



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 02:04 am GMT

PDB ID : 2X7O  
Title : CRYSTAL STRUCTURE OF TGFBR1 COMPLEXED WITH AN INDOLINONE INHIBITOR  
Authors : Roth, G.J.; Heckel, A.; Brandl, T.; Grauert, M.; Hoerer, S.; Kley, J.T.; Schnapp, G.; Baum, P.; Mennerich, D.; Schnapp, A.; Park, J.E.  
Deposited on : 2010-03-03  
Resolution : 3.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

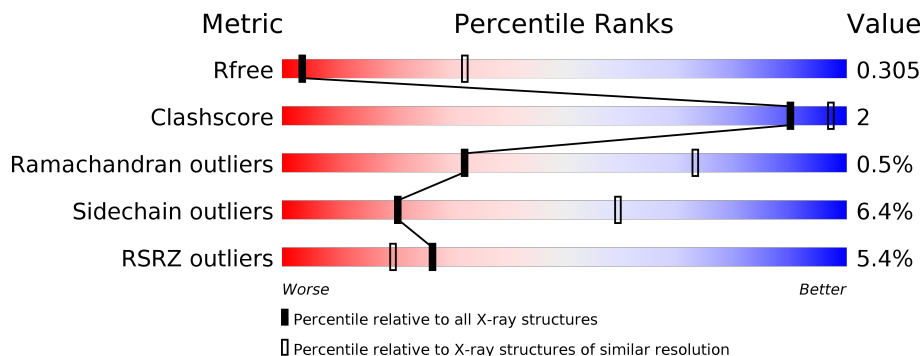
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.70 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))
$R_{free}$	100719	1234 (3.90-3.50)
Clashscore	112137	1377 (3.90-3.50)
Ramachandran outliers	110173	1323 (3.90-3.50)
Sidechain outliers	110143	1320 (3.90-3.50)
RSRZ outliers	101464	1262 (3.90-3.50)

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	342	<div> <div>4%</div> <div> <div></div> <div>84%</div> <div>12%</div> <div></div> </div> <div></div> </div>
1	B	342	<div> <div>2%</div> <div> <div></div> <div>85%</div> <div>11%</div> <div></div> </div> <div></div> </div>
1	C	342	<div> <div>11%</div> <div> <div></div> <div>86%</div> <div>11%</div> <div></div> </div> <div></div> </div>
1	D	342	<div> <div>3%</div> <div> <div></div> <div>87%</div> <div>10%</div> <div></div> </div> <div></div> </div>
1	E	342	<div> <div>5%</div> <div> <div></div> <div>85%</div> <div>11%</div> <div></div> </div> <div></div> </div>

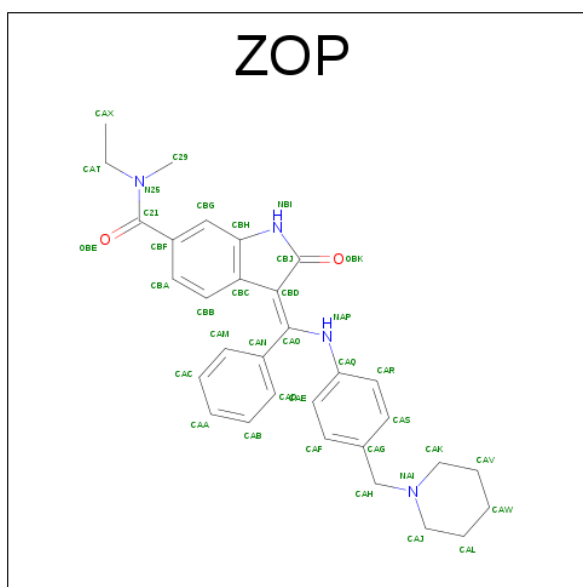


In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called TGF-BETA RECEPTOR TYPE I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	330	Total 2629	C 1658	N 471	O 484	S 16	0	0	0
1	B	330	Total 2629	C 1658	N 471	O 484	S 16	0	0	0
1	C	330	Total 2629	C 1658	N 471	O 484	S 16	0	0	0
1	D	330	Total 2629	C 1658	N 471	O 484	S 16	0	0	0
1	E	330	Total 2629	C 1658	N 471	O 484	S 16	0	0	0

- Molecule 2 is (3Z)-N-ETHYL-N-METHYL-2-OXO-3-(PHENYL{[4-(PIPERIDIN-1-YLME THYL)PHENYL]AMINO}METHYLIDENE)-2,3-DIHYDRO-1H-INDOLE-6-CARBOXAM IDE (three-letter code: ZOP) (formula: C<sub>31</sub>H<sub>34</sub>N<sub>4</sub>O<sub>2</sub>).

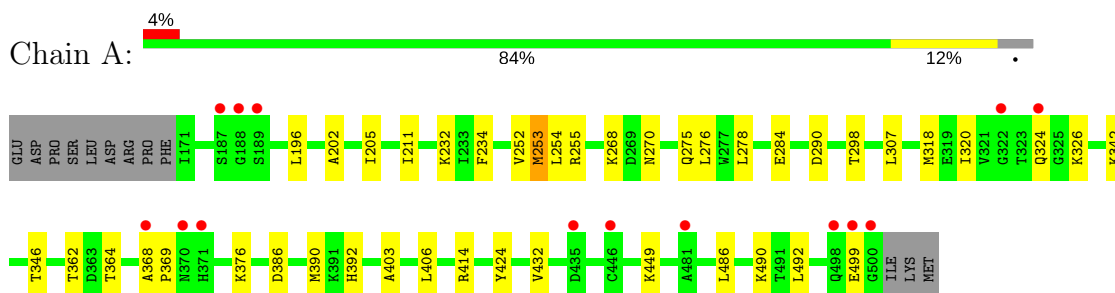


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			37	31	4	2		
2	B	1	Total	C	N	O	0	0
			37	31	4	2		
2	C	1	Total	C	N	O	0	0
			37	31	4	2		
2	D	1	Total	C	N	O	0	0
			37	31	4	2		
2	E	1	Total	C	N	O	0	0
			37	31	4	2		

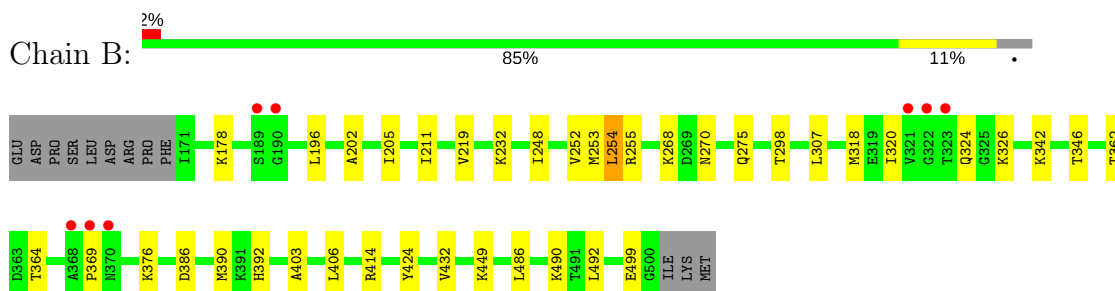
### 3 Residue-property plots

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

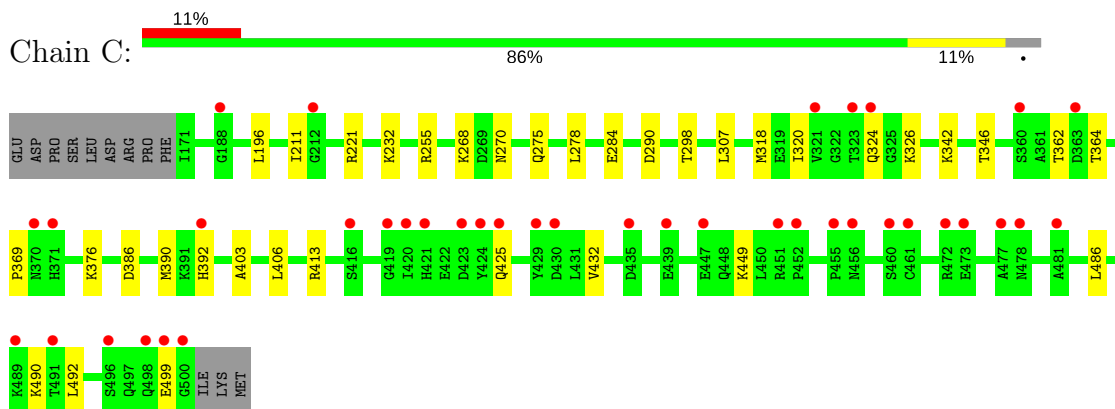
#### • Molecule 1: TGF-BETA RECEPTOR TYPE I



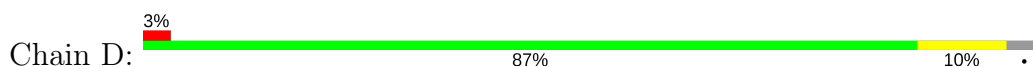
#### • Molecule 1: TGF-BETA RECEPTOR TYPE I

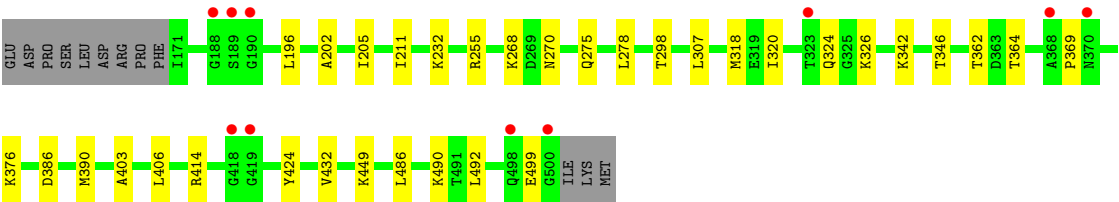


#### • Molecule 1: TGF-BETA RECEPTOR TYPE I

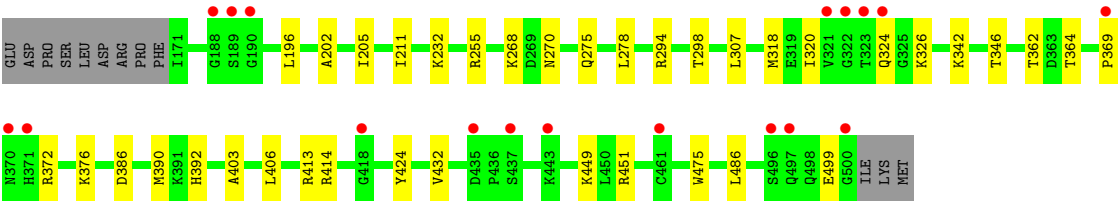
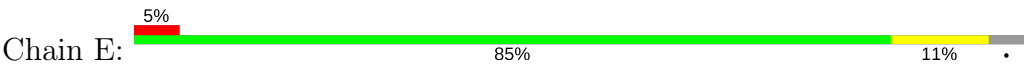


#### • Molecule 1: TGF-BETA RECEPTOR TYPE I





• Molecule 1: TGF-BETA RECEPTOR TYPE I



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	179.93Å 246.56Å 131.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	22.72 – 3.70 22.72 – 3.70	Depositor EDS
% Data completeness (in resolution range)	78.6 (22.72-3.70) 78.6 (22.72-3.70)	Depositor EDS
$R_{merge}$	0.02	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	13.06 (at 3.73Å)	Xtriage
Refinement program	BUSTER 2.9.3	Depositor
R, $R_{free}$	0.267 , 0.273 0.300 , 0.305	Depositor DCC
$R_{free}$ test set	1220 reflections (5.08%)	DCC
Wilson B-factor (Å <sup>2</sup> )	50.7	Xtriage
Anisotropy	0.064	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 28.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.55$ , $\langle L^2 \rangle = 0.40$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.80	EDS
Total number of atoms	13330	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.35% 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: ZOP

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	0.37	0/2682	0.56	0/3622
1	B	0.37	0/2682	0.56	0/3622
1	C	0.38	0/2682	0.55	0/3622
1	D	0.37	0/2682	0.55	0/3622
1	E	0.37	0/2682	0.55	0/3622
All	All	0.37	0/13410	0.55	0/18110

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	2629	0	2631	14	0
1	B	2629	0	2631	12	0
1	C	2629	0	2631	9	0
1	D	2629	0	2631	10	0
1	E	2629	0	2631	12	0
2	A	37	0	34	4	0
2	B	37	0	34	1	0
2	C	37	0	34	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	37	0	34	3	0
2	E	37	0	34	4	0
All	All	13330	0	13325	56	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 2.

All (56) 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:B:232:LYS:HB2	2:B:600:ZOP:H293	1.58	0.84
1:D:232:LYS:HB2	2:D:600:ZOP:H293	1.59	0.84
1:A:232:LYS:HB2	2:A:600:ZOP:H293	1.62	0.82
1:E:232:LYS:HB2	2:E:600:ZOP:H293	1.65	0.78
1:C:232:LYS:HB2	2:C:600:ZOP:H293	1.64	0.77
1:A:290:ASP:HB3	2:A:600:ZOP:HAL2	1.80	0.62
1:E:369:PRO:HB2	1:E:390:MET:HB3	1.84	0.60
1:B:252:VAL:HG23	1:B:254:LEU:HD23	1.82	0.60
1:C:369:PRO:HB2	1:C:390:MET:HB3	1.84	0.60
1:A:369:PRO:HB2	1:A:390:MET:HB3	1.83	0.59
1:B:369:PRO:HB2	1:B:390:MET:HB3	1.84	0.59
1:D:369:PRO:HB2	1:D:390:MET:HB3	1.84	0.58
1:C:278:LEU:HD23	2:C:600:ZOP:HAT1	1.85	0.57
1:C:413:ARG:HH22	1:C:425:GLN:HB2	1.75	0.51
1:E:268:LYS:HB2	1:E:275:GLN:HB2	1.94	0.50
1:B:268:LYS:HB2	1:B:275:GLN:HB2	1.94	0.49
1:D:268:LYS:HB2	1:D:275:GLN:HB2	1.93	0.49
1:A:268:LYS:HB2	1:A:275:GLN:HB2	1.94	0.49
1:C:268:LYS:HB2	1:C:275:GLN:HB2	1.93	0.48
1:A:414:ARG:HH21	1:A:424:TYR:H	1.61	0.48
1:A:368:ALA:HB2	1:B:178:LYS:HD3	1.95	0.48
1:C:403:ALA:HA	1:C:406:LEU:HD12	1.96	0.48
1:A:403:ALA:HA	1:A:406:LEU:HD12	1.96	0.48
1:A:320:ILE:HD12	1:A:326:LYS:HG2	1.96	0.48
1:D:320:ILE:HD12	1:D:326:LYS:HG2	1.96	0.47
1:C:320:ILE:HD12	1:C:326:LYS:HG2	1.96	0.47
1:D:403:ALA:HA	1:D:406:LEU:HD12	1.96	0.47
1:B:403:ALA:HA	1:B:406:LEU:HD12	1.96	0.47
1:B:414:ARG:HD2	1:B:424:TYR:HB2	1.96	0.47
1:E:320:ILE:HD12	1:E:326:LYS:HG2	1.96	0.47
1:B:320:ILE:HD12	1:B:326:LYS:HG2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:414:ARG:HH21	1:E:424:TYR:H	1.63	0.46
1:E:403:ALA:HA	1:E:406:LEU:HD12	1.96	0.46
1:D:342:LYS:HD3	1:D:346:THR:HB	1.99	0.44
1:B:342:LYS:HD3	1:B:346:THR:HB	1.99	0.44
1:E:294:ARG:HH11	2:E:600:ZOP:HAW1	1.82	0.44
1:E:342:LYS:HD3	1:E:346:THR:HB	1.99	0.44
1:A:211:ILE:HG23	2:A:600:ZOP:HAD	1.99	0.43
1:C:342:LYS:HD3	1:C:346:THR:HB	2.00	0.43
1:A:253:MET:O	1:A:253:MET:HG3	2.19	0.43
1:D:414:ARG:HH21	1:D:424:TYR:H	1.67	0.43
1:B:211:ILE:HD12	1:B:219:VAL:HG12	1.99	0.43
1:A:278:LEU:HD23	2:A:600:ZOP:HAT1	2.00	0.42
1:A:342:LYS:HD3	1:A:346:THR:HB	2.01	0.42
1:E:211:ILE:HG23	2:E:600:ZOP:HAD	2.01	0.42
1:D:211:ILE:HG23	2:D:600:ZOP:HAD	2.00	0.42
1:A:234:PHE:HB2	1:A:276:LEU:HB2	2.02	0.42
1:C:290:ASP:HB3	2:C:600:ZOP:HAL2	2.01	0.42
1:B:202:ALA:HA	1:B:205:ILE:HD12	2.02	0.41
1:E:202:ALA:HA	1:E:205:ILE:HD12	2.03	0.41
1:B:248:ILE:O	1:B:252:VAL:HG22	2.20	0.41
1:D:202:ALA:HA	1:D:205:ILE:HD12	2.02	0.40
1:D:278:LEU:HD23	2:D:600:ZOP:HAT1	2.02	0.40
1:A:202:ALA:HA	1:A:205:ILE:HD12	2.02	0.40
1:E:278:LEU:HD23	2:E:600:ZOP:HAT1	2.03	0.40
1:E:451:ARG:HG2	1:E:475:TRP:HB3	2.04	0.40

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	328/342 (96%)	306 (93%)	20 (6%)	2 (1%)	28 70

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	328/342 (96%)	306 (93%)	19 (6%)	3 (1%)	20	64
1	C	328/342 (96%)	305 (93%)	22 (7%)	1 (0%)	44	80
1	D	328/342 (96%)	305 (93%)	22 (7%)	1 (0%)	44	80
1	E	328/342 (96%)	306 (93%)	21 (6%)	1 (0%)	44	80
All	All	1640/1710 (96%)	1528 (93%)	104 (6%)	8 (0%)	32	73

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	255	ARG
1	B	254	LEU
1	B	255	ARG
1	C	255	ARG
1	D	255	ARG
1	E	255	ARG
1	B	253	MET
1	A	252	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	282/294 (96%)	262 (93%)	20 (7%)	17	56
1	B	282/294 (96%)	265 (94%)	17 (6%)	22	61
1	C	282/294 (96%)	262 (93%)	20 (7%)	17	56
1	D	282/294 (96%)	266 (94%)	16 (6%)	24	63
1	E	282/294 (96%)	265 (94%)	17 (6%)	22	61
All	All	1410/1470 (96%)	1320 (94%)	90 (6%)	20	59

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	196	LEU
1	A	253	MET
1	A	254	LEU
1	A	270	ASN
1	A	284	GLU
1	A	298	THR
1	A	307	LEU
1	A	318	MET
1	A	324	GLN
1	A	362	THR
1	A	364	THR
1	A	376	LYS
1	A	386	ASP
1	A	392	HIS
1	A	432	VAL
1	A	449	LYS
1	A	486	LEU
1	A	490	LYS
1	A	492	LEU
1	A	499	GLU
1	B	196	LEU
1	B	270	ASN
1	B	298	THR
1	B	307	LEU
1	B	318	MET
1	B	324	GLN
1	B	362	THR
1	B	364	THR
1	B	376	LYS
1	B	386	ASP
1	B	392	HIS
1	B	432	VAL
1	B	449	LYS
1	B	486	LEU
1	B	490	LYS
1	B	492	LEU
1	B	499	GLU
1	C	196	LEU
1	C	211	ILE
1	C	221	ARG
1	C	270	ASN
1	C	284	GLU
1	C	298	THR

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Mol	Chain	Res	Type
1	C	307	LEU
1	C	318	MET
1	C	324	GLN
1	C	362	THR
1	C	364	THR
1	C	376	LYS
1	C	386	ASP
1	C	392	HIS
1	C	432	VAL
1	C	449	LYS
1	C	486	LEU
1	C	490	LYS
1	C	492	LEU
1	C	499	GLU
1	D	196	LEU
1	D	270	ASN
1	D	298	THR
1	D	307	LEU
1	D	318	MET
1	D	324	GLN
1	D	362	THR
1	D	364	THR
1	D	376	LYS
1	D	386	ASP
1	D	432	VAL
1	D	449	LYS
1	D	486	LEU
1	D	490	LYS
1	D	492	LEU
1	D	499	GLU
1	E	196	LEU
1	E	270	ASN
1	E	298	THR
1	E	307	LEU
1	E	318	MET
1	E	324	GLN
1	E	362	THR
1	E	364	THR
1	E	372	ARG
1	E	376	LYS
1	E	386	ASP
1	E	392	HIS

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Mol	Chain	Res	Type
1	E	413	ARG
1	E	432	VAL
1	E	449	LYS
1	E	486	LEU
1	E	499	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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](#)

5 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	$\# Z  > 2$
2	ZOP	A	600	-	40,41,41	1.24	2 (5%)	54,57,57	1.30	6 (11%)
2	ZOP	B	600	-	40,41,41	1.29	3 (7%)	54,57,57	1.38	6 (11%)
2	ZOP	C	600	-	40,41,41	1.25	3 (7%)	54,57,57	1.39	8 (14%)
2	ZOP	D	600	-	40,41,41	1.23	3 (7%)	54,57,57	1.42	5 (9%)
2	ZOP	E	600	-	40,41,41	1.28	4 (10%)	54,57,57	1.45	5 (9%)

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
2	ZOP	A	600	-	-	0/26/46/46	0/5/5/5
2	ZOP	B	600	-	-	0/26/46/46	0/5/5/5
2	ZOP	C	600	-	-	0/26/46/46	0/5/5/5
2	ZOP	D	600	-	-	0/26/46/46	0/5/5/5
2	ZOP	E	600	-	-	0/26/46/46	0/5/5/5

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	600	ZOP	CBD-CBJ	-2.86	1.43	1.50
2	E	600	ZOP	CBD-CBJ	-2.82	1.43	1.50
2	D	600	ZOP	CBD-CBJ	-2.73	1.44	1.50
2	A	600	ZOP	CBD-CBJ	-2.66	1.44	1.50
2	C	600	ZOP	CBD-CBJ	-2.65	1.44	1.50
2	C	600	ZOP	CBJ-NBI	-2.44	1.33	1.36
2	A	600	ZOP	CBJ-NBI	-2.25	1.33	1.36
2	E	600	ZOP	CBJ-NBI	-2.17	1.33	1.36
2	D	600	ZOP	CBJ-NBI	-2.04	1.34	1.36
2	C	600	ZOP	CAM-CAN	2.01	1.42	1.39
2	E	600	ZOP	C21-N25	2.03	1.38	1.34
2	B	600	ZOP	C21-N25	2.04	1.38	1.34
2	E	600	ZOP	CBG-CBF	2.05	1.42	1.39
2	D	600	ZOP	C21-N25	2.05	1.38	1.34
2	B	600	ZOP	CBG-CBF	2.18	1.42	1.39

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	600	ZOP	CAG-CAH-NAI	-3.87	105.73	113.17
2	D	600	ZOP	CAG-CAH-NAI	-3.78	105.89	113.17
2	B	600	ZOP	CAG-CAH-NAI	-3.63	106.18	113.17
2	A	600	ZOP	CBG-CBH-CBC	-3.12	119.72	122.44
2	B	600	ZOP	CBG-CBH-CBC	-2.82	119.98	122.44
2	D	600	ZOP	CBG-CBH-CBC	-2.72	120.07	122.44
2	E	600	ZOP	CBG-CBH-CBC	-2.61	120.16	122.44
2	C	600	ZOP	CBG-CBH-CBC	-2.44	120.31	122.44
2	C	600	ZOP	CAG-CAH-NAI	-2.19	108.95	113.17
2	C	600	ZOP	CBD-CAO-NAP	-2.16	116.17	118.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	600	ZOP	CAG-CAH-NAI	-2.11	109.11	113.17
2	C	600	ZOP	CAM-CAN-CAO	-2.03	118.32	120.75
2	B	600	ZOP	CAO-CBD-CBJ	2.07	126.44	122.64
2	C	600	ZOP	CAQ-NAP-CAO	2.18	134.81	127.79
2	A	600	ZOP	CAO-CBD-CBJ	2.20	126.67	122.64
2	C	600	ZOP	CBF-C21-N25	2.25	121.97	118.47
2	A	600	ZOP	CBF-C21-N25	2.34	122.10	118.47
2	D	600	ZOP	CBF-C21-N25	2.47	122.31	118.47
2	B	600	ZOP	CBF-C21-N25	2.61	122.53	118.47
2	D	600	ZOP	CAN-CAO-NAP	2.67	122.77	119.14
2	B	600	ZOP	CAN-CAO-NAP	2.81	122.96	119.14
2	E	600	ZOP	CAN-CAO-NAP	2.83	122.99	119.14
2	A	600	ZOP	CAN-CAO-NAP	2.85	123.02	119.14
2	E	600	ZOP	CBF-C21-N25	2.87	122.94	118.47
2	C	600	ZOP	CAN-CAO-NAP	3.26	123.58	119.14
2	E	600	ZOP	CBD-CBJ-NBI	5.02	110.09	106.84
2	B	600	ZOP	CBD-CBJ-NBI	5.08	110.12	106.84
2	D	600	ZOP	CBD-CBJ-NBI	5.14	110.17	106.84
2	A	600	ZOP	CBD-CBJ-NBI	5.19	110.20	106.84
2	C	600	ZOP	CBD-CBJ-NBI	5.30	110.27	106.84

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	600	ZOP	4	0
2	B	600	ZOP	1	0
2	C	600	ZOP	3	0
2	D	600	ZOP	3	0
2	E	600	ZOP	4	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

### 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	330/342 (96%)	0.17	14 (4%) 37 27	19, 52, 81, 91	0
1	B	330/342 (96%)	0.13	8 (2%) 59 47	19, 51, 81, 92	0
1	C	330/342 (96%)	0.62	39 (11%) 5 5	20, 53, 82, 92	0
1	D	330/342 (96%)	0.16	10 (3%) 51 38	18, 52, 82, 91	0
1	E	330/342 (96%)	0.24	18 (5%) 26 18	19, 52, 82, 92	0
All	All	1650/1710 (96%)	0.26	89 (5%) 26 19	18, 52, 82, 92	0

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	496	SER	4.7
1	C	500	GLY	4.2
1	C	423	ASP	3.9
1	C	455	PRO	3.7
1	C	481	ALA	3.7
1	E	189	SER	3.7
1	C	424	TYR	3.5
1	C	452	PRO	3.4
1	C	421	HIS	3.4
1	C	370	ASN	3.3
1	E	321	VAL	3.3
1	C	371	HIS	3.3
1	A	188	GLY	3.2
1	C	477	ALA	3.2
1	A	187	SER	3.1
1	C	451	ARG	3.1
1	C	360	SER	3.1
1	A	435	ASP	3.1
1	C	416	SER	3.1
1	B	370	ASN	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	425	GLN	3.1
1	E	370	ASN	3.1
1	A	499	GLU	3.0
1	E	496	SER	3.0
1	D	189	SER	2.9
1	E	323	THR	2.9
1	C	456	ASN	2.9
1	E	190	GLY	2.9
1	B	322	GLY	2.8
1	A	500	GLY	2.8
1	C	419	GLY	2.8
1	E	322	GLY	2.8
1	D	419	GLY	2.8
1	C	420	ILE	2.8
1	E	443	LYS	2.7
1	C	188	GLY	2.7
1	C	324	GLN	2.7
1	D	370	ASN	2.6
1	D	190	GLY	2.6
1	C	491	THR	2.5
1	D	500	GLY	2.5
1	C	472	ARG	2.5
1	C	363	ASP	2.5
1	D	368	ALA	2.5
1	A	370	ASN	2.4
1	B	190	GLY	2.4
1	E	435	ASP	2.4
1	C	323	THR	2.4
1	C	430	ASP	2.4
1	B	321	VAL	2.4
1	C	473	GLU	2.3
1	C	461	CYS	2.3
1	E	369	PRO	2.3
1	E	500	GLY	2.3
1	E	324	GLN	2.3
1	A	498	GLN	2.2
1	C	498	GLN	2.2
1	B	323	THR	2.2
1	C	460	SER	2.2
1	C	499	GLU	2.2
1	B	368	ALA	2.2
1	B	369	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	497	GLN	2.2
1	C	447	GLU	2.2
1	E	437	SER	2.2
1	C	392	HIS	2.2
1	A	322	GLY	2.1
1	D	418	GLY	2.1
1	A	368	ALA	2.1
1	E	418	GLY	2.1
1	C	321	VAL	2.1
1	C	429	TYR	2.1
1	D	188	GLY	2.1
1	A	481	ALA	2.1
1	B	189	SER	2.1
1	C	489	LYS	2.1
1	C	212	GLY	2.1
1	C	439	GLU	2.1
1	C	478	ASN	2.1
1	D	323	THR	2.1
1	A	189	SER	2.0
1	E	188	GLY	2.1
1	C	435	ASP	2.0
1	D	498	GLN	2.0
1	A	371	HIS	2.0
1	E	461	CYS	2.0
1	E	371	HIS	2.0
1	A	324	GLN	2.0
1	A	446	CYS	2.0

## 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 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
2	ZOP	C	600	37/37	0.76	0.38	0.76	76,79,81,81	0
2	ZOP	B	600	37/37	0.86	0.31	0.54	25,29,48,49	0
2	ZOP	E	600	37/37	0.86	0.30	0.27	34,40,51,52	0
2	ZOP	A	600	37/37	0.89	0.28	0.04	30,33,44,44	0
2	ZOP	D	600	37/37	0.89	0.26	-0.24	31,33,51,52	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.