



# wwPDB X-ray Structure Validation Summary Report i

Feb 28, 2014 – 02:22 AM GMT

PDB ID : 1OSG  
Title : Complex between BAFF and a BR3 derived peptide presented in a beta-hairpin scaffold  
Authors : Gordon, N.C.; Pan, B.; Hymowitz, S.G.; Yin, J.P.; Kelley, R.F.; Cochran, A.G.; Yan, M.; Dixit, V.M.; Fairbrother, W.J.; Starovasnik, M.A.  
Deposited on : 2003-03-19  
Resolution : 3.00 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

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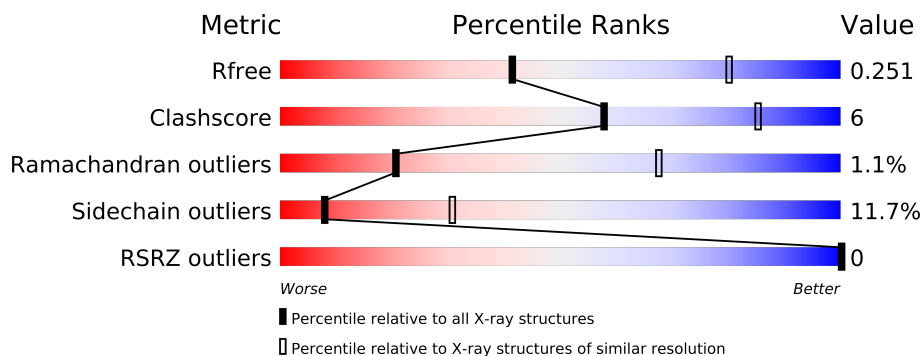
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 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 3.00 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	1216 (3.00-3.00)
Clashscore	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)
RSRZ outliers	66119	1217 (3.00-3.00)

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. 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	208	
1	B	208	
1	C	208	
1	D	208	
1	E	208	
1	F	208	
2	G	12	
2	H	12	
2	I	12	
2	J	12	
2	K	12	
2	L	12	

The following table lists non-polymeric compounds that are outliers for geometric or electron-

density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	MG	A	701	-	X
3	MG	A	702	-	X
3	MG	D	802	-	X
3	MG	E	801	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7531 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 Tumor necrosis factor ligand superfamily member 13B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	144	Total	C	N	O	S	0	0	0
			1143	736	184	218	5			
1	B	144	Total	C	N	O	S	0	0	0
			1143	736	184	218	5			
1	C	144	Total	C	N	O	S	0	0	0
			1143	736	184	218	5			
1	D	144	Total	C	N	O	S	0	0	0
			1143	736	184	218	5			
1	E	144	Total	C	N	O	S	0	0	0
			1143	736	184	218	5			
1	F	144	Total	C	N	O	S	0	0	0
			1143	736	184	218	5			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	78	GLY	-	CLONING ARTIFACT	UNP Q9Y275
A	79	SER	-	CLONING ARTIFACT	UNP Q9Y275
A	80	HIS	-	CLONING ARTIFACT	UNP Q9Y275
A	81	MET	-	CLONING ARTIFACT	UNP Q9Y275
B	78	GLY	-	CLONING ARTIFACT	UNP Q9Y275
B	79	SER	-	CLONING ARTIFACT	UNP Q9Y275
B	80	HIS	-	CLONING ARTIFACT	UNP Q9Y275
B	81	MET	-	CLONING ARTIFACT	UNP Q9Y275
C	78	GLY	-	CLONING ARTIFACT	UNP Q9Y275
C	79	SER	-	CLONING ARTIFACT	UNP Q9Y275
C	80	HIS	-	CLONING ARTIFACT	UNP Q9Y275
C	81	MET	-	CLONING ARTIFACT	UNP Q9Y275
D	78	GLY	-	CLONING ARTIFACT	UNP Q9Y275
D	79	SER	-	CLONING ARTIFACT	UNP Q9Y275
D	80	HIS	-	CLONING ARTIFACT	UNP Q9Y275
D	81	MET	-	CLONING ARTIFACT	UNP Q9Y275
E	78	GLY	-	CLONING ARTIFACT	UNP Q9Y275

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Chain	Residue	Modelled	Actual	Comment	Reference
E	79	SER	-	CLONING ARTIFACT	UNP Q9Y275
E	80	HIS	-	CLONING ARTIFACT	UNP Q9Y275
E	81	MET	-	CLONING ARTIFACT	UNP Q9Y275
F	78	GLY	-	CLONING ARTIFACT	UNP Q9Y275
F	79	SER	-	CLONING ARTIFACT	UNP Q9Y275
F	80	HIS	-	CLONING ARTIFACT	UNP Q9Y275
F	81	MET	-	CLONING ARTIFACT	UNP Q9Y275

- Molecule 2 is a protein called BR3 derived PEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	12	Total	C	N	O	S	0	0	0
			109	72	21	14	2			
2	J	12	Total	C	N	O	S	0	0	0
			109	72	21	14	2			
2	H	12	Total	C	N	O	S	0	0	0
			109	72	21	14	2			
2	I	12	Total	C	N	O	S	0	0	0
			104	69	19	14	2			
2	K	12	Total	C	N	O	S	0	0	0
			109	72	21	14	2			
2	L	12	Total	C	N	O	S	0	0	0
			109	72	21	14	2			

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Mg	0	0
			2	2		
3	D	1	Total	Mg	0	0
			1	1		
3	E	1	Total	Mg	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	O	0	0
			3	3		
4	B	4	Total	O	0	0
			4	4		

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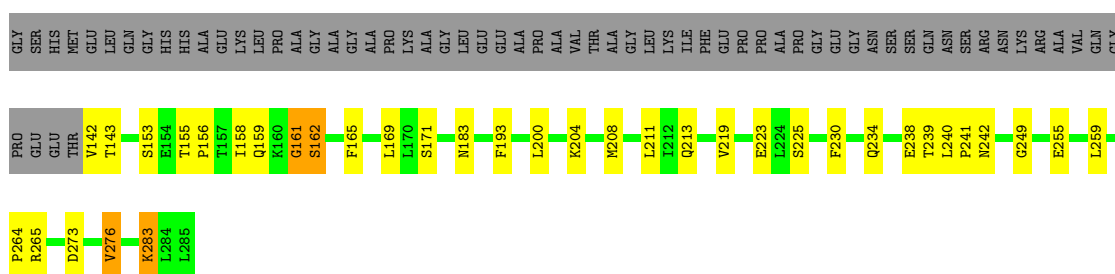
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	1	Total 1	O 1	0	0
4	E	3	Total 3	O 3	0	0
4	F	5	Total 5	O 5	0	0
4	G	1	Total 1	O 1	0	0
4	I	1	Total 1	O 1	0	0
4	K	1	Total 1	O 1	0	0
4	L	1	Total 1	O 1	0	0

### 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.

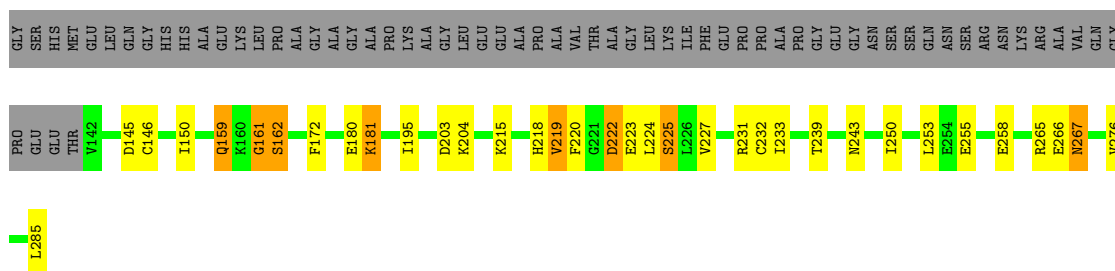
- Molecule 1: Tumor necrosis factor ligand superfamily member 13B

Chain A:



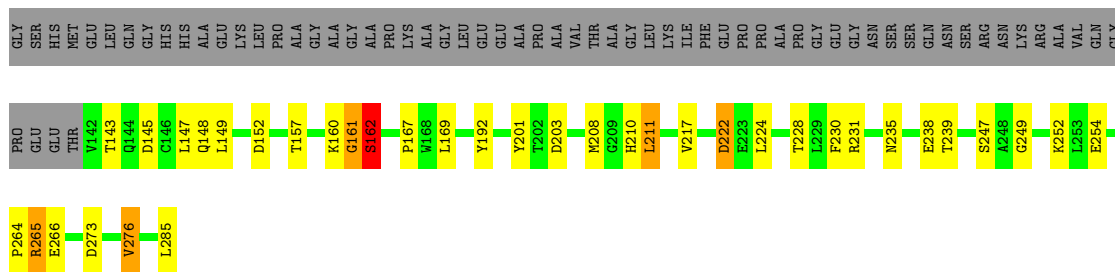
- Molecule 1: Tumor necrosis factor ligand superfamily member 13B

Chain B:



- Molecule 1: Tumor necrosis factor ligand superfamily member 13B

Chain C:



- Molecule 1: Tumor necrosis factor ligand superfamily member 13B

Chain D:

GLY SER HIS MET GLU LEU GLN GLY HIS HIS ALA ALA LYS LEU PRO ALA GLY ALA GLY ALA PRO PRO LYS ALA GLY LEU GLU GLU ALA PRO VAL THR ALA GLY LEU LYS ILE PHE GLU PRO PRO ALA PRO GLY GLY GLY ASN SER GLN ASN SER ARG ASN LYS ARG ALA VAL GLN GLY

PRO GLU THR V142 T143 Q144 D145 D152 T155 Q159 K160 G161 S162 L169 K181 E182 N183 Y192 T202 D203 Q213 R214 D222 E223 L224 F230 R233 C232 I233 N235 E238 T239 L240 P241 N242 G249 T250 Q260 V276 L282 L285

- Molecule 1: Tumor necrosis factor ligand superfamily member 13B

Chain E: 

GLY SER HIS MET GLU LEU GLN GLY HIS HIS ALA ALA LYS LEU PRO ALA GLY ALA GLY ALA PRO PRO LYS ALA GLY LEU GLU GLU ALA PRO VAL THR ALA GLY LEU LYS ILE PHE GLU PRO PRO ALA PRO GLY GLY GLY ASN SER SER GLN ASN SER ARG ASN LYS ARG ALA VAL GLN GLY

PRO GLU THR V142 D145 Q148 L149 D152 S153 E154 I158 T159 K160 L169 F165 V166 E167 W168 L169 L170 K173 R174 E180 K181 E182 N183 L186 V187 K188 F193 Q198 V199 L200 D203 L211 I212 Q213 R214 R215 K216 V217 H218 D222 E223 L224 R231

N235 L240 P241 N242 S247 Q260 P264 R265 E266 N267 Q269 V276 T277 K283 L284 L285

- Molecule 1: Tumor necrosis factor ligand superfamily member 13B

Chain F: 

GLY SER HIS MET GLU LEU GLN GLY HIS HIS ALA ALA LYS LEU PRO ALA GLY ALA GLY ALA PRO PRO LYS ALA GLY LEU GLU GLU ALA PRO VAL THR ALA GLY LEU LYS ILE PHE GLU PRO PRO ALA PRO GLY GLY GLY ASN SER SER GLN ASN SER ARG ASN LYS ARG ALA VAL GLN GLY

PRO GLU THR V142 T143 Q144 D145 Q148 T157 G161 P167 V168 L169 F172 E180 N183 D203 L211 H218 V219 S225 L226 V227 T228 C232 T239 N242 E254 D257 P264 R265 V276 L282 K283 L284 L285

- Molecule 2: BR3 derived PEPTIDE

Chain G: 

C23 H24 W25 D26 H31 C34

- Molecule 2: BR3 derived PEPTIDE

Chain J: 

C23 D26 V33 C34

- Molecule 2: BR3 derived PEPTIDE

Chain H: 

C23 L28 C34

- Molecule 2: BR3 derived PEPTIDE

Chain I: 

C23 D26 C34



- Molecule 2: BR3 derived PEPTIDE

Chain K: 



- Molecule 2: BR3 derived PEPTIDE

Chain L: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	121.63Å 121.63Å 157.21Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 3.00 29.85 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.6 (30.00-3.00) 99.7 (29.85-3.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.18 (at 3.00Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.213 , 0.286 0.193 , 0.251	Depositor DCC
$R_{free}$ test set	2536 reflections (10.67%)	DCC
Wilson B-factor (Å <sup>2</sup> )	53.3	Xtriage
Anisotropy	0.013	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 16.6	EDS
Estimated twinning fraction	0.056 for h,-h-k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 26307 reflections (0.004%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	7531	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.67% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities 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: MG

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	0.62	0/1165	0.80	1/1574 (0.1%)
1	B	0.59	0/1165	0.78	3/1574 (0.2%)
1	C	0.59	0/1165	0.77	4/1574 (0.3%)
1	D	0.58	0/1165	0.80	3/1574 (0.2%)
1	E	0.56	0/1165	0.82	3/1574 (0.2%)
1	F	0.59	0/1165	0.78	3/1574 (0.2%)
2	G	0.48	0/114	0.83	1/156 (0.6%)
2	H	0.50	0/114	0.71	0/156
2	I	0.54	0/108	0.80	1/148 (0.7%)
2	J	0.54	0/114	0.74	1/156 (0.6%)
2	K	0.48	0/114	0.85	1/156 (0.6%)
2	L	0.48	0/114	0.87	1/156 (0.6%)
All	All	0.58	0/7668	0.79	22/10372 (0.2%)

There are no bond length outliers.

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	26	ASP	CB-CG-OD2	6.87	124.48	118.30
1	F	203	ASP	CB-CG-OD2	6.74	124.37	118.30
1	B	203	ASP	CB-CG-OD2	6.64	124.28	118.30
1	E	152	ASP	CB-CG-OD2	6.50	124.15	118.30
1	B	145	ASP	CB-CG-OD2	6.39	124.05	118.30

There are no chirality outliers.

There are no planarity outliers.

## 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	1143	0	1145	17	0
1	B	1143	0	1145	17	0
1	C	1143	0	1145	18	0
1	D	1143	0	1145	18	0
1	E	1143	0	1145	24	0
1	F	1143	0	1145	13	0
2	G	109	0	98	1	0
2	H	109	0	98	1	0
2	I	104	0	93	0	0
2	J	109	0	98	1	0
2	K	109	0	98	2	0
2	L	109	0	98	4	0
3	A	2	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
4	A	3	0	0	0	0
4	B	4	0	0	0	0
4	D	1	0	0	0	0
4	E	3	0	0	0	0
4	F	5	0	0	0	0
4	G	1	0	0	0	0
4	I	1	0	0	0	0
4	K	1	0	0	0	0
4	L	1	0	0	1	0
All	All	7531	0	7453	94	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 6.

The worst 5 of 94 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:250:ILE:H	1:E:148:GLN:HE22	1.27	0.82
1:A:242:ASN:H	1:C:235:ASN:HD21	1.35	0.73
1:D:235:ASN:HD21	1:E:242:ASN:H	1.40	0.70

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:161:GLY:O	1:C:162:SER:HB2	1.92	0.69
1:A:264:PRO:O	1:A:265:ARG:HD3	1.95	0.67

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	142/208 (68%)	134 (94%)	7 (5%)	1 (1%)	30	78
1	B	142/208 (68%)	132 (93%)	8 (6%)	2 (1%)	16	60
1	C	142/208 (68%)	132 (93%)	8 (6%)	2 (1%)	16	60
1	D	142/208 (68%)	133 (94%)	6 (4%)	3 (2%)	11	47
1	E	142/208 (68%)	132 (93%)	9 (6%)	1 (1%)	30	78
1	F	142/208 (68%)	134 (94%)	7 (5%)	1 (1%)	30	78
2	G	10/12 (83%)	10 (100%)	0	0	100	100
2	H	10/12 (83%)	9 (90%)	1 (10%)	0	100	100
2	I	10/12 (83%)	9 (90%)	1 (10%)	0	100	100
2	J	10/12 (83%)	10 (100%)	0	0	100	100
2	K	10/12 (83%)	10 (100%)	0	0	100	100
2	L	10/12 (83%)	10 (100%)	0	0	100	100
All	All	912/1320 (69%)	855 (94%)	47 (5%)	10 (1%)	21	67

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	162	SER
1	D	161	GLY
1	F	161	GLY
1	A	161	GLY
1	C	161	GLY

### 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	126/171 (74%)	111 (88%)	15 (12%)	8	30
1	B	126/171 (74%)	107 (85%)	19 (15%)	4	20
1	C	126/171 (74%)	112 (89%)	14 (11%)	9	34
1	D	126/171 (74%)	111 (88%)	15 (12%)	8	30
1	E	126/171 (74%)	110 (87%)	16 (13%)	6	27
1	F	126/171 (74%)	113 (90%)	13 (10%)	10	38
2	G	12/12 (100%)	12 (100%)	0	100	100
2	H	12/12 (100%)	12 (100%)	0	100	100
2	I	11/12 (92%)	11 (100%)	0	100	100
2	J	12/12 (100%)	10 (83%)	2 (17%)	3	16
2	K	12/12 (100%)	12 (100%)	0	100	100
2	L	12/12 (100%)	9 (75%)	3 (25%)	1	4
All	All	827/1098 (75%)	730 (88%)	97 (12%)	8	31

5 of 97 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	247	SER
1	D	181	LYS
1	F	265	ARG
1	C	265	ARG
1	D	155	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	267	ASN
1	D	234	GLN
1	F	218	HIS
1	D	159	GLN
1	D	235	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 ⓘ

Of 4 ligands modelled in this entry, 4 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.

### 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, 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	144/208 (69%)	-0.36	0 100 100	19, 29, 44, 51	0
1	B	144/208 (69%)	-0.32	0 100 100	20, 31, 49, 61	0
1	C	144/208 (69%)	-0.34	0 100 100	20, 31, 44, 51	0
1	D	144/208 (69%)	-0.29	0 100 100	20, 31, 59, 79	0
1	E	144/208 (69%)	-0.36	0 100 100	20, 31, 44, 51	0
1	F	144/208 (69%)	-0.36	0 100 100	17, 29, 44, 51	0
2	G	12/12 (100%)	0.13	0 100 100	38, 54, 63, 64	0
2	H	12/12 (100%)	0.30	0 100 100	38, 54, 62, 64	0
2	I	12/12 (100%)	0.34	0 100 100	39, 54, 63, 64	0
2	J	12/12 (100%)	0.47	0 100 100	38, 54, 63, 64	0
2	K	12/12 (100%)	0.35	0 100 100	38, 54, 63, 65	0
2	L	12/12 (100%)	0.23	0 100 100	38, 54, 63, 64	0
All	All	936/1320 (70%)	-0.29	0 100 100	17, 31, 56, 79	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, 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	MG	A	702	1/1	0.78	26.66	58,58,58,58	0
3	MG	A	701	1/1	0.56	17.97	56,56,56,56	0
3	MG	E	801	1/1	0.61	17.85	75,75,75,75	0
3	MG	D	802	1/1	0.47	12.11	48,48,48,48	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.