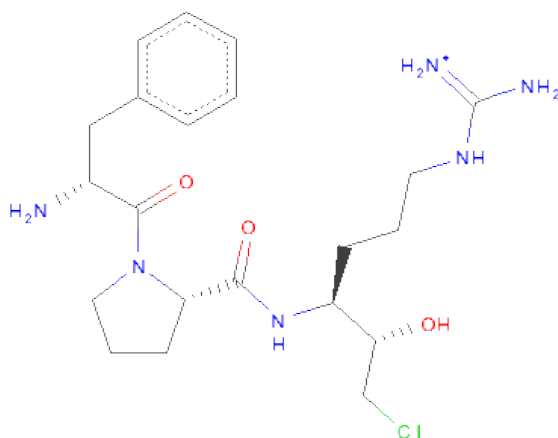
- Molecule 4 is a protein called Fibrinogen beta chain.

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

- Molecule 5 is a protein called Fibrinogen gamma chain.

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

- 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: $C_{21}H_{34}ClN_6O_3$).



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

- Molecule 7 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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: 



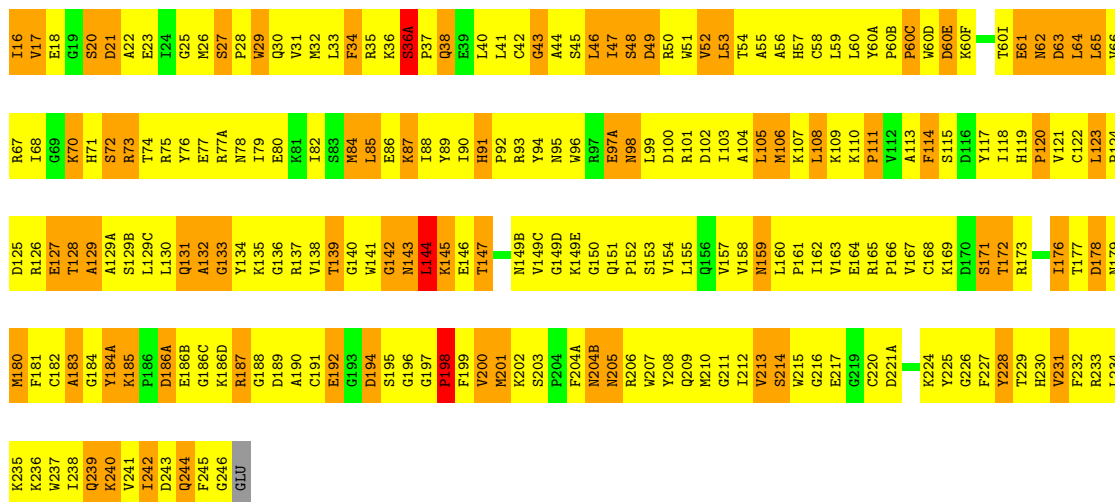
- Molecule 1: Thrombin light chain

Chain D: 



- Molecule 2: Thrombin heavy chain

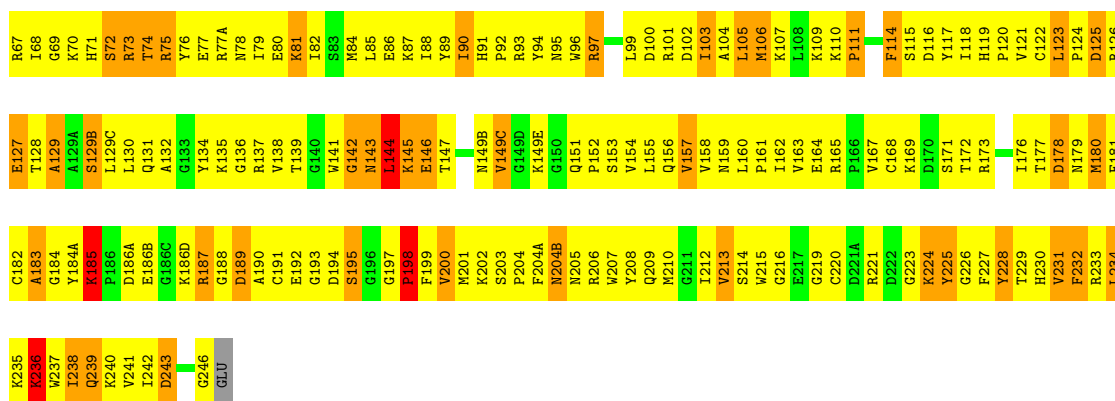
Chain B: 



- Molecule 2: Thrombin heavy chain

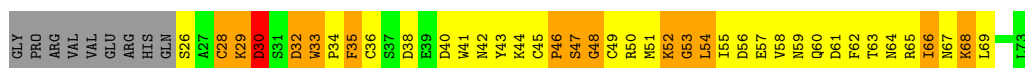
Chain E: 





- Molecule 3: Fibrinogen alpha chain

Chain G:



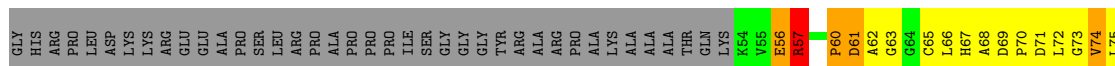
- Molecule 3: Fibrinogen alpha chain

Chain J:



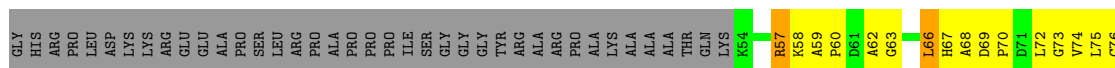
- Molecule 4: Fibrinogen beta chain

Chain H:



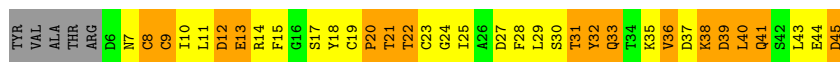
- Molecule 4: Fibrinogen beta chain

Chain K:



- Molecule 5: Fibrinogen gamma chain

Chain I:



- Molecule 5: Fibrinogen gamma chain

Chain L: 

TYR	V2	A3	T4	R5	D6	M7	C8	C9	I10	L11	D12	E13	R14	F15	G16	S17	Y18	C19	P20	T21	T22	C23	Q24	I25	A26	D27	F28	L29	S30	T31	Y32	Q33	V36	D37	K38	D39	L40	Q41	S42	L43	E44	D45
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4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	0.00 (at 3.24Å)	Xtriage
Refinement program	SHELX-97	Depositor
R, R_{free}	0.221 , 0.290 0.218 , 0.283	Depositor DCC
R_{free} test set	1246 reflections (9.90%)	DCC
Wilson B-factor (Å ²)	60.4	Xtriage
Anisotropy	0.236	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 18.5	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	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	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 ²)	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.*

¹Intensities estimated from amplitudes.

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 102.

The worst 5 of 1379 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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

5.3.1 Protein backbone ⓘ

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	1
2	B	256/259 (99%)	179 (70%)	57 (22%)	20 (8%)	1	26
2	E	256/259 (99%)	174 (68%)	55 (22%)	27 (10%)	1	16
3	G	46/57 (81%)	27 (59%)	14 (30%)	5 (11%)	1	15
3	J	46/57 (81%)	28 (61%)	13 (28%)	5 (11%)	1	15
4	H	50/91 (55%)	36 (72%)	7 (14%)	7 (14%)	0	9
4	K	50/91 (55%)	36 (72%)	11 (22%)	3 (6%)	2	35
5	I	38/45 (84%)	22 (58%)	10 (26%)	6 (16%)	0	6
5	L	42/45 (93%)	29 (69%)	5 (12%)	8 (19%)	0	3
All	All	844/976 (86%)	563 (67%)	185 (22%)	96 (11%)	1	14

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
2	B	127	GLU
2	B	129	ALA

5.3.2 Protein sidechains ⓘ

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	10
1	D	28/31 (90%)	22 (79%)	6 (21%)	1	10
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	5
4	H	41/72 (57%)	29 (71%)	12 (29%)	0	4
4	K	41/72 (57%)	35 (85%)	6 (15%)	5	28
5	I	36/41 (88%)	24 (67%)	12 (33%)	0	3
5	L	39/41 (95%)	32 (82%)	7 (18%)	2	17
All	All	743/844 (88%)	551 (74%)	192 (26%)	1	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
3	G	67	ASN
4	K	101	ASN
2	E	204(B)	ASN
2	B	149(B)	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	30,31,32	1.12	2 (6%)	39,41,42	1.32	4 (10%)
7	PO4	B	248	-	4,4,4	0.66	0	6,6,6	0.31	0
6	OG6	E	1	2	30,31,32	0.77	1 (3%)	39,41,42	0.79	1 (2%)
7	PO4	E	2	-	4,4,4	0.66	0	6,6,6	0.31	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	OG6	B	1	2	-	0/31/41/43	0/2/2/2
7	PO4	B	248	-	-	0/0/0/0	0/0/0/0
6	OG6	E	1	2	-	0/31/41/43	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	-3.46	1.22	1.41
6	E	1	0G6	O2-C2	-3.38	1.22	1.41
6	B	1	0G6	CZ1-NH2	-2.21	1.27	1.32

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	1	0G6	C2-CA2-N2	-3.95	102.62	110.29
6	B	1	0G6	CB2-CG2-CD3	3.37	120.57	111.94
6	E	1	0G6	CB2-CA2-C2	-2.85	108.77	113.02
6	B	1	0G6	CE2-CD2-CG	2.14	124.21	120.64
6	B	1	0G6	CG2-CB2-CA2	2.08	117.31	113.69

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	A	32/36 (88%)	-0.61	0 100 100	28, 28, 28, 28	0
1	D	32/36 (88%)	-0.63	0 100 100	28, 28, 28, 28	0
2	B	258/259 (99%)	-0.55	0 100 100	28, 28, 28, 28	0
2	E	258/259 (99%)	-0.54	0 100 100	28, 28, 28, 28	0
3	G	45/57 (78%)	-0.56	0 100 100	28, 28, 28, 28	0
3	J	45/57 (78%)	-0.63	0 100 100	28, 28, 28, 28	0
4	H	52/91 (57%)	-0.58	0 100 100	28, 28, 28, 28	0
4	K	52/91 (57%)	-0.61	0 100 100	28, 28, 28, 28	0
5	I	40/45 (88%)	-0.62	0 100 100	28, 28, 28, 28	0
5	L	44/45 (97%)	-0.61	0 100 100	28, 28, 28, 28	0
All	All	858/976 (87%)	-0.57	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 ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
7	PO4	B	248	5/5	0.11	-	27,27,27,27	0
7	PO4	E	2	5/5	0.17	-	27,27,27,27	0
6	0G6	E	1	30/31	0.16	-	27,27,27,27	0
6	0G6	B	1	30/31	0.14	-	27,27,27,27	0

6.5 Other polymers ⓘ

There are no such residues in this entry.