



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 09:58 AM GMT

PDB ID : 3KCF
Title : Crystal structure of TGFbRI complexed with a pyrazolone inhibitor
Authors : Boriack-Sjodin, P.A.
Deposited on : 2009-10-21
Resolution : 2.80 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
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

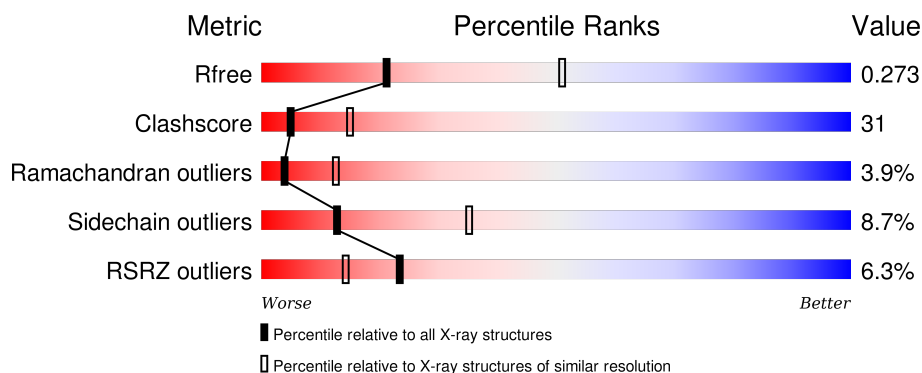
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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>8%</div> <div>45%</div> <div>44%</div> <div>6%</div> <div>.</div> </div>
1	B	342	<div> <div>2%</div> <div>51%</div> <div>38%</div> <div>6%</div> <div>5%</div> </div>
1	C	342	<div> <div>12%</div> <div>37%</div> <div>51%</div> <div>8%</div> <div>.</div> </div>
1	D	342	<div> <div>4%</div> <div>52%</div> <div>38%</div> <div>6%</div> <div>.</div> </div>
1	E	342	<div> <div>4%</div> <div>54%</div> <div>35%</div> <div>7%</div> <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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PO4	B	11	-	-	X	-
3	PO4	D	14	-	-	-	X
3	PO4	D	15	-	-	X	X
3	PO4	E	2	-	-	X	X
3	PO4	E	3	-	-	X	-

2 Entry composition [i](#)

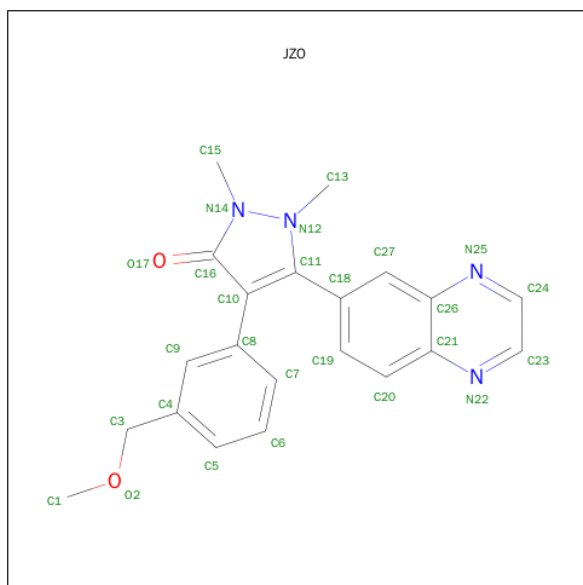
There are 4 unique types of molecules in this entry. The entry contains 13297 atoms, of which 0 are hydrogens and 0 are deuteriums.

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-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	328	Total	C	N	O	S	0	0	0
			2617	1650	469	482	16			
1	B	324	Total	C	N	O	S	0	0	0
			2590	1636	463	475	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 4-[3-(METHOXYMETHYL)PHENYL]-1,2-DIMETHYL-5-QUINOXALIN-6-YL-1,2-DIHYDRO-3H-PYRAZOL-3-ONE (three-letter code: JZO) (formula: C₂₁H₂₀N₄O₂).



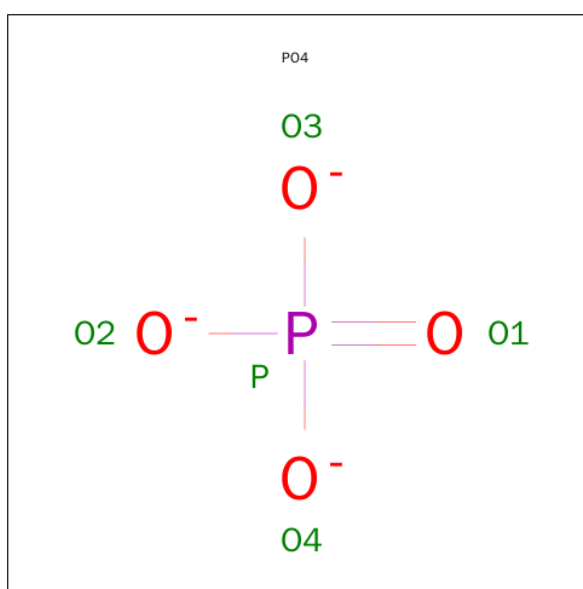
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			27	21	4	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			27	21	4	2		
2	C	1	Total	C	N	O	0	0
			27	21	4	2		
2	D	1	Total	C	N	O	0	0
			27	21	4	2		
2	E	1	Total	C	N	O	0	0
			27	21	4	2		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		
3	E	1	Total	O	P	0	0
			5	4	1		
3	E	1	Total	O	P	0	0
			5	4	1		
3	E	1	Total	O	P	0	0
			5	4	1		

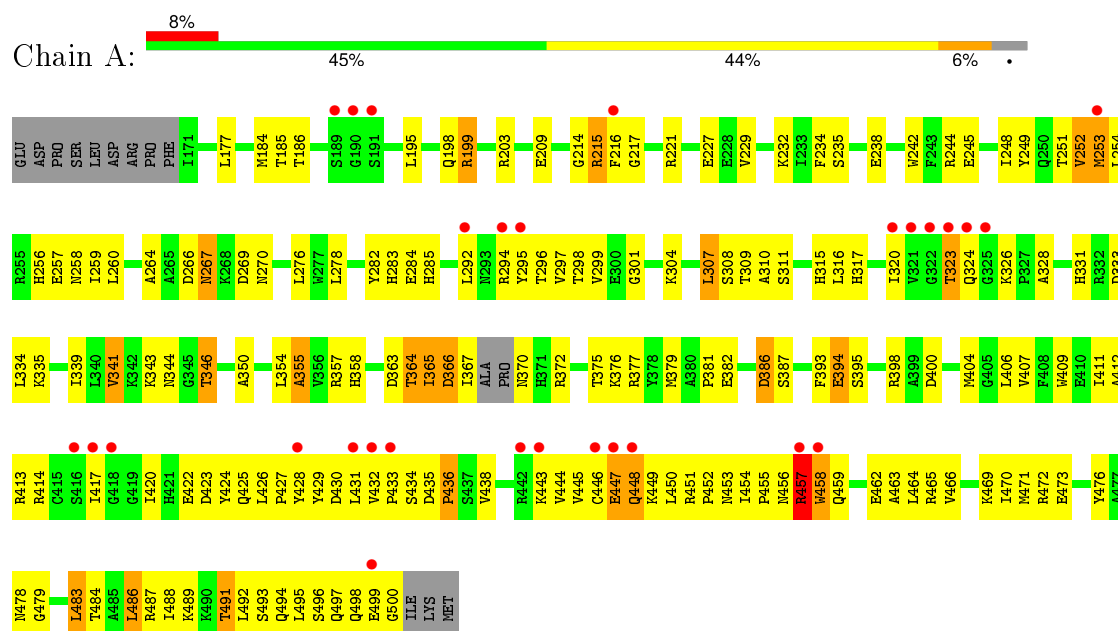
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	O	0	0
			1	1		
4	C	1	Total	O	0	0
			1	1		
4	E	1	Total	O	0	0
			1	1		

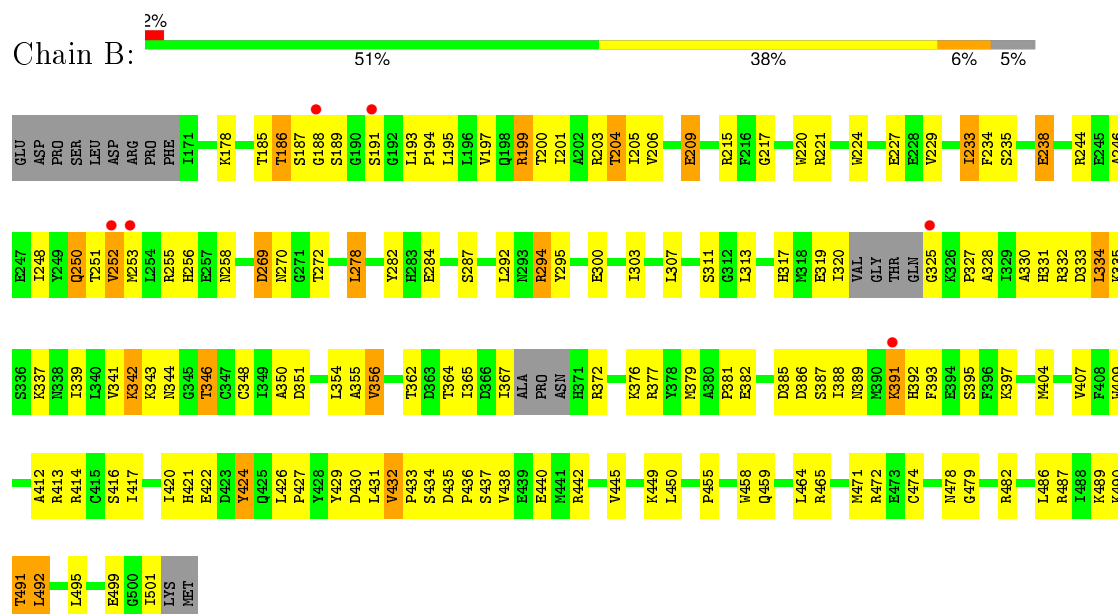
3 Residue-property plots

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: TGF-beta receptor type-1



• Molecule 1: TGF-beta receptor type-1



Chain C:

Position	Residue	Type
1	Q448	Yellow
2	K449	Yellow
3	P381	Yellow
4	L450	Yellow
5	R382	Yellow
6	R451	Yellow
7	P452	Yellow
8	P455	Yellow
9	M456	Yellow
10	R457	Yellow
11	K458	Yellow
12	Q459	Yellow
13	S460	Yellow
14	C461	Yellow
15	E462	Yellow
16	A463	Yellow
17	L464	Yellow
18	R465	Yellow
19	V466	Yellow
20	M467	Yellow
21	G468	Yellow
22	K469	Yellow
23	L470	Yellow
24	M471	Yellow
25	R472	Yellow
26	E473	Yellow
27	C474	Yellow
28	M475	Yellow
29	V476	Yellow
30	A477	Yellow
31	M478	Yellow
32	G479	Yellow
33	A480	Yellow
34	A481	Yellow
35	R482	Yellow
36	L483	Yellow
37	T484	Yellow
38	A485	Yellow
39	L486	Yellow
40	R487	Yellow
41	V488	Yellow
42	K489	Yellow
43	K490	Yellow
44	T491	Yellow
45	S493	Yellow
46	Q494	Yellow
47	L495	Yellow
48	S496	Yellow
49	Q497	Yellow
50	D498	Yellow
51	E499	Yellow
52	G500	Yellow
53	I501	Yellow
54	L502	Yellow
55	K503	Yellow
56	L504	Yellow
57	K505	Yellow
58	L506	Yellow
59	K507	Yellow
60	L508	Yellow
61	K509	Yellow
62	L510	Yellow
63	K511	Yellow
64	L512	Yellow
65	K513	Yellow
66	L514	Yellow
67	K515	Yellow
68	L516	Yellow
69	K517	Yellow
70	L518	Yellow
71	K519	Yellow
72	L520	Yellow
73	K521	Yellow
74	L522	Yellow
75	K523	Yellow
76	L524	Yellow
77	K525	Yellow
78	L526	Yellow
79	K527	Yellow
80	L528	Yellow
81	K529	Yellow
82	L530	Yellow
83	K531	Yellow
84	L532	Yellow
85	K533	Yellow
86	L534	Yellow
87	K535	Yellow
88	L536	Yellow
89	K537	Yellow
90	L538	Yellow
91	K539	Yellow
92	L540	Yellow
93	K541	Yellow
94	L542	Yellow
95	K543	Yellow
96	L544	Yellow
97	K545	Yellow
98	L546	Yellow
99	K547	Yellow
100	L548	Yellow
101	K549	Yellow
102	L550	Yellow
103	K551	Yellow
104	L552	Yellow
105	K553	Yellow
106	L554	Yellow
107	K555	Yellow
108	L556	Yellow
109	K557	Yellow
110	L558	Yellow
111	K559	Yellow
112	L560	Yellow
113	K561	Yellow
114	L562	Yellow
115	K563	Yellow
116	L564	Yellow
117	K565	Yellow
118	L566	Yellow
119	K567	Yellow
120	L568	Yellow
121	K569	Yellow
122	L570	Yellow
123	K571	Yellow
124	L572	Yellow
125	K573	Yellow
126	L574	Yellow
127	K575	Yellow
128	L576	Yellow
129	K577	Yellow
130	L578	Yellow
131	K579	Yellow
132	L580	Yellow
133	K581	Yellow
134	L582	Yellow
135	K583	Yellow
136	L584	Yellow
137	K585	Yellow
138	L586	Yellow
139	K587	Yellow
140	L588	Yellow
141	K589	Yellow
142	L590	Yellow
143	K591	Yellow
144	L592	Yellow
145	K593	Yellow
146	L594	Yellow
147	K595	Yellow
148	L596	Yellow
14		

Chain D:

4% 52% 38% 6%

Amino Acid	Count
GLU	1
ASP	1
PRQ	1
SER	1
LEU	1
ASP	1
ARG	1
PRQ	1
PHE	1
I171	1
K178	1
D179	1
L180	1
I181	1
M184	1
T185	1
V197	1
Q198	1
R199	1
T201	1
I201	1
A202	1
R203	1
T204	1
I205	1
V206	1
L207	1
Q208	1
E209	1
G214	1
R215	1
F216	1
G217	1
W224	1
E227	1
E228	1
V229	1
A230	1
V231	1
K232	1
I233	1
S235	1
S236	1
R237	1
E238	1
V341	1
K342	1
R343	1
N344	1
G345	1
T346	1
C347	1
C348	1
I349	1
A350	1
V356	1
R357	1
T364	1
I365	1
D366	1
I367	1
A368	1
R369	1
N370	1
H371	1
R372	1
K376	1
R377	1
V378	1
M379	1
A380	1
P381	1
E382	1
I388	1
N389	1
M390	1
K391	1
K397	1
A403	1
M404	1
V407	1
R413	1
R414	1
C415	1
S416	1
I417	1
G418	1
I420	1
H421	1
E422	1
D423	1
Y424	1
Q425	1
L426	1
Y428	1
D430	1
L431	1
V432	1
P433	1
A434	1
D435	1
P436	1
A437	1
V438	1
E439	1
E440	1
N441	1
K443	1
V444	1
V445	1
E446	1
E447	1
Q448	1
K449	1
L450	1
N453	1
L454	1
P455	1
N456	1
R457	1
V458	1
Q459	1
S460	1
C461	1
E462	1
A463	1
L464	1
R465	1
R469	1
R472	1
E473	1
R482	1
L486	1
R487	1
K490	1
T491	1
L492	1
Q498	1
E499	1
G500	1
I1E	1
LYS	1
MET	1

Chain E:

S434	D435	P436	S437	E440	Y441	R442	R443	Y444	Y445	C446	E447	Q448	R449	L450	R451	I454	P455	I456	R457	Y458	Q459	S460	C461	L464	R465	Y466	Y467	Y471	R472	E473	G479	R482	L483	R487	L488	R489	R490	L492	S493	Q494	Q497	Q498	E499	G500	ILE	LYS	MEI
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	174.03Å 249.08Å 138.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.86 – 2.80 49.59 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.6 (34.86-2.80) 99.7 (49.59-2.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.12 (at 2.81Å)	Xtriage
Refinement program	CNX 2005	Depositor
R, R_{free}	0.235 , 0.278 0.232 , 0.273	Depositor DCC
R_{free} test set	3747 reflections (5.37%)	DCC
Wilson B-factor (Å ²)	50.2	Xtriage
Anisotropy	0.249	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 65.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 73507 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	13297	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.45% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: JZO, 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	0.36	1/2668 (0.0%)	0.58	0/3600
1	B	0.40	0/2640	0.65	0/3560
1	C	0.34	0/2682	0.61	0/3622
1	D	0.39	0/2682	0.69	0/3622
1	E	0.41	0/2682	0.67	0/3622
All	All	0.38	1/13354 (0.0%)	0.64	0/18026

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
1	B	0	1
1	D	0	1
1	E	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	245	GLU	N-CA	5.55	1.57	1.46

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	424	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	D	424	TYR	Sidechain
1	E	424	TYR	Sidechain

5.2 Too-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 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	2617	0	2618	170	0
1	B	2590	0	2595	119	0
1	C	2629	0	2631	251	0
1	D	2629	0	2631	151	0
1	E	2629	0	2631	132	0
2	A	27	0	20	1	0
2	B	27	0	20	0	0
2	C	27	0	20	3	0
2	D	27	0	20	3	0
2	E	27	0	20	1	0
3	A	15	0	0	0	0
3	B	15	0	0	4	0
3	C	5	0	0	1	0
3	D	15	0	0	2	0
3	E	15	0	0	4	0
4	A	1	0	0	1	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
All	All	13297	0	13206	823	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 31.

The worst 5 of 823 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:E:216:PHE:HB3	1:E:238:GLU:HG2	1.22	1.10
1:A:443:LYS:HG2	1:A:448:GLN:HE21	1.19	1.08
1:C:461:CYS:HB2	1:C:464:LEU:HD23	1.35	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:367:ILE:HG13	1:D:369:PRO:HD3	1.40	1.04
1:E:253:MET:HB2	1:E:326:LYS:HB3	1.41	1.01

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	324/342 (95%)	262 (81%)	44 (14%)	18 (6%)	2	6
1	B	318/342 (93%)	281 (88%)	31 (10%)	6 (2%)	10	32
1	C	328/342 (96%)	251 (76%)	61 (19%)	16 (5%)	3	8
1	D	328/342 (96%)	276 (84%)	38 (12%)	14 (4%)	3	10
1	E	328/342 (96%)	291 (89%)	28 (8%)	9 (3%)	6	21
All	All	1626/1710 (95%)	1361 (84%)	202 (12%)	63 (4%)	4	12

5 of 63 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	215	ARG
1	A	252	VAL
1	A	366	ASP
1	A	447	GLU
1	B	235	SER

5.3.2 Protein sidechains [i](#)

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	281/294 (96%)	264 (94%)	17 (6%)	24	56
1	B	278/294 (95%)	252 (91%)	26 (9%)	11	31
1	C	282/294 (96%)	256 (91%)	26 (9%)	11	32
1	D	282/294 (96%)	255 (90%)	27 (10%)	10	29
1	E	282/294 (96%)	256 (91%)	26 (9%)	11	32
All	All	1405/1470 (96%)	1283 (91%)	122 (9%)	13	35

5 of 122 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	296	THR
1	C	483	LEU
1	E	364	THR
1	C	297	VAL
1	C	379	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 50 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	459	GLN
1	D	258	ASN
1	E	448	GLN
1	C	478	ASN
1	D	250	GLN

5.3.3 RNA ⓘ

There are no RNA molecules 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

18 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	JZO	A	1	-	25,30,30	1.49	6 (24%)	35,43,43	1.49	7 (20%)
3	PO4	A	21	-	4,4,4	1.09	0	6,6,6	0.27	0
3	PO4	A	22	-	4,4,4	1.14	0	6,6,6	0.27	0
3	PO4	A	9	-	4,4,4	1.16	0	6,6,6	0.27	0
3	PO4	B	11	-	4,4,4	1.13	0	6,6,6	0.27	0
3	PO4	B	12	-	4,4,4	1.19	0	6,6,6	0.27	0
2	JZO	B	2	-	25,30,30	1.47	6 (24%)	35,43,43	1.45	6 (17%)
3	PO4	B	6	-	4,4,4	1.01	0	6,6,6	0.27	0
3	PO4	C	10	-	4,4,4	1.07	0	6,6,6	0.27	0
2	JZO	C	3	-	25,30,30	1.43	5 (20%)	35,43,43	1.53	8 (22%)
3	PO4	D	13	-	4,4,4	1.13	0	6,6,6	0.27	0
3	PO4	D	14	-	4,4,4	1.21	0	6,6,6	0.27	0
3	PO4	D	15	-	4,4,4	1.27	0	6,6,6	0.27	0
2	JZO	D	4	-	25,30,30	1.54	7 (28%)	35,43,43	1.48	8 (22%)
3	PO4	E	1	-	4,4,4	1.13	0	6,6,6	0.27	0
3	PO4	E	2	-	4,4,4	1.18	0	6,6,6	0.27	0
3	PO4	E	3	-	4,4,4	1.22	0	6,6,6	0.27	0
2	JZO	E	5	-	25,30,30	1.49	5 (20%)	35,43,43	1.55	7 (20%)

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	JZO	A	1	-	-	0/11/11/11	0/4/4/4
3	PO4	A	21	-	-	0/0/0/0	0/0/0/0
3	PO4	A	22	-	-	0/0/0/0	0/0/0/0
3	PO4	A	9	-	-	0/0/0/0	0/0/0/0
3	PO4	B	11	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PO4	B	12	-	-	0/0/0/0	0/0/0/0
2	JZO	B	2	-	-	0/11/11/11	0/4/4/4
3	PO4	B	6	-	-	0/0/0/0	0/0/0/0
3	PO4	C	10	-	-	0/0/0/0	0/0/0/0
2	JZO	C	3	-	-	0/11/11/11	0/4/4/4
3	PO4	D	13	-	-	0/0/0/0	0/0/0/0
3	PO4	D	14	-	-	0/0/0/0	0/0/0/0
3	PO4	D	15	-	-	0/0/0/0	0/0/0/0
2	JZO	D	4	-	-	0/11/11/11	0/4/4/4
3	PO4	E	1	-	-	0/0/0/0	0/0/0/0
3	PO4	E	2	-	-	0/0/0/0	0/0/0/0
3	PO4	E	3	-	-	0/0/0/0	0/0/0/0
2	JZO	E	5	-	-	0/11/11/11	0/4/4/4

The worst 5 of 29 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	4	JZO	C6-C5	2.01	1.43	1.38
2	B	2	JZO	C19-C18	2.04	1.43	1.39
2	A	1	JZO	C6-C7	2.04	1.43	1.38
2	C	3	JZO	C24-N25	2.05	1.36	1.32
2	C	3	JZO	C19-C18	2.06	1.43	1.39

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	5	JZO	C15-N14-C16	-3.76	124.52	129.59
2	C	3	JZO	C15-N14-C16	-3.67	124.65	129.59
2	A	1	JZO	C15-N14-C16	-3.51	124.86	129.59
2	B	2	JZO	C15-N14-C16	-3.46	124.94	129.59
2	D	4	JZO	C15-N14-C16	-2.93	125.65	129.59

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	JZO	1	0
3	B	11	PO4	2	0
3	B	12	PO4	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	6	PO4	1	0
3	C	10	PO4	1	0
2	C	3	JZO	3	0
3	D	14	PO4	1	0
3	D	15	PO4	2	0
2	D	4	JZO	3	0
3	E	2	PO4	2	0
3	E	3	PO4	3	0
2	E	5	JZO	1	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, 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	328/342 (95%)	0.48	29 (8%) 12 6	23, 67, 105, 113	0
1	B	324/342 (94%)	-0.04	6 (1%) 70 59	17, 38, 68, 98	0
1	C	330/342 (96%)	0.64	40 (12%) 6 3	21, 71, 100, 110	0
1	D	330/342 (96%)	0.09	15 (4%) 37 26	20, 43, 82, 93	0
1	E	330/342 (96%)	0.01	13 (3%) 43 31	18, 37, 76, 93	0
All	All	1642/1710 (96%)	0.24	103 (6%) 23 14	17, 47, 96, 113	0

The worst 5 of 103 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	324	GLN	6.0
1	C	252	VAL	5.9
1	C	497	GLN	5.4
1	D	323	THR	5.4
1	E	370	ASN	4.9

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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	PO4	D	15	5/5	0.94	0.34	4.43	2,7,8,8	5
3	PO4	D	14	5/5	0.95	0.32	4.23	21,21,21,22	5
3	PO4	E	2	5/5	0.98	0.23	2.58	7,8,10,11	5
3	PO4	B	12	5/5	0.98	0.20	1.76	15,16,16,18	5
3	PO4	E	3	5/5	0.98	0.25	1.58	1,1,2,3	5
2	JZO	E	5	27/27	0.97	0.19	0.90	25,28,32,32	0
2	JZO	A	1	27/27	0.98	0.21	0.84	26,30,34,39	0
2	JZO	D	4	27/27	0.97	0.20	0.81	25,28,35,39	0
3	PO4	B	11	5/5	0.97	0.24	0.76	1,2,6,6	5
2	JZO	C	3	27/27	0.96	0.21	0.64	41,47,49,50	0
2	JZO	B	2	27/27	0.98	0.17	-0.04	17,22,26,30	0
3	PO4	A	22	5/5	0.93	0.23	-0.25	19,20,22,23	5
3	PO4	A	21	5/5	0.94	0.22	-0.41	35,36,36,37	5
3	PO4	D	13	5/5	0.97	0.14	-0.75	54,54,55,56	0
3	PO4	B	6	5/5	0.95	0.15	-1.03	37,37,38,40	0
3	PO4	E	1	5/5	0.97	0.15	-1.03	44,44,46,46	0
3	PO4	A	9	5/5	0.94	0.16	-1.05	69,70,70,71	0
3	PO4	C	10	5/5	0.89	0.18	-1.50	61,61,63,63	0

6.5 Other polymers

There are no such residues in this entry.