



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:28 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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

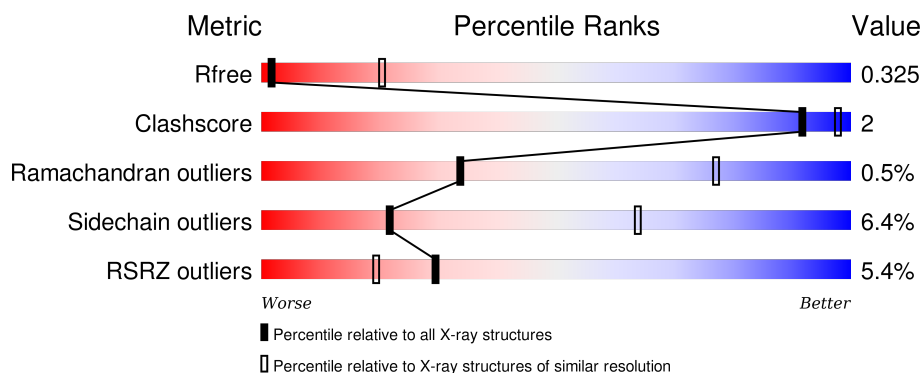
1 Overall quality at a glance

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}	91344	1101 (3.90-3.50)
Clashscore	102246	1224 (3.90-3.50)
Ramachandran outliers	100387	1172 (3.90-3.50)
Sidechain outliers	100360	1170 (3.90-3.50)
RSRZ outliers	91569	1108 (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 ≥ 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>84%12%.</div> </div>
1	B	342	<div> <div>2%</div> <div>85%11%.</div> </div>
1	C	342	<div> <div>11%</div> <div>86%11%.</div> </div>
1	D	342	<div> <div>3%</div> <div>87%10%.</div> </div>
1	E	342	<div> <div>6%</div> <div>85%11%.</div> </div>

2 Entry composition [i](#)

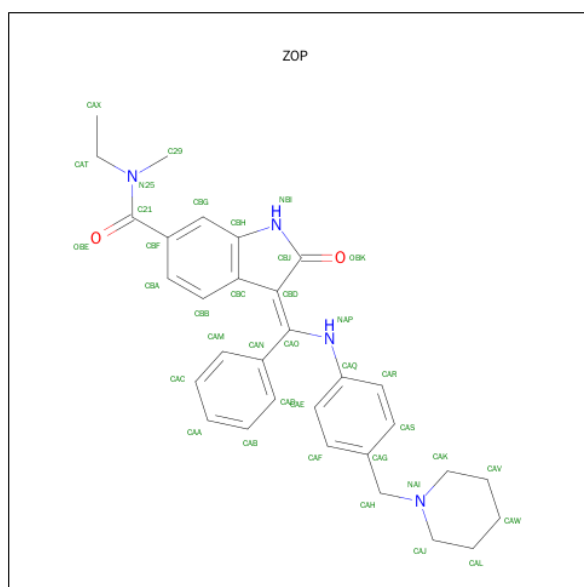
There are 2 unique types of molecules in this entry. The entry contains 13330 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

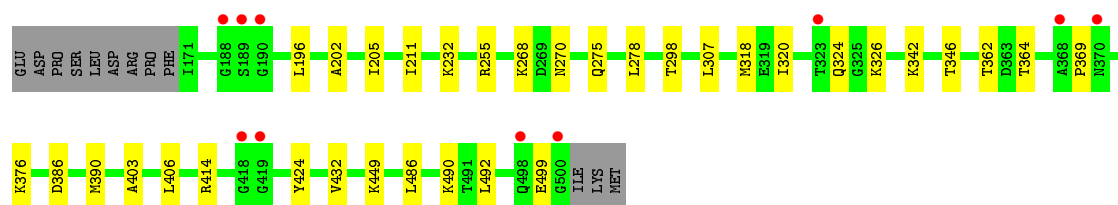
- Molecule 1 is a protein called TGF-BETA RECEPTOR TYPE I.

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

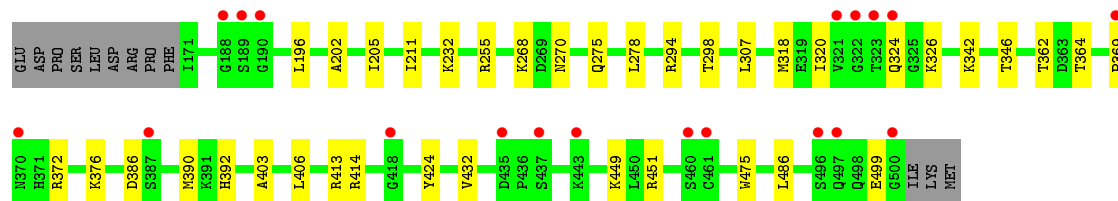
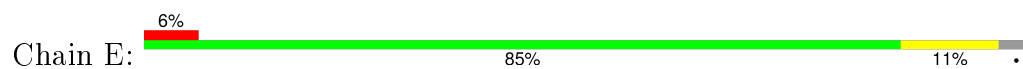
- Molecule 2 is (3Z)-N-ETHYL-N-METHYL-2-OXO-3-(PHENYL{[4-(PIPERIDIN-1-YLMETHYL)PHENYL]AMINO}METHYLIDENE)-2,3-DIHYDRO-1H-INDOLE-6-CARBOXAMIDE (three-letter code: ZOP) (formula: C₃₁H₃₄N₄O₂).



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		



• 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, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	13.06 (at 3.73Å)	Xtriage
Refinement program	BUSTER 2.9.3	Depositor
R, R_{free}	0.267 , 0.273 0.317 , 0.325	Depositor DCC
R_{free} test set	1260 reflections (5.09%)	DCC
Wilson B-factor (Å ²)	50.7	Xtriage
Anisotropy	0.064	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 28.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.55$, $\langle L^2 \rangle = 0.40$	Xtriage
Outliers	0 of 24744 reflections	Xtriage
F_o, F_c correlation	0.80	EDS
Total number of atoms	13330	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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 [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:C:403:ALA:HA	1:C:406:LEU:HD12	1.96	0.48
1:A:368:ALA:HB2	1:B:178:LYS:HD3	1.95	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:C:290:ASP:HB3	2:C:600:ZOP:HAL2	2.01	0.42
1:A:234:PHE:HB2	1:A:276:LEU:HB2	2.02	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:278:LEU:HD23	2:D:600:ZOP:HAT1	2.02	0.40
1:D:202:ALA:HA	1:D:205:ILE:HD12	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%)	30 75

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	328/342 (96%)	306 (93%)	19 (6%)	3 (1%)	21	68
1	C	328/342 (96%)	305 (93%)	22 (7%)	1 (0%)	46	83
1	D	328/342 (96%)	305 (93%)	22 (7%)	1 (0%)	46	83
1	E	328/342 (96%)	306 (93%)	21 (6%)	1 (0%)	46	83
All	All	1640/1710 (96%)	1528 (93%)	104 (6%)	8 (0%)	34	77

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%)	18	60
1	B	282/294 (96%)	265 (94%)	17 (6%)	24	66
1	C	282/294 (96%)	262 (93%)	20 (7%)	18	60
1	D	282/294 (96%)	266 (94%)	16 (6%)	25	68
1	E	282/294 (96%)	265 (94%)	17 (6%)	24	66
All	All	1410/1470 (96%)	1320 (94%)	90 (6%)	22	64

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	1.20	2 (5%)	56,57,57	1.33	7 (12%)
2	ZOP	B	600	-	40,41,41	1.25	3 (7%)	56,57,57	1.41	8 (14%)
2	ZOP	C	600	-	40,41,41	1.21	2 (5%)	56,57,57	1.40	8 (14%)
2	ZOP	D	600	-	40,41,41	1.19	2 (5%)	56,57,57	1.42	6 (10%)
2	ZOP	E	600	-	40,41,41	1.24	3 (7%)	56,57,57	1.47	6 (10%)

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 (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	600	ZOP	CBD-CBJ	-2.76	1.43	1.50
2	E	600	ZOP	CBD-CBJ	-2.73	1.43	1.50
2	D	600	ZOP	CBD-CBJ	-2.64	1.44	1.50
2	A	600	ZOP	CBD-CBJ	-2.56	1.44	1.50
2	C	600	ZOP	CBD-CBJ	-2.56	1.44	1.50
2	C	600	ZOP	CBJ-NBI	-2.39	1.33	1.36
2	A	600	ZOP	CBJ-NBI	-2.21	1.33	1.36
2	E	600	ZOP	CBJ-NBI	-2.13	1.33	1.36
2	D	600	ZOP	CBJ-NBI	-2.01	1.34	1.36
2	E	600	ZOP	CBG-CBF	2.04	1.42	1.39
2	B	600	ZOP	CAR-CAQ	2.05	1.42	1.39
2	B	600	ZOP	CBG-CBF	2.17	1.42	1.39

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	600	ZOP	CAG-CAH-NAI	-3.84	105.73	113.16
2	D	600	ZOP	CAG-CAH-NAI	-3.75	105.89	113.16
2	B	600	ZOP	CAG-CAH-NAI	-3.61	106.18	113.16
2	A	600	ZOP	CBG-CBH-CBC	-3.11	119.72	122.46
2	B	600	ZOP	CAN-CAO-CBD	-2.99	119.01	122.41
2	B	600	ZOP	CBG-CBH-CBC	-2.81	119.98	122.46
2	A	600	ZOP	CAN-CAO-CBD	-2.79	119.24	122.41
2	D	600	ZOP	CBG-CBH-CBC	-2.71	120.07	122.46
2	E	600	ZOP	CBG-CBH-CBC	-2.60	120.16	122.46
2	C	600	ZOP	CBD-CAO-NAP	-2.59	116.17	118.17
2	E	600	ZOP	CAN-CAO-CBD	-2.47	119.61	122.41
2	C	600	ZOP	CBG-CBH-CBC	-2.43	120.31	122.46
2	D	600	ZOP	CAN-CAO-CBD	-2.26	119.84	122.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	600	ZOP	CAG-CAH-NAI	-2.18	108.95	113.16
2	A	600	ZOP	CAG-CAH-NAI	-2.09	109.11	113.16
2	C	600	ZOP	CAK-NAI-CAJ	2.02	113.28	108.90
2	B	600	ZOP	CAK-NAI-CAJ	2.08	113.39	108.90
2	B	600	ZOP	CAO-CBD-CBJ	2.11	126.44	122.58
2	C	600	ZOP	CBF-C21-N25	2.13	121.97	118.56
2	C	600	ZOP	CAQ-NAP-CAO	2.13	134.81	127.70
2	A	600	ZOP	CBF-C21-N25	2.21	122.10	118.56
2	A	600	ZOP	CAO-CBD-CBJ	2.23	126.67	122.58
2	D	600	ZOP	CBF-C21-N25	2.35	122.31	118.56
2	B	600	ZOP	CBF-C21-N25	2.48	122.53	118.56
2	D	600	ZOP	CAN-CAO-NAP	2.67	122.77	119.24
2	E	600	ZOP	CBF-C21-N25	2.74	122.94	118.56
2	B	600	ZOP	CAN-CAO-NAP	2.82	122.96	119.24
2	E	600	ZOP	CAN-CAO-NAP	2.84	122.99	119.24
2	A	600	ZOP	CAN-CAO-NAP	2.87	123.02	119.24
2	C	600	ZOP	CAN-CAO-NAP	3.28	123.58	119.24
2	E	600	ZOP	CBD-CBJ-NBI	4.91	110.09	106.83
2	B	600	ZOP	CBD-CBJ-NBI	4.96	110.12	106.83
2	D	600	ZOP	CBD-CBJ-NBI	5.02	110.17	106.83
2	A	600	ZOP	CBD-CBJ-NBI	5.07	110.20	106.83
2	C	600	ZOP	CBD-CBJ-NBI	5.17	110.27	106.83

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 ⓘ

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	330/342 (96%)	0.19	13 (3%) 43 29	19, 52, 81, 91	0
1	B	330/342 (96%)	0.16	8 (2%) 62 46	19, 51, 81, 92	0
1	C	330/342 (96%)	0.64	39 (11%) 6 5	20, 53, 82, 92	0
1	D	330/342 (96%)	0.19	10 (3%) 54 37	18, 52, 82, 91	0
1	E	330/342 (96%)	0.27	19 (5%) 26 16	19, 52, 82, 92	0
All	All	1650/1710 (96%)	0.29	89 (5%) 29 19	18, 52, 82, 92	0

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	496	SER	4.8
1	C	500	GLY	4.1
1	C	423	ASP	3.9
1	E	189	SER	3.7
1	C	481	ALA	3.7
1	C	455	PRO	3.7
1	C	424	TYR	3.6
1	C	452	PRO	3.4
1	C	370	ASN	3.4
1	C	421	HIS	3.3
1	E	321	VAL	3.3
1	A	187	SER	3.2
1	C	477	ALA	3.2
1	C	360	SER	3.2
1	A	188	GLY	3.2
1	C	416	SER	3.2
1	A	435	ASP	3.2
1	C	371	HIS	3.2
1	B	370	ASN	3.1
1	E	370	ASN	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	499	GLU	3.1
1	C	425	GLN	3.1
1	E	496	SER	3.1
1	C	451	ARG	3.1
1	D	189	SER	3.0
1	C	456	ASN	2.9
1	E	323	THR	2.9
1	E	190	GLY	2.8
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	324	GLN	2.7
1	C	188	GLY	2.7
1	D	370	ASN	2.6
1	C	491	THR	2.6
1	C	363	ASP	2.6
1	D	190	GLY	2.5
1	C	461	CYS	2.5
1	D	368	ALA	2.5
1	D	500	GLY	2.5
1	E	435	ASP	2.5
1	A	370	ASN	2.5
1	C	430	ASP	2.5
1	C	472	ARG	2.4
1	C	323	THR	2.4
1	B	190	GLY	2.4
1	C	473	GLU	2.4
1	B	321	VAL	2.4
1	E	324	GLN	2.3
1	E	369	PRO	2.3
1	C	460	SER	2.3
1	C	499	GLU	2.3
1	E	500	GLY	2.3
1	A	498	GLN	2.3
1	C	498	GLN	2.3
1	C	447	GLU	2.3
1	E	437	SER	2.2
1	B	323	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	368	ALA	2.2
1	E	497	GLN	2.2
1	B	369	PRO	2.2
1	E	461	CYS	2.2
1	A	368	ALA	2.2
1	A	446	CYS	2.2
1	B	189	SER	2.1
1	C	439	GLU	2.1
1	A	322	GLY	2.1
1	C	321	VAL	2.1
1	D	418	GLY	2.1
1	C	429	TYR	2.1
1	E	418	GLY	2.1
1	A	189	SER	2.1
1	A	481	ALA	2.1
1	C	478	ASN	2.1
1	C	392	HIS	2.1
1	C	435	ASP	2.1
1	D	323	THR	2.1
1	D	498	GLN	2.1
1	D	188	GLY	2.1
1	C	212	GLY	2.1
1	C	489	LYS	2.0
1	E	387	SER	2.0
1	A	324	GLN	2.0
1	E	188	GLY	2.0
1	E	460	SER	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, 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	RSCC	RSR	LLDF	B-factors(Å ²)	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.