



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 21, 2020 – 07:53 AM BST

PDB ID : 3UGX  
Title : Crystal Structure of Visual Arrestin  
Authors : Batra-Safferling, R.; Granzin, J.  
Deposited on : 2011-11-03  
Resolution : 2.65 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
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) : 2.13.1

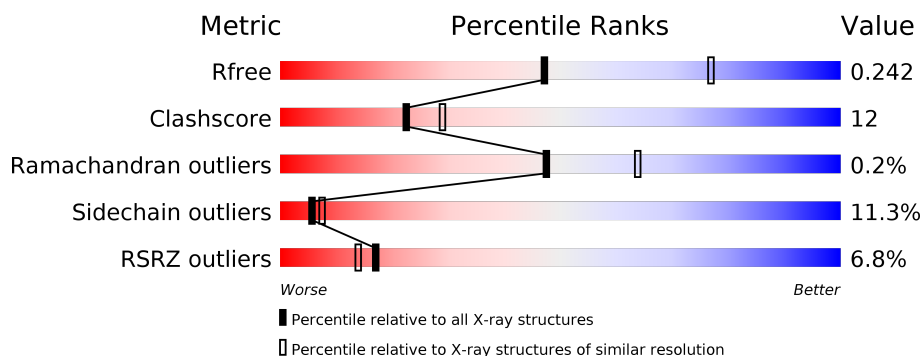
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.65 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))
$R_{free}$	130704	1426 (2.66-2.62)
Clashscore	141614	1472 (2.66-2.62)
Ramachandran outliers	138981	1446 (2.66-2.62)
Sidechain outliers	138945	1446 (2.66-2.62)
RSRZ outliers	127900	1408 (2.66-2.62)

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 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	A	414	<div> <div>3%</div> <div> <div></div> <div>67%</div> <div>19%</div> <div>•</div> <div>11%</div> </div> </div>
1	B	414	<div> <div>8%</div> <div> <div></div> <div>56%</div> <div>26%</div> <div>•</div> <div>15%</div> </div> </div>
1	C	414	<div> <div>4%</div> <div> <div></div> <div>66%</div> <div>16%</div> <div>•</div> <div>14%</div> </div> </div>
1	D	414	<div> <div>9%</div> <div> <div></div> <div>59%</div> <div>22%</div> <div>•</div> <div>16%</div> </div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PTD	A	410	-	-	X	-
2	PTD	C	406	-	-	X	-
5	IMD	B	405	-	-	X	-

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 11230 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 S-arrestin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	369	Total	C	N	O	S	0	1	0
			2859	1832	474	544	9			
1	B	352	Total	C	N	O	S	0	0	0
			2662	1709	437	507	9			
1	C	358	Total	C	N	O	S	0	0	0
			2772	1783	461	520	8			
1	D	348	Total	C	N	O	S	0	0	0
			2608	1680	432	487	9			

There are 40 discrepancies between the modelled and reference sequences:

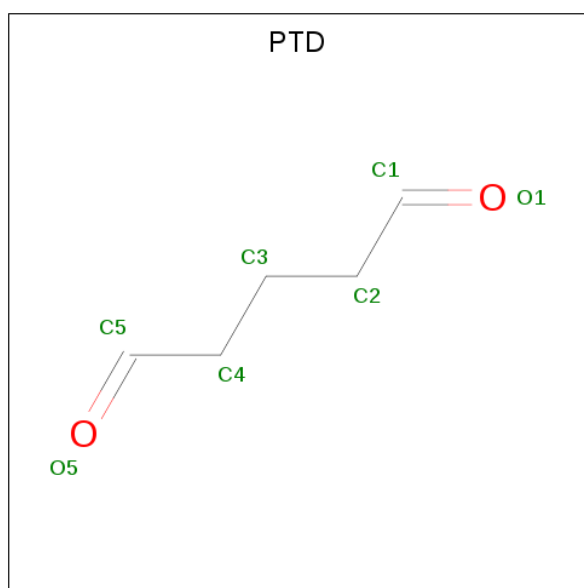
Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	ALA	-	EXPRESSION TAG	UNP P08168
A	-8	SER	-	EXPRESSION TAG	UNP P08168
A	-7	TRP	-	EXPRESSION TAG	UNP P08168
A	-6	SER	-	EXPRESSION TAG	UNP P08168
A	-5	HIS	-	EXPRESSION TAG	UNP P08168
A	-4	PRO	-	EXPRESSION TAG	UNP P08168
A	-3	GLN	-	EXPRESSION TAG	UNP P08168
A	-2	PHE	-	EXPRESSION TAG	UNP P08168
A	-1	GLU	-	EXPRESSION TAG	UNP P08168
A	0	LYS	-	EXPRESSION TAG	UNP P08168
B	-9	ALA	-	EXPRESSION TAG	UNP P08168
B	-8	SER	-	EXPRESSION TAG	UNP P08168
B	-7	TRP	-	EXPRESSION TAG	UNP P08168
B	-6	SER	-	EXPRESSION TAG	UNP P08168
B	-5	HIS	-	EXPRESSION TAG	UNP P08168
B	-4	PRO	-	EXPRESSION TAG	UNP P08168
B	-3	GLN	-	EXPRESSION TAG	UNP P08168
B	-2	PHE	-	EXPRESSION TAG	UNP P08168
B	-1	GLU	-	EXPRESSION TAG	UNP P08168
B	0	LYS	-	EXPRESSION TAG	UNP P08168
C	-9	ALA	-	EXPRESSION TAG	UNP P08168

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-8	SER	-	EXPRESSION TAG	UNP P08168
C	-7	TRP	-	EXPRESSION TAG	UNP P08168
C	-6	SER	-	EXPRESSION TAG	UNP P08168
C	-5	HIS	-	EXPRESSION TAG	UNP P08168
C	-4	PRO	-	EXPRESSION TAG	UNP P08168
C	-3	GLN	-	EXPRESSION TAG	UNP P08168
C	-2	PHE	-	EXPRESSION TAG	UNP P08168
C	-1	GLU	-	EXPRESSION TAG	UNP P08168
C	0	LYS	-	EXPRESSION TAG	UNP P08168
D	-9	ALA	-	EXPRESSION TAG	UNP P08168
D	-8	SER	-	EXPRESSION TAG	UNP P08168
D	-7	TRP	-	EXPRESSION TAG	UNP P08168
D	-6	SER	-	EXPRESSION TAG	UNP P08168
D	-5	HIS	-	EXPRESSION TAG	UNP P08168
D	-4	PRO	-	EXPRESSION TAG	UNP P08168
D	-3	GLN	-	EXPRESSION TAG	UNP P08168
D	-2	PHE	-	EXPRESSION TAG	UNP P08168
D	-1	GLU	-	EXPRESSION TAG	UNP P08168
D	0	LYS	-	EXPRESSION TAG	UNP P08168

- Molecule 2 is PENTANEDIAL (three-letter code: PTD) (formula: C<sub>5</sub>H<sub>8</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			7	5	2		
2	A	1	Total	C	O	0	0
			7	5	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			7	5	2		
2	A	1	Total	C	O	0	0
			7	5	2		
2	A	1	Total	C	O	0	0
			7	5	2		
2	A	1	Total	C	O	0	0
			7	5	2		
2	A	1	Total	C	O	0	0
			7	5	2		
2	B	1	Total	C	O	0	0
			7	5	2		
2	B	1	Total	C	O	0	0
			7	5	2		
2	C	1	Total	C	O	0	0
			7	5	2		
2	C	1	Total	C	O	0	0
			7	5	2		
2	C	1	Total	C	O	0	0
			7	5	2		
2	D	1	Total	C	O	0	0
			7	5	2		

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

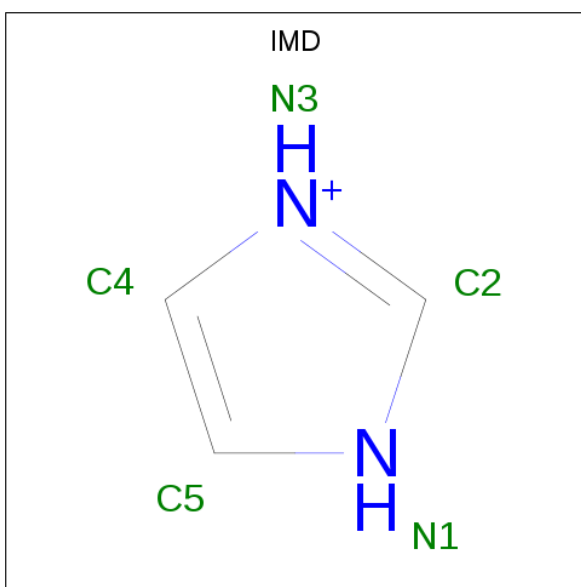
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Na	0	0
			1	1		
3	A	1	Total	Na	0	0
			1	1		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is IMIDAZOLE (three-letter code: IMD) (formula: C<sub>3</sub>H<sub>5</sub>N<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	N	0	0
			5	3	2		
5	D	1	Total	C	N	0	0
			5	3	2		
5	D	1	Total	C	N	0	0
			5	3	2		

- Molecule 6 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	1	Total	K	0	0
			1	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	68	Total	O	0	0
			68	68		
7	B	31	Total	O	0	0
			31	31		
7	C	45	Total	O	0	0
			45	45		
7	D	41	Total	O	0	0
			41	41		



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.

Chain A:

3%

67%

19%

11%

ALA  
SER  
TRP  
TRP  
SER  
HIS  
PRO  
GLN  
PHE  
GLU  
LYS  
MET  
LYS  
ALA  
LYS  
PRO  
ALA  
PRO  
H9  
H10  
K14  
K15  
I16  
S17  
K20  
L26  
I32  
V35  
V38  
V44  
D48  
P49  
K53  
G54  
R56  
V59  
R66  
I72  
R80  
L83  
Y84  
P93  
S97

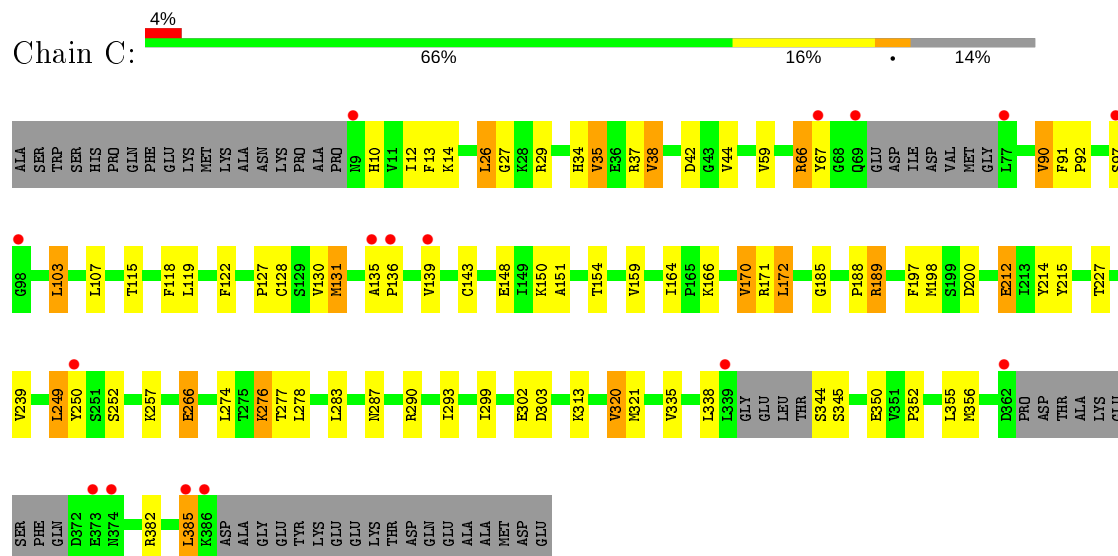
G98  
A99  
T100  
L103  
Q104  
K109  
T115  
Y116  
L126  
P127  
K128  
S129  
V130  
A135  
P136  
Q137  
D138  
V139  
G140  
K150  
A153  
T154  
H155  
I164  
L172  
Q178  
H179  
M184  
G185  
R189  
S193  
W194  
Q195  
F196  
F197  
M198  
S208  
L209  
E212  
I213  
Y214  
Y215  
K232  
V241  
T245  
L249  
Y250  
S251  
S252  
D253  
Y254  
Y255  
E262  
E266  
M271  
L274  
T275  
K276  
T277  
L278  
T279  
L280  
S309  
V320  
K321  
G322  
K330  
L338  
L339  
L342  
S345  
F346  
V347  
E350  
M356  
E361  
D362  
PRO  
ASP  
THR  
ALA  
LYS  
GLU  
SER  
PHE  
GLN  
D372  
P372

Chain B:

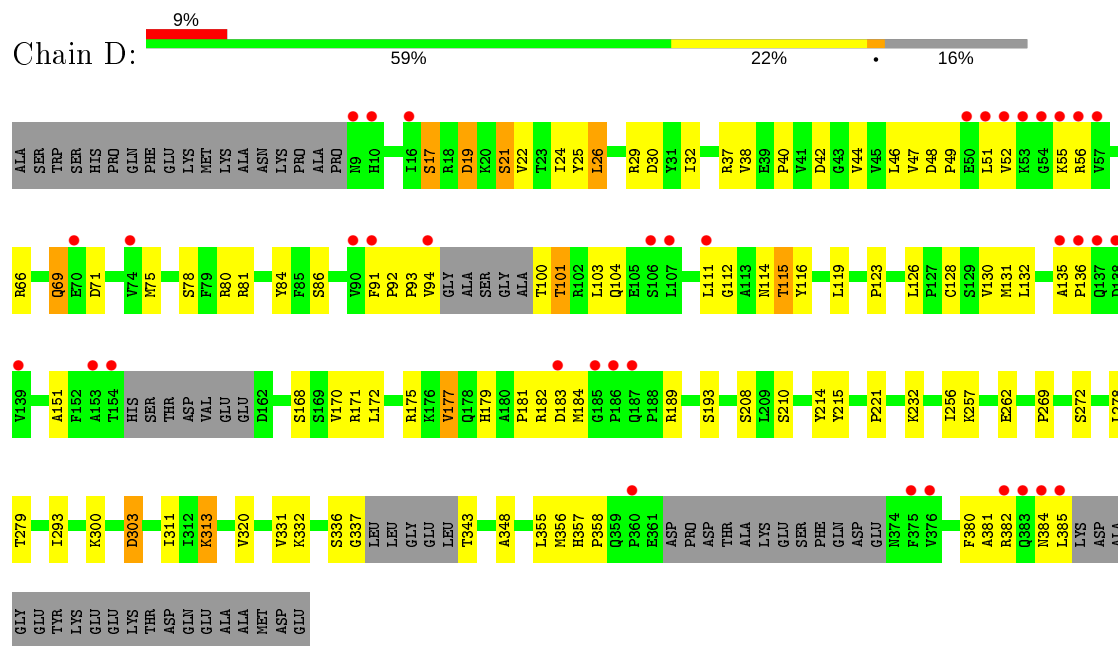
8% 56% 26% 15%

ALA SER TRP SER HIS PRO GLN PHE GLU ASP MET LYS ASN LYS PRO ALA PRO ASN HIS V11 I12 F13 K14 K15 I16 S17 R18 D19 K20 S21 I24 Y25 L26 G27 K28 H34 V35 F36 R37 V38 E39 V44 V45 L46 V47 D48 P49 E50 L51 V52 R53 G54 K55 R56 V57 V58 V59 T154 H155 S156 T157 D158 V159 Q69 E70 D71 P72 I73 D73 V74 W75 G76 Y84 F85 S86 P92 P93 V94 G95 I96 SER G98 A99 T100 T101 R102 H103 L103 Q104 L107 L111 T115 Y116 L119 L126 P127 C128 S129 V130 M131 A135 P136 V139 F147 E148 I149 K150 A151 F152 A153 K167 S168 S169 V170 R171 L172 L173 L174 P181 Q187 P188 R189 A192 V193 W194 S199 D200 L209 E212 V215 E231 K232 K235 K236 T237 K238 V239 E242 L249 V250 S251 S252 I256 K257 F258 E263 E266 T279 L280 V281 P282 L283 V286 N287 R290 I293 A294 L295 L299 K300 H301 E302 D303 K313 K330 V331 K332 L333 T334 L338 LEU GLY GLU LEU T343 S344 V347 A348 T349 E350 K356 E361 K362 P363 ASP THR ALA GLU PHE GLN ASP

- Molecule 1: S-arrestin



- Molecule 1: S-arrestin



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	168.36Å 184.33Å 90.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.89 – 2.65 32.89 – 2.65	Depositor EDS
% Data completeness (in resolution range)	98.6 (32.89-2.65) 98.3 (32.89-2.65)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.46 (at 2.65Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, $R_{free}$	0.209 , 0.253 0.196 , 0.242	Depositor DCC
$R_{free}$ test set	4083 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	49.8	Xtriage
Anisotropy	0.428	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 57.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	11230	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% 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, 0.333 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: NA, K, PTD, IMD, EDO

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	0.42	0/2919	0.62	0/3969
1	B	0.38	0/2712	0.58	0/3698
1	C	0.40	0/2827	0.59	0/3841
1	D	0.42	0/2660	0.60	0/3632
All	All	0.40	0/11118	0.60	0/15140

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	2859	0	2852	57	0
1	B	2662	0	2615	77	0
1	C	2772	0	2776	55	0
1	D	2608	0	2538	68	0
2	A	56	0	64	13	0
2	B	14	0	16	0	0
2	C	21	0	24	11	0
2	D	7	0	8	0	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
4	A	8	0	12	1	0
4	B	4	0	6	0	0
4	C	12	0	18	1	0
4	D	4	0	6	2	0
5	B	5	0	5	4	0
5	D	10	0	10	4	0
6	C	1	0	0	0	0
7	A	68	0	0	1	0
7	B	31	0	0	2	0
7	C	45	0	0	4	0
7	D	41	0	0	1	0
All	All	11230	0	10950	255	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 12.

The worst 5 of 255 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:D:128:CYS:H	5:D:406:IMD:H5	1.14	1.07
1:A:128:CYS:HB2	2:A:410:PTD:HC31	1.53	0.91
1:D:313:LYS:HG2	7:D:442:HOH:O	1.70	0.90
1:A:72:ILE:HG21	1:A:80:ARG:HD2	1.57	0.87
1:D:128:CYS:H	5:D:406:IMD:C5	1.88	0.86

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	366/414 (88%)	358 (98%)	7 (2%)	1 (0%)	41	56
1	B	342/414 (83%)	332 (97%)	9 (3%)	1 (0%)	41	56
1	C	350/414 (84%)	344 (98%)	5 (1%)	1 (0%)	41	56
1	D	338/414 (82%)	332 (98%)	6 (2%)	0	100	100
All	All	1396/1656 (84%)	1366 (98%)	27 (2%)	3 (0%)	47	64

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	35	VAL
1	B	35	VAL
1	C	35	VAL

### 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	315/368 (86%)	283 (90%)	32 (10%)	7	9
1	B	287/368 (78%)	244 (85%)	43 (15%)	3	3
1	C	304/368 (83%)	282 (93%)	22 (7%)	14	21
1	D	276/368 (75%)	239 (87%)	37 (13%)	4	4
All	All	1182/1472 (80%)	1048 (89%)	134 (11%)	6	7

5 of 134 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	232	LYS
1	C	10	HIS
1	D	210	SER
1	B	251	SER
1	B	287	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	137	GLN
1	C	178	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](#)

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 27 ligands modelled in this entry, 3 are monoatomic - leaving 24 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).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	EDO	C	411	-	3,3,3	0.48	0	2,2,2	0.26	0
2	PTD	A	407	-	6,6,6	1.96	2 (33%)	5,5,5	1.06	0
5	IMD	B	405	-	3,5,5	0.37	0	4,5,5	0.62	0
4	EDO	C	410	-	3,3,3	0.53	0	2,2,2	0.27	0
2	PTD	B	407	-	6,6,6	1.97	2 (33%)	5,5,5	1.13	0
4	EDO	D	408	-	3,3,3	0.51	0	2,2,2	0.08	0
4	EDO	C	409	-	3,3,3	0.46	0	2,2,2	0.40	0
4	EDO	B	409	-	3,3,3	0.43	0	2,2,2	0.42	0
2	PTD	A	411	-	6,6,6	1.93	2 (33%)	5,5,5	1.23	0
2	PTD	C	406	-	6,6,6	1.95	2 (33%)	5,5,5	1.07	0
5	IMD	D	406	-	3,5,5	0.44	0	4,5,5	0.54	0
5	IMD	D	405	-	3,5,5	0.43	0	4,5,5	0.64	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	PTD	B	406	-	6,6,6	1.98	2 (33%)	5,5,5	1.16	0
4	EDO	A	414	-	3,3,3	0.44	0	2,2,2	0.21	0
2	PTD	C	407	-	6,6,6	1.99	2 (33%)	5,5,5	0.99	0
2	PTD	A	410	-	6,6,6	2.07	2 (33%)	5,5,5	1.18	0
2	PTD	A	406	-	6,6,6	2.01	2 (33%)	5,5,5	1.34	0
2	PTD	C	405	-	6,6,6	1.99	2 (33%)	5,5,5	1.07	0
2	PTD	A	412	-	6,6,6	1.96	2 (33%)	5,5,5	1.11	0
2	PTD	D	407	-	6,6,6	1.98	2 (33%)	5,5,5	1.27	0
2	PTD	A	408	-	6,6,6	1.97	2 (33%)	5,5,5	1.07	0
2	PTD	A	409	-	6,6,6	2.00	2 (33%)	5,5,5	1.15	0
4	EDO	A	415	-	3,3,3	0.48	0	2,2,2	0.31	0
2	PTD	A	405	-	6,6,6	1.98	2 (33%)	5,5,5	1.15	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
4	EDO	C	411	-	-	1/1/1/1	-
2	PTD	A	407	-	-	1/2/4/4	-
5	IMD	B	405	-	-	-	0/1/1/1
4	EDO	C	410	-	-	0/1/1/1	-
2	PTD	B	407	-	-	1/2/4/4	-
4	EDO	D	408	-	-	0/1/1/1	-
2	PTD	B	406	-	-	1/2/4/4	-
4	EDO	B	409	-	-	1/1/1/1	-
2	PTD	A	411	-	-	2/2/4/4	-
2	PTD	C	406	-	-	0/2/4/4	-
5	IMD	D	406	-	-	-	0/1/1/1
5	IMD	D	405	-	-	-	0/1/1/1
4	EDO	C	409	-	-	1/1/1/1	-
2	PTD	A	412	-	-	2/2/4/4	-
2	PTD	C	407	-	-	1/2/4/4	-
2	PTD	A	410	-	-	0/2/4/4	-
2	PTD	A	406	-	-	0/2/4/4	-
2	PTD	C	405	-	-	2/2/4/4	-
4	EDO	A	414	-	-	1/1/1/1	-
2	PTD	D	407	-	-	2/2/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PTD	A	408	-	-	0/2/4/4	-
2	PTD	A	409	-	-	1/2/4/4	-
4	EDO	A	415	-	-	1/1/1/1	-
2	PTD	A	405	-	-	1/2/4/4	-

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	410	PTD	O5-C5	3.64	1.40	1.19
2	A	410	PTD	O1-C1	3.46	1.39	1.19
2	A	409	PTD	O5-C5	3.44	1.39	1.19
2	A	406	PTD	O1-C1	3.42	1.39	1.19
2	C	407	PTD	O1-C1	3.42	1.39	1.19

There are no bond angle outliers.

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	411	PTD	C1-C2-C3-C4
2	A	411	PTD	C2-C3-C4-C5
2	B	406	PTD	C2-C3-C4-C5
2	C	405	PTD	C1-C2-C3-C4
2	A	409	PTD	C1-C2-C3-C4

There are no ring outliers.

13 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	407	PTD	3	0
5	B	405	IMD	4	0
4	D	408	EDO	2	0
4	C	409	EDO	1	0
2	C	406	PTD	6	0
5	D	406	IMD	3	0
5	D	405	IMD	1	0
2	C	407	PTD	3	0
2	A	410	PTD	5	0
2	C	405	PTD	2	0
2	A	409	PTD	2	0
4	A	415	EDO	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	405	PTD	3	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	369/414 (89%)	-0.07	12 (3%) 46 43	23, 42, 90, 133	0
1	B	352/414 (85%)	0.27	32 (9%) 9 7	29, 58, 120, 140	0
1	C	358/414 (86%)	-0.04	16 (4%) 33 30	25, 47, 90, 162	0
1	D	348/414 (84%)	0.22	37 (10%) 6 4	26, 52, 117, 141	0
All	All	1427/1656 (86%)	0.09	97 (6%) 17 14	23, 48, 114, 162	0

The worst 5 of 97 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	98	GLY	6.2
1	B	99	ALA	5.5
1	D	376	VAL	5.4
1	D	375	PHE	5.3
1	D	385	LEU	5.0

### 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<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	B-factors( $\text{\AA}^2$ )	Q<0.9
2	PTD	A	407	7/7	0.64	0.26	62,70,78,82	0
2	PTD	C	405	7/7	0.68	0.33	69,72,76,77	0
2	PTD	B	406	7/7	0.78	0.20	69,73,81,83	0
2	PTD	A	411	7/7	0.79	0.29	65,71,75,77	0
2	PTD	A	410	7/7	0.81	0.36	55,56,62,63	0
2	PTD	B	407	7/7	0.83	0.23	62,65,71,74	0
2	PTD	C	407	7/7	0.85	0.30	57,64,71,76	0
2	PTD	A	412	7/7	0.85	0.22	59,63,72,72	0
2	PTD	C	406	7/7	0.86	0.32	60,63,84,92	0
5	IMD	B	405	5/5	0.86	0.26	86,89,89,89	0
4	EDO	B	409	4/4	0.88	0.33	55,60,61,70	0
2	PTD	D	407	7/7	0.88	0.20	52,61,69,69	0
2	PTD	A	408	7/7	0.88	0.20	68,70,72,72	0
2	PTD	A	409	7/7	0.88	0.21	45,54,76,77	0
4	EDO	C	409	4/4	0.89	0.27	58,59,63,65	0
2	PTD	A	405	7/7	0.91	0.24	42,48,72,75	0
6	K	C	408	1/1	0.93	0.28	88,88,88,88	0
4	EDO	D	408	4/4	0.93	0.39	62,63,63,63	0
4	EDO	A	415	4/4	0.93	0.23	59,63,64,68	0
3	NA	B	408	1/1	0.93	0.36	45,45,45,45	0
2	PTD	A	406	7/7	0.94	0.32	27,35,36,38	0
3	NA	A	413	1/1	0.96	0.23	34,34,34,34	0
5	IMD	D	406	5/5	0.96	0.25	80,81,88,91	0
5	IMD	D	405	5/5	0.96	0.22	72,73,74,75	0
4	EDO	C	411	4/4	0.97	0.23	60,65,78,85	0
4	EDO	A	414	4/4	0.98	0.24	36,39,41,49	0
4	EDO	C	410	4/4	0.99	0.18	26,30,37,38	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.