



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 31, 2017 – 02:32 AM EDT

PDB ID : 3FAA
Title : Crystal structure of TGFbRI complexed with a 2-aminoimidazole inhibitor
Authors : Boriack-Sjodin, P.A.; Fitch, C.
Deposited on : unknown
Resolution : 3.35 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
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) : rb-20030345

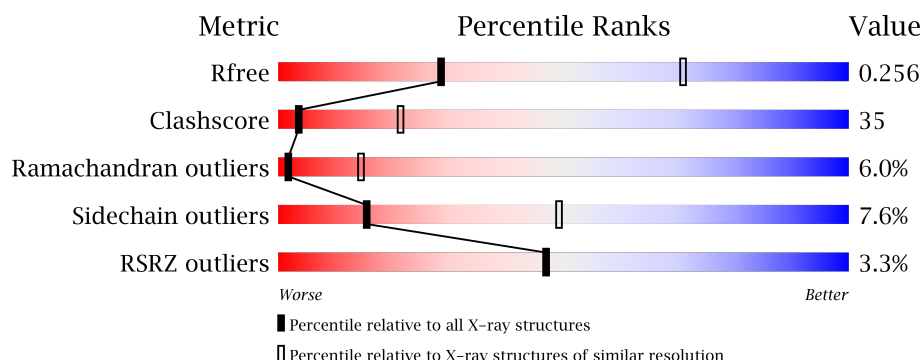
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.35 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	1156 (3.42-3.30)
Clashscore	112137	1231 (3.42-3.30)
Ramachandran outliers	110173	1212 (3.42-3.30)
Sidechain outliers	110143	1211 (3.42-3.30)
RSRZ outliers	101464	1165 (3.42-3.30)

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>2%</div> <div>44%</div> <div>45%</div> <div>7%</div> <div>.</div> </div>
1	B	342	<div> <div>50%</div> <div>36%</div> <div>8%</div> <div>5%</div> </div>
1	C	342	<div> <div>12%</div> <div>32%</div> <div>56%</div> <div>8%</div> <div>.</div> </div>
1	D	342	<div> <div>0%</div> <div>45%</div> <div>45%</div> <div>6%</div> <div>.</div> </div>
1	E	342	<div> <div>0%</div> <div>46%</div> <div>43%</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	A	9	-	-	X	-
3	PO4	B	12	-	-	-	X
3	PO4	D	13	-	-	X	-
3	PO4	D	14	-	-	-	X
3	PO4	D	24	-	-	-	X
3	PO4	E	2	-	-	X	-

2 Entry composition [i](#)

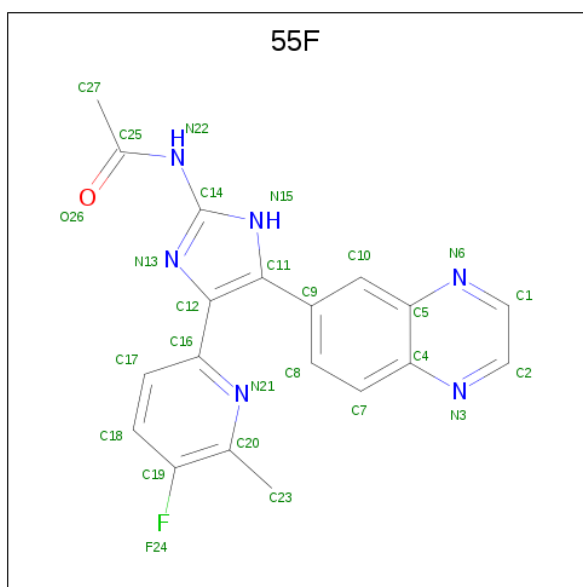
There are 3 unique types of molecules in this entry. The entry contains 13294 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 N-[4-(5-fluoro-6-methylpyridin-2-yl)-5-quinoxalin-6-yl]-1H-imidazol-2-yl]acetamide (three-letter code: 55F) (formula: C₁₉H₁₅FN₆O).



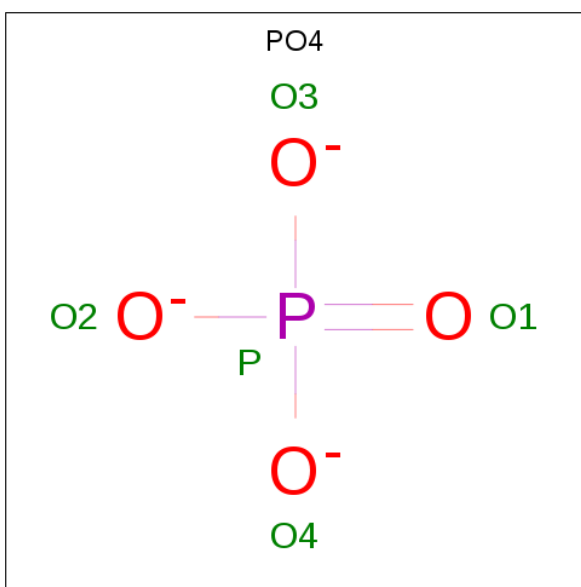
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			27	19	1	6	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	F	N	O	0	0
			27	19	1	6	1		
2	C	1	Total	C	F	N	O	0	0
			27	19	1	6	1		
2	D	1	Total	C	F	N	O	0	0
			27	19	1	6	1		
2	E	1	Total	C	F	N	O	0	0
			27	19	1	6	1		

- 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		

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 ($\text{RSRZ} > 2$). 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:

2%

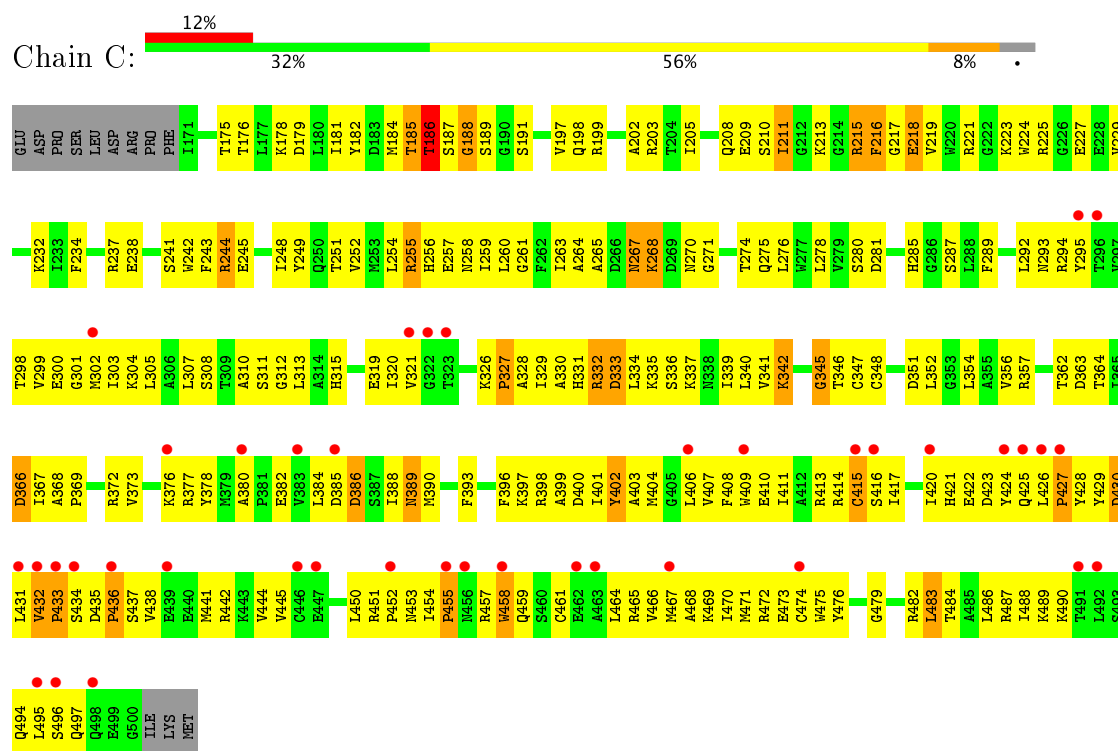
44%

45%

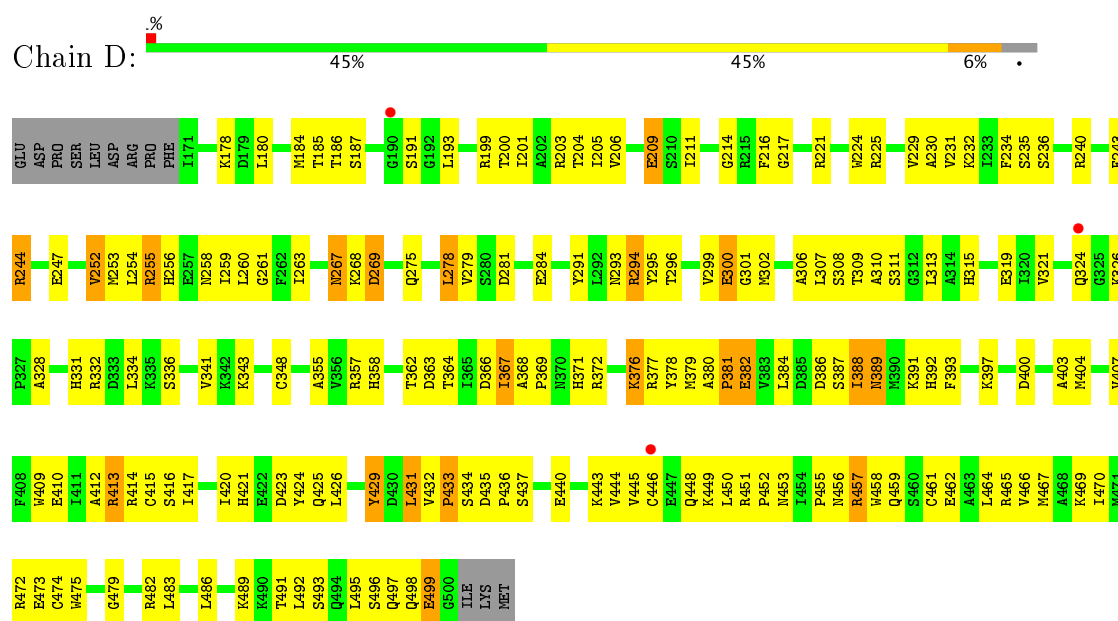
7%

- Chain B:
-
- | Amino Acid | Frequency (%) |
|------------|---------------|
| GLU | 50 |
| ASP | 50 |
| PRO | 50 |
| SER | 50 |
| LEU | 50 |
| ASP | 50 |
| ARG | 50 |
| PRO | 50 |
| PHE | 50 |
| I171 | 50 |
| S172 | 50 |
| E173 | 50 |
| G174 | 50 |
| T175 | 50 |
| K178 | 50 |
| D179 | 50 |
| L180 | 50 |
| I181 | 50 |
| M184 | 50 |
| G188 | 50 |
| S189 | 50 |
| G190 | 50 |
| S191 | 50 |
| G192 | 50 |
| L193 | 50 |
| P194 | 50 |
| V197 | 50 |
| Q198 | 50 |
| R199 | 50 |
| T200 | 50 |
| I201 | 50 |
| A202 | 50 |
| R203 | 50 |
| T204 | 50 |
| T205 | 50 |
| T206 | 50 |
| L207 | 50 |
| Q208 | 50 |
| E209 | 50 |
| R215 | 50 |
| F216 | 50 |
| G217 | 50 |
| R221 | 50 |
| W224 | 50 |
| R225 | 50 |
| G226 | 50 |
| E227 | 50 |
| E228 | 50 |
| V229 | 50 |
| K232 | 50 |
| L233 | 50 |
| F234 | 50 |
| E238 | 36 |
| R244 | 36 |
| T248 | 36 |
| T251 | 36 |
| V252 | 36 |
| R253 | 36 |
| L254 | 36 |
| R255 | 36 |
| R256 | 36 |
| E257 | 36 |
| N258 | 36 |
| T259 | 36 |
| T263 | 36 |
| A264 | 36 |
| R268 | 36 |
| D269 | 36 |
| N270 | 36 |
| G271 | 36 |
| L278 | 36 |
| H283 | 36 |
| S287 | 36 |
| L288 | 36 |
| L292 | 36 |
| N293 | 36 |
| R294 | 36 |
| E300 | 36 |
| G301 | 36 |
| P302 | 36 |
| I303 | 36 |
| K304 | 36 |
| L307 | 36 |
| S308 | 36 |
| T309 | 36 |
| A310 | 36 |
| S311 | 36 |
| G312 | 36 |
| L313 | 36 |
| L316 | 36 |
| E319 | 36 |
| I320 | 36 |
| VAL | 36 |
| GLY | 36 |
| THR | 36 |
| GLN | 36 |
| G325 | 36 |
| V326 | 36 |
| P327 | 36 |
| A328 | 36 |
| I329 | 36 |
| A330 | 36 |
| K331 | 36 |
| R332 | 36 |
| D333 | 36 |
| E410 | 36 |
| L334 | 36 |
| K335 | 36 |
| S336 | 36 |
| K337 | 36 |
| K338 | 36 |
| L339 | 36 |
| L340 | 36 |
| V341 | 36 |
| G348 | 36 |
| I349 | 36 |
| A350 | 36 |
| D351 | 36 |
| A355 | 36 |
| V356 | 36 |
| D359 | 36 |
| T362 | 36 |
| D363 | 36 |
| T364 | 36 |
| I365 | 36 |
| D366 | 36 |
| I367 | 36 |
| ALA | 36 |
| PRO | 36 |
| ASN | 36 |
| H371 | 36 |
| R372 | 36 |
| K376 | 36 |
| K379 | 36 |
| A380 | 36 |
| P381 | 36 |
| S382 | 36 |
| V383 | 36 |
| N456 | 36 |
| L457 | 36 |
| D385 | 36 |
| D386 | 36 |
| S387 | 36 |
| L388 | 36 |
| N389 | 36 |
| N390 | 36 |
| K391 | 36 |
| E394 | 36 |
| R398 | 36 |
| M404 | 36 |
| G405 | 36 |
| L406 | 36 |
| W409 | 36 |
| E410 | 36 |
| I411 | 36 |
| A412 | 36 |
| R413 | 36 |
| R414 | 36 |
| C415 | 36 |
| K438 | 36 |
| S416 | 36 |
| I417 | 36 |
| I420 | 36 |
| H421 | 36 |
| D423 | 36 |
| Y424 | 36 |
| Y428 | 36 |
| L431 | 36 |
| V432 | 36 |
| S433 | 36 |
| S434 | 36 |
| D435 | 36 |
| P436 | 36 |
| S437 | 36 |
| V438 | 36 |
| E439 | 36 |
| E440 | 36 |
| R441 | 36 |
| R442 | 36 |
| K443 | 36 |
| V444 | 36 |
| V445 | 36 |
| C446 | 36 |
| E447 | 36 |
| K448 | 36 |
| K449 | 36 |
| L450 | 36 |
| R451 | 36 |
| P455 | 36 |
| A463 | 36 |
| L464 | 36 |
| R465 | 36 |
| V466 | 36 |
| M467 | 36 |
| E467 | 36 |
| R471 | 36 |
| M472 | 36 |
| E473 | 36 |
| G474 | 36 |
| W475 | 36 |
| G479 | 36 |
| R482 | 36 |
| L483 | 36 |
| L486 | 36 |
| R487 | 36 |
| I488 | 36 |
| K489 | 36 |
| K490 | 36 |
| I491 | 36 |
| L492 | 36 |
| S493 | 36 |
| S49 | |

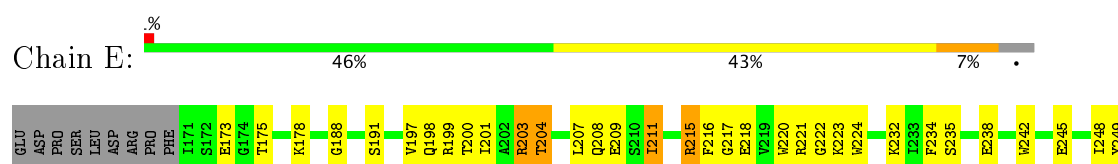
• Molecule 1: TGF-beta receptor type-1



• Molecule 1: TGF-beta receptor type-1



• Molecule 1: TGF-beta receptor type-1



Q250	Q324	Q402	Q473
T251	Q325	A403	M478
V252	M253	M404	G479
	I329		
H256	A330	M409	R482
F257	H331	E410	L483
I258	R332	I411	
I259	D333	A412	L486
L260	I334	R413	R487
G261	K335		I488
F262	S336	I417	K489
I263			K490
A264	L340	I420	T491
	V341	H421	L492
		E422	S493
I267	M344	D423	Q494
G271	G345	Y424	L495
	T346	Q425	S496
L276	C347	L426	Q497
M277		P427	Q498
L278	D351	Y428	E499
		Y429	G500
D281	L354	V432	I1E
	A355	P433	LYS
H285	V356	S434	MET
	R357	D435	
		P436	
L288	S360		
		E440	
L292	D366	M441	
I293	I367	R442	
R294	A368	K443	
I295	P369	V444	
T296	M370	V445	
V297	H371	C446	
T298	R372	E447	
V299	V373	Q448	
E300		K449	
G301	K376	L450	
M302	R377	R451	
I303	Y378	P452	
K304	M379	M453	
L305	A380	L454	
A306	P381	P455	
L307	E382		
S308	V383	Q459	
T309	I384	S460	
A310	D385	C461	
S311	D386	E462	
G312	S387	A463	
L313	I388	L464	
A314	M389	R465	
H315	M390	V466	
L316	K391	M467	
H317	H392	L468	
K318	F393	K469	
E319	E394	I470	
	R398	M471	
G322		R472	
T323			

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	174.86Å 248.85Å 138.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.00 – 3.35 47.69 – 3.19	Depositor EDS
% Data completeness (in resolution range)	99.8 (35.00-3.35) 98.4 (47.69-3.19)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.09 (at 3.19Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.228 , 0.271 0.212 , 0.256	Depositor DCC
R_{free} test set	2200 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	82.5	Xtriage
Anisotropy	0.285	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 71.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	13294	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% 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, 0.333 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: PO4, 55F

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	0/2668	0.62	1/3600 (0.0%)
1	B	0.46	0/2640	0.66	0/3560
1	C	0.37	0/2682	0.64	0/3622
1	D	0.44	0/2682	0.67	0/3622
1	E	0.48	0/2682	0.70	0/3622
All	All	0.42	0/13354	0.66	1/18026 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	268	LYS	N-CA-C	5.35	125.44	111.00

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	2617	0	2618	189	0
1	B	2590	0	2595	150	0
1	C	2629	0	2631	259	0
1	D	2629	0	2631	165	0
1	E	2629	0	2631	167	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	27	0	15	1	0
2	B	27	0	15	2	0
2	C	27	0	15	1	0
2	D	27	0	15	0	0
2	E	27	0	15	2	0
3	A	15	0	0	2	0
3	B	15	0	0	1	0
3	C	5	0	0	0	0
3	D	15	0	0	2	0
3	E	15	0	0	2	0
All	All	13294	0	13181	919	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 35.

The worst 5 of 919 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:417:ILE:HD11	1:D:457:ARG:HH12	1.08	1.11
1:E:367:ILE:HD13	1:E:370:ASN:HD21	1.21	1.02
1:D:367:ILE:HG13	1:D:369:PRO:HD3	1.39	1.02
1:A:417:ILE:HD11	1:A:457:ARG:HH12	1.26	0.99
1:E:256:HIS:HD2	1:E:258:ASN:H	0.99	0.98

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%)	240 (74%)	61 (19%)	23 (7%)	1	11
1	B	318/342 (93%)	259 (81%)	43 (14%)	16 (5%)	2	19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	328/342 (96%)	239 (73%)	61 (19%)	28 (8%)	1	7
1	D	328/342 (96%)	266 (81%)	51 (16%)	11 (3%)	4	29
1	E	328/342 (96%)	272 (83%)	37 (11%)	19 (6%)	2	15
All	All	1626/1710 (95%)	1276 (78%)	253 (16%)	97 (6%)	2	14

5 of 97 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	252	VAL
1	A	447	GLU
1	B	191	SER
1	B	252	VAL
1	B	386	ASP

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	281/294 (96%)	261 (93%)	20 (7%)	17	53
1	B	278/294 (95%)	252 (91%)	26 (9%)	10	36
1	C	282/294 (96%)	266 (94%)	16 (6%)	24	61
1	D	282/294 (96%)	259 (92%)	23 (8%)	13	45
1	E	282/294 (96%)	260 (92%)	22 (8%)	15	47
All	All	1405/1470 (96%)	1298 (92%)	107 (8%)	15	49

5 of 107 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	215	ARG
1	C	415	CYS
1	E	379	MET
1	C	216	PHE
1	C	268	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 53 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	453	ASN
1	D	256	HIS
1	E	425	GLN
1	C	459	GLN
1	C	494	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	$\# Z > 2$
3	PO4	A	21	-	4,4,4	1.39	0	6,6,6	0.42	0
3	PO4	A	26	-	4,4,4	1.35	0	6,6,6	0.39	0
2	55F	A	601	-	30,30,30	1.67	10 (33%)	32,43,43	1.72	6 (18%)
3	PO4	A	9	-	4,4,4	1.32	0	6,6,6	0.40	0
3	PO4	B	12	-	4,4,4	1.44	0	6,6,6	0.38	0
3	PO4	B	23	-	4,4,4	1.43	0	6,6,6	0.39	0
3	PO4	B	6	-	4,4,4	1.36	0	6,6,6	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	55F	B	601	-	30,30,30	1.67	9 (30%)	32,43,43	1.76	7 (21%)
3	PO4	C	10	-	4,4,4	1.29	0	6,6,6	0.41	0
2	55F	C	601	-	30,30,30	1.71	8 (26%)	32,43,43	1.72	7 (21%)
3	PO4	D	13	-	4,4,4	1.34	0	6,6,6	0.43	0
3	PO4	D	14	-	4,4,4	1.44	0	6,6,6	0.39	0
3	PO4	D	24	-	4,4,4	1.38	0	6,6,6	0.39	0
2	55F	D	601	-	30,30,30	1.67	7 (23%)	32,43,43	1.74	7 (21%)
3	PO4	E	1	-	4,4,4	1.38	0	6,6,6	0.41	0
3	PO4	E	2	-	4,4,4	1.39	0	6,6,6	0.41	0
3	PO4	E	22	-	4,4,4	1.37	0	6,6,6	0.42	0
2	55F	E	601	-	30,30,30	1.54	8 (26%)	32,43,43	1.71	7 (21%)

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
3	PO4	A	21	-	-	0/0/0/0	0/0/0/0
3	PO4	A	26	-	-	0/0/0/0	0/0/0/0
2	55F	A	601	-	-	0/8/12/12	0/4/4/4
3	PO4	A	9	-	-	0/0/0/0	0/0/0/0
3	PO4	B	12	-	-	0/0/0/0	0/0/0/0
3	PO4	B	23	-	-	0/0/0/0	0/0/0/0
3	PO4	B	6	-	-	0/0/0/0	0/0/0/0
2	55F	B	601	-	-	0/8/12/12	0/4/4/4
3	PO4	C	10	-	-	0/0/0/0	0/0/0/0
2	55F	C	601	-	-	0/8/12/12	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	24	-	-	0/0/0/0	0/0/0/0
2	55F	D	601	-	-	0/8/12/12	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	22	-	-	0/0/0/0	0/0/0/0
2	55F	E	601	-	-	0/8/12/12	0/4/4/4

The worst 5 of 42 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	601	55F	C14-N13	-3.67	1.28	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	601	55F	C9-C11	-2.84	1.46	1.49
2	B	601	55F	C14-N13	-2.82	1.30	1.34
2	C	601	55F	C9-C11	-2.76	1.46	1.49
2	A	601	55F	C9-C11	-2.73	1.46	1.49

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	55F	C14-N22-C25	-4.84	122.80	130.28
2	D	601	55F	C14-N22-C25	-4.74	122.95	130.28
2	C	601	55F	C14-N22-C25	-4.49	123.33	130.28
2	E	601	55F	C14-N22-C25	-4.48	123.36	130.28
2	B	601	55F	C14-N22-C25	-4.14	123.88	130.28

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	55F	1	0
3	A	9	PO4	2	0
3	B	23	PO4	1	0
2	B	601	55F	2	0
2	C	601	55F	1	0
3	D	13	PO4	2	0
3	E	2	PO4	2	0
2	E	601	55F	2	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 [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, 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%)	0.14	8 (2%) 59 60	31, 89, 131, 142	0
1	B	324/342 (94%)	-0.15	0 100 100	27, 51, 84, 105	0
1	C	330/342 (96%)	0.55	40 (12%) 5 4	28, 101, 138, 144	0
1	D	330/342 (96%)	-0.11	3 (0%) 84 86	31, 58, 97, 109	0
1	E	330/342 (96%)	-0.11	3 (0%) 84 86	26, 51, 86, 109	0
All	All	1642/1710 (96%)	0.07	54 (3%) 47 47	26, 63, 128, 144	0

The worst 5 of 54 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	491	THR	5.6
1	C	496	SER	4.9
1	C	495	LEU	4.7
1	C	322	GLY	4.4
1	E	369	PRO	4.2

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
3	PO4	D	14	5/5	0.93	0.40	4.76	21,22,22,23	5
3	PO4	D	24	5/5	0.93	0.29	2.42	29,29,31,31	5
3	PO4	B	12	5/5	0.92	0.33	2.10	20,21,22,23	5
2	55F	E	601	27/27	0.95	0.27	1.64	36,40,59,62	0
2	55F	D	601	27/27	0.96	0.26	1.32	48,49,58,61	0
3	PO4	B	23	5/5	0.93	0.25	1.31	31,31,32,32	5
3	PO4	C	10	5/5	0.88	0.30	1.30	103,104,104,105	0
3	PO4	E	2	5/5	0.95	0.29	1.22	7,8,8,9	5
2	55F	A	601	27/27	0.95	0.28	0.64	46,53,65,67	0
3	PO4	E	1	5/5	0.93	0.24	0.61	89,89,90,90	0
2	55F	B	601	27/27	0.96	0.23	0.56	29,39,49,52	0
2	55F	C	601	27/27	0.91	0.26	0.47	73,79,81,81	0
3	PO4	E	22	5/5	0.95	0.21	0.04	18,18,20,20	5
3	PO4	A	26	5/5	0.93	0.24	-0.56	48,48,48,49	5
3	PO4	A	21	5/5	0.91	0.20	-1.20	36,36,37,38	5
3	PO4	B	6	5/5	0.96	0.13	-2.05	60,63,63,65	0
3	PO4	D	13	5/5	0.95	0.12	-2.30	82,82,83,84	0
3	PO4	A	9	5/5	0.88	0.17	-	103,103,104,104	0

6.5 Other polymers ⓘ

There are no such residues in this entry.