wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 08:37 AM GMT

PDB ID	:	3FAA
Title	:	Crystal structure of TGFbRI complexed with a 2-aminoimidazole inhibitor
Authors	:	Boriack-Sjodin, P.A.; Fitch, C.
Deposited on	:	2008-11-16
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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

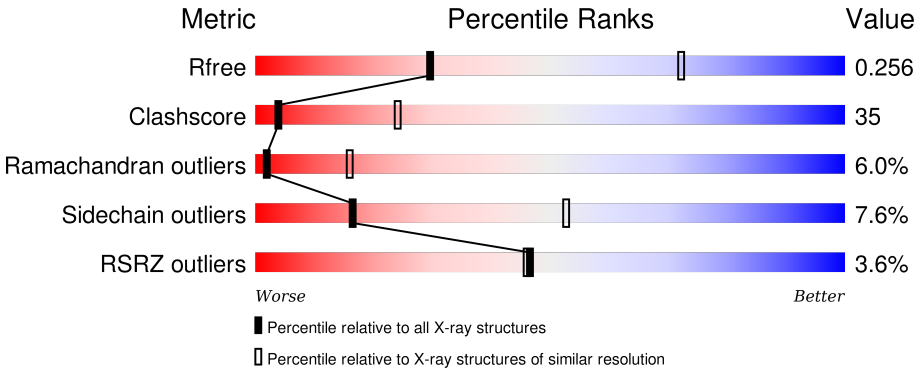
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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}	91344	1005 (3.42-3.30)
Clashscore	102246	1076 (3.42-3.30)
Ramachandran outliers	100387	1059 (3.42-3.30)
Sidechain outliers	100360	1058 (3.42-3.30)
RSRZ outliers	91569	1010 (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 <=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	3% 44% 45% 7% ·
1	B	342	50% 36% 8% 5%
1	C	342	12% 32% 56% 8% ·
1	D	342	% 45% 45% 6% ·
1	E	342	% 46% 43% 7% ·

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

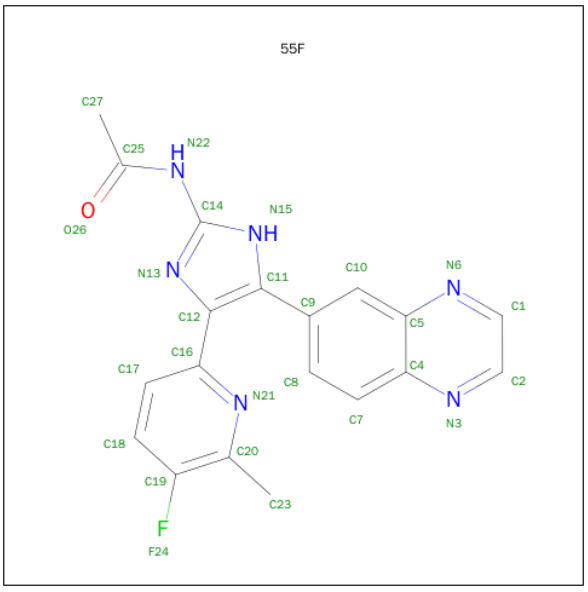
There are 3 unique types of molecules in this entry. The entry contains 13294 atoms, of which 0 are hydrogens and 0 are deuteriums.

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: $C_{19}H_{15}FN_6O$).



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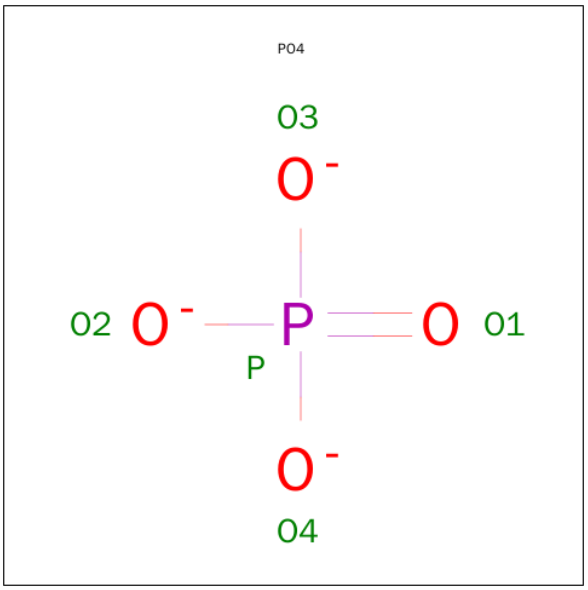
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	F	N	O	0	0
			27	19	1	6	1		
2	C	1	Total	C	F	N	O	0	0
			27	19	1	6	1		
2	D	1	Total	C	F	N	O	0	0
			27	19	1	6	1		
2	E	1	Total	C	F	N	O	0	0
			27	19	1	6	1		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

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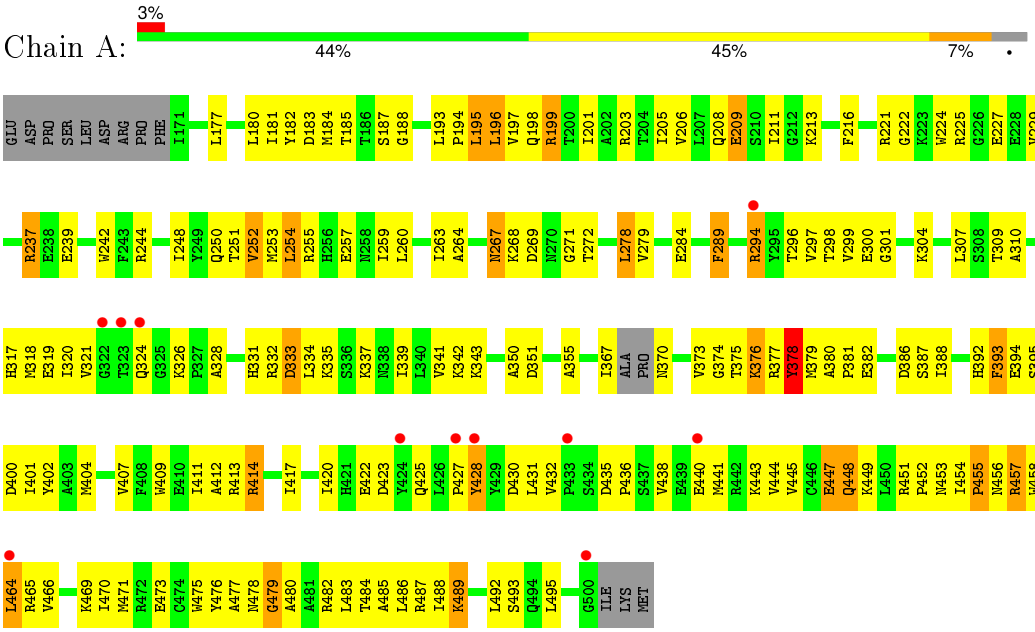
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total O P 5 4 1	0	0
3	A	1	Total O P 5 4 1	0	0
3	E	1	Total O P 5 4 1	0	0
3	B	1	Total O P 5 4 1	0	0
3	D	1	Total O P 5 4 1	0	0
3	A	1	Total O P 5 4 1	0	0

3 Residue-property plots (i)

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.

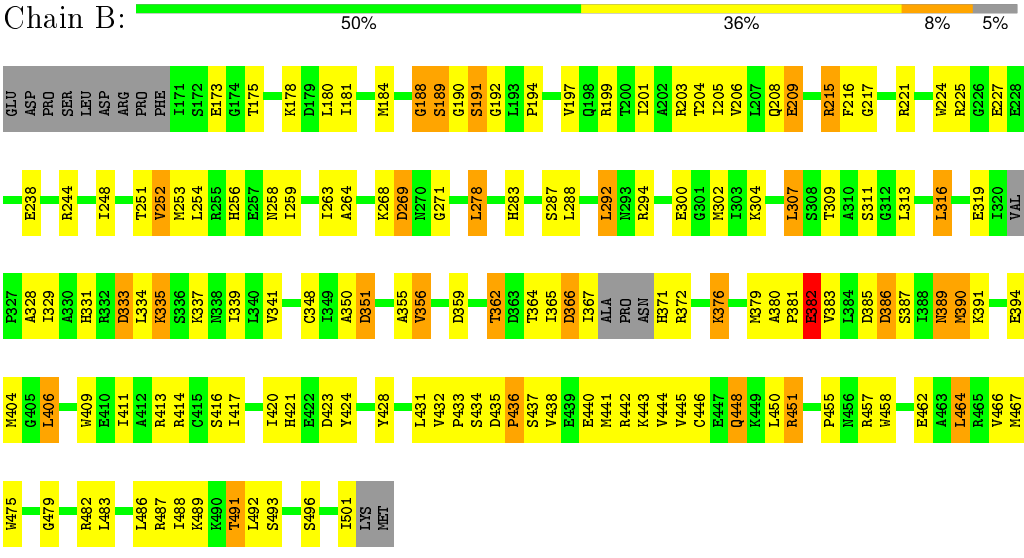
- Molecule 1: TGF-beta receptor type-1

Chain A:



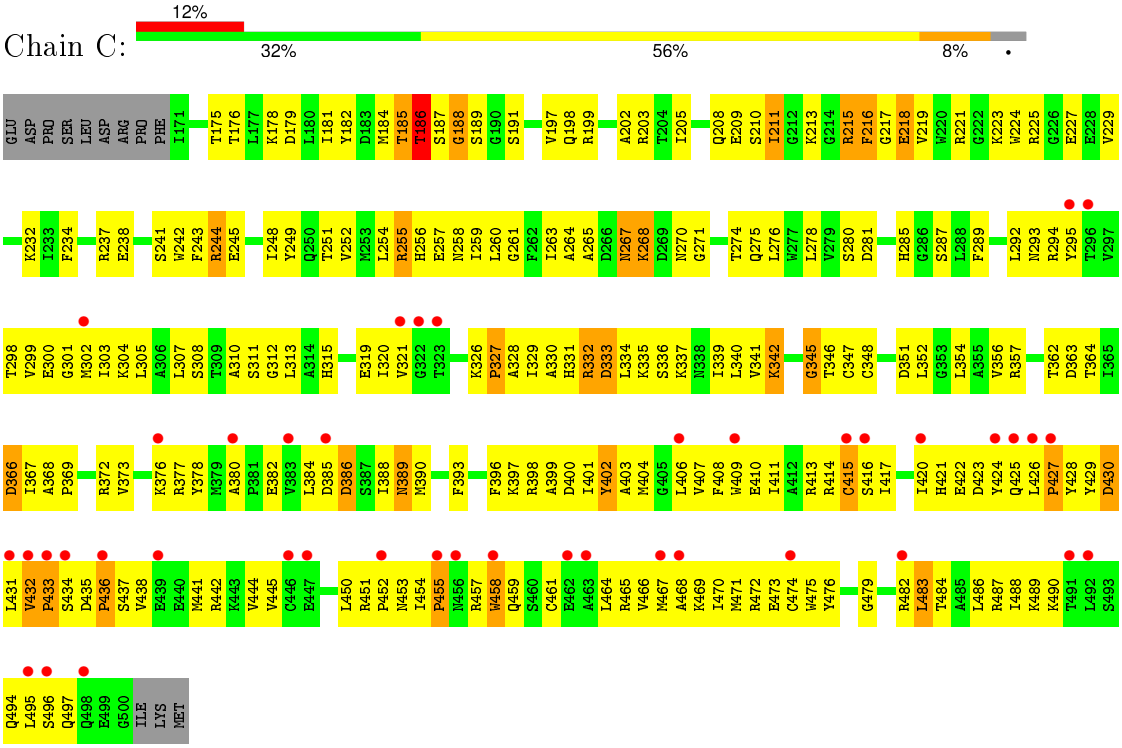
- Molecule 1: TGF-beta receptor type-1

Chain B:



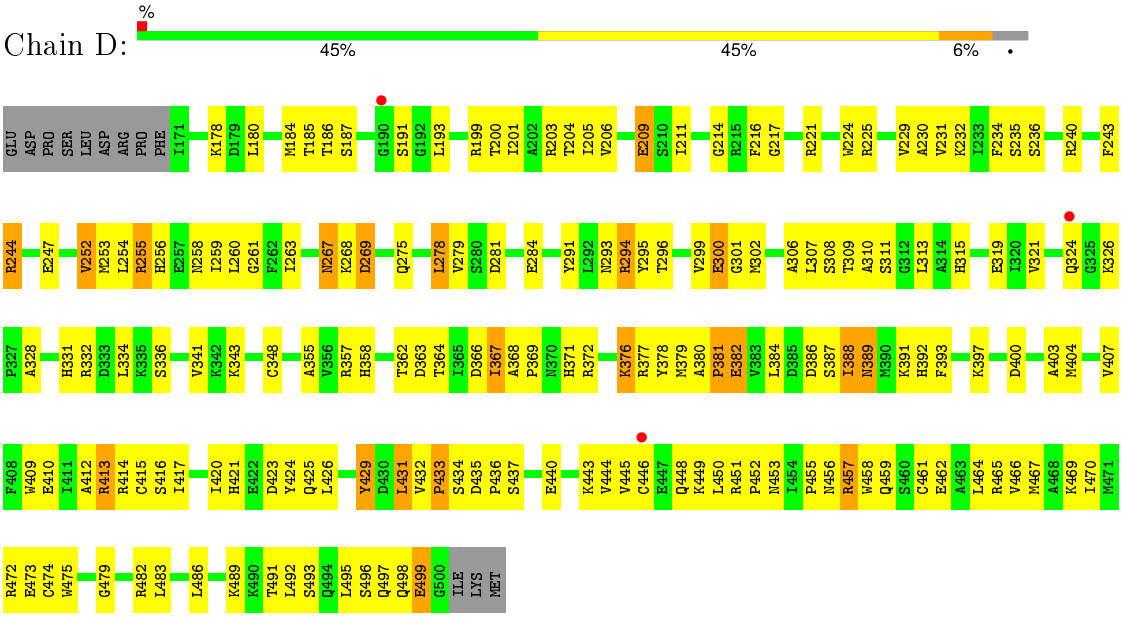
• Molecule 1: TGF-beta receptor type-1

Chain C:



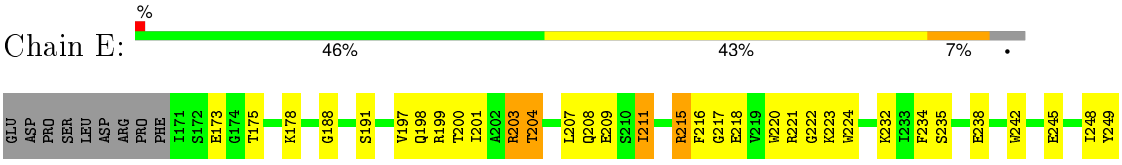
• Molecule 1: TGF-beta receptor type-1

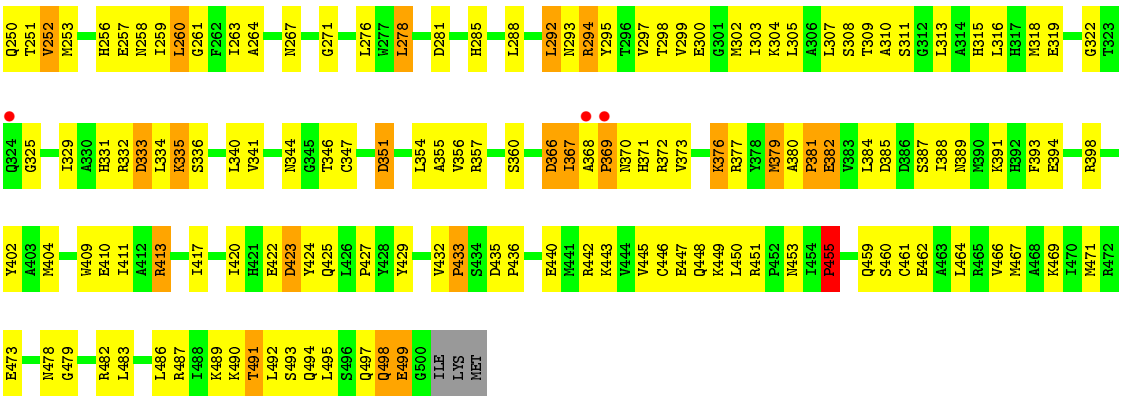
Chain D:



• Molecule 1: TGF-beta receptor type-1

Chain E:




Q250 T251 V252 M253 H256 E257 N258 I259 L260 G261 F262 I263 A264 N267 G271 L276 W277 L278 D281 H285 L288 L292 N293 R294 Y295 T296 V297 T298 V299 E300 G301 M302 I303 K304 L305 A306 L307 S308 T309 A310 S311 G312 L313 A314 H315 L316 H317 M318 E319 G322 T323
Q324 G325 I329 A330 H331 R332 D333 L334 K335 S336 L340 V341 N344 G345 T346 C347 D351 L354 A355 V356 R357 S360 D366 I367 A368 P369 N370 H371 R372 V373 K376 R377 Y378 M379 A380 P381 E382 V383 L384 D385 D386 S387 I388 N389 M390 K391 H392 F393 E394 R398
Y402 A403 M404 W409 E410 I411 A412 R413 I417 I420 H421 E422 D423 Y424 Q425 L426 P427 Y428 Y429 V432 P433 S434 D435 P436 E440 M441 R442 K443 V444 V445 C446 E447 Q448 K449 L450 R451 P452 N453 I454 P455 Q459 S460 C461 E462 A463 L464 R465 V466 M467 A468 K469 I470 M471 R472
E473 N478 G479 R482 L483 L486 R487 I488 K489 K490 T491 L492 S493 Q494 L495 S496 Q497 Q498 E499 G500 ILE LYS MET

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 49780 reflections	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: 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(^{o})	Ideal(^{o})
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

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 12
1	B	318/342 (93%)	259 (81%)	43 (14%)	16 (5%)	3 21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	328/342 (96%)	239 (73%)	61 (19%)	28 (8%)	1 8
1	D	328/342 (96%)	266 (81%)	51 (16%)	11 (3%)	5 33
1	E	328/342 (96%)	272 (83%)	37 (11%)	19 (6%)	2 17
All	All	1626/1710 (95%)	1276 (78%)	253 (16%)	97 (6%)	2 16

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 (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%)	261 (93%)	20 (7%)	18 56
1	B	278/294 (95%)	252 (91%)	26 (9%)	11 39
1	C	282/294 (96%)	266 (94%)	16 (6%)	25 64
1	D	282/294 (96%)	259 (92%)	23 (8%)	14 48
1	E	282/294 (96%)	260 (92%)	22 (8%)	16 51
All	All	1405/1470 (96%)	1298 (92%)	107 (8%)	16 53

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 (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)

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	1.15	0	6,6,6	0.27	0
3	PO4	A	26	-	4,4,4	1.13	0	6,6,6	0.27	0
2	55F	A	601	-	30,30,30	1.65	10 (33%)	30,43,43	1.63	5 (16%)
3	PO4	A	9	-	4,4,4	1.09	0	6,6,6	0.27	0
3	PO4	B	12	-	4,4,4	1.21	0	6,6,6	0.27	0
3	PO4	B	23	-	4,4,4	1.19	0	6,6,6	0.27	0
3	PO4	B	6	-	4,4,4	1.13	0	6,6,6	0.27	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	1.65	9 (30%)	30,43,43	1.70	5 (16%)
3	PO4	C	10	-	4,4,4	1.06	0	6,6,6	0.27	0
2	55F	C	601	-	30,30,30	1.71	9 (30%)	30,43,43	1.62	6 (20%)
3	PO4	D	13	-	4,4,4	1.11	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	24	-	4,4,4	1.15	0	6,6,6	0.27	0
2	55F	D	601	-	30,30,30	1.67	9 (30%)	30,43,43	1.65	6 (20%)
3	PO4	E	1	-	4,4,4	1.15	0	6,6,6	0.27	0
3	PO4	E	2	-	4,4,4	1.16	0	6,6,6	0.27	0
3	PO4	E	22	-	4,4,4	1.13	0	6,6,6	0.27	0
2	55F	E	601	-	30,30,30	1.52	9 (30%)	30,43,43	1.65	6 (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
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	-	-	0/7/12/12	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	-	-	0/7/12/12	0/4/4/4
3	PO4	C	10	-	-	0/0/0/0	0/0/0/0
2	55F	C	601	-	-	0/7/12/12	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	-	-	0/7/12/12	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	-	-	0/7/12/12	0/4/4/4

The worst 5 of 46 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	601	55F	C14-N13	-3.51	1.28	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	601	55F	C9-C11	-2.76	1.46	1.49
2	B	601	55F	C14-N13	-2.70	1.30	1.34
2	C	601	55F	C9-C11	-2.68	1.46	1.49
2	A	601	55F	C9-C11	-2.65	1.46	1.49

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	601	55F	C14-N22-C25	-4.74	122.80	130.17
2	D	601	55F	C14-N22-C25	-4.64	122.95	130.17
2	C	601	55F	C14-N22-C25	-4.39	123.33	130.17
2	E	601	55F	C14-N22-C25	-4.38	123.36	130.17
2	B	601	55F	C14-N22-C25	-4.05	123.88	130.17

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 (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^{th} 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%)	0.17	11 (3%) 49 49	31, 89, 131, 142	0
1	B	324/342 (94%)	-0.13	0 100 100	27, 51, 84, 105	0
1	C	330/342 (96%)	0.59	42 (12%) 5 4	28, 101, 138, 144	0
1	D	330/342 (96%)	-0.09	3 (0%) 85 87	31, 58, 97, 109	0
1	E	330/342 (96%)	-0.08	3 (0%) 85 87	26, 51, 86, 109	0
All	All	1642/1710 (96%)	0.09	59 (3%) 46 46	26, 63, 128, 144	0

The worst 5 of 59 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	491	THR	5.7
1	C	496	SER	5.0
1	C	495	LEU	4.8
1	C	322	GLY	4.6
1	E	369	PRO	4.3

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, 95^{th} 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 (i)

There are no such residues in this entry.