



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 16, 2016 – 08:53 AM EDT

PDB ID : 5KX8
Title : Irak4-inhibitor co-structure
Authors : Fischmann, T.O.
Deposited on : 2016-07-20
Resolution : 2.67 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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027939
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) : rb-20027939

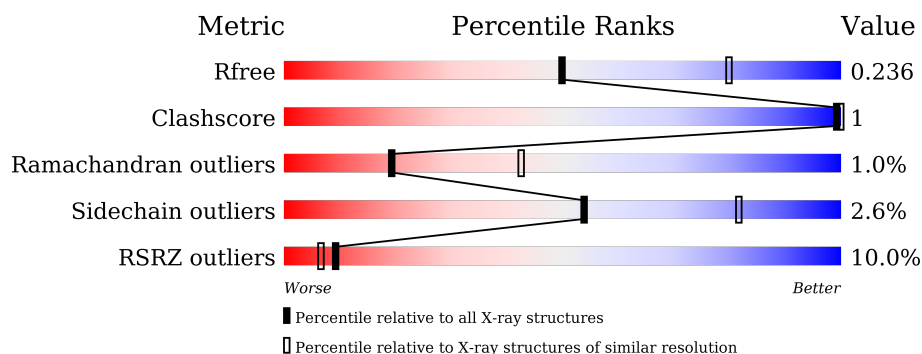
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.67 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	2780 (2.70-2.66)
Clashscore	102246	3138 (2.70-2.66)
Ramachandran outliers	100387	3089 (2.70-2.66)
Sidechain outliers	100360	3089 (2.70-2.66)
RSRZ outliers	91569	2789 (2.70-2.66)

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	301	<div> <div>15%</div> <div>92%</div> <div>• •</div> </div>
1	B	301	<div> <div>11%</div> <div>90%</div> <div>• 7%</div> </div>
1	C	301	<div> <div>5%</div> <div>91%</div> <div>5% •</div> </div>
1	D	301	<div> <div>6%</div> <div>91%</div> <div>• 5%</div> </div>

2 Entry composition [i](#)

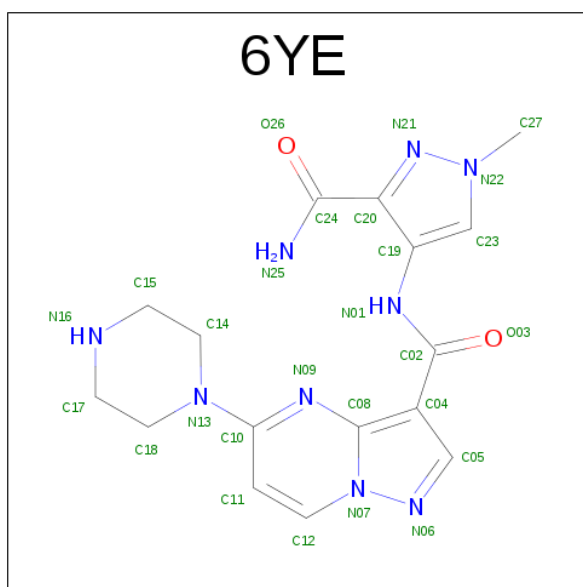
There are 3 unique types of molecules in this entry. The entry contains 9115 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Interleukin-1 receptor-associated kinase 4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	288	Total	C	N	O	P	S	0	0	3
			2262	1415	382	448	3	14			
1	B	281	Total	C	N	O	P	S	0	0	2
			2204	1381	371	435	3	14			
1	C	290	Total	C	N	O	P	S	0	0	3
			2260	1415	379	449	3	14			
1	D	286	Total	C	N	O	P	S	0	0	1
			2254	1412	380	445	3	14			

- Molecule 2 is {N}-(3-aminocarbonyl-1-methyl-pyrazol-4-yl)-5-piperazin-1-yl-pyrazolo[1,5-a]pyrimidine-3-carboxamide (three-letter code: 6YE) (formula: C₁₆H₁₉N₉O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			27	16	9	2		
2	B	1	Total	C	N	O	0	0
			27	16	9	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	0
			27	16	9	2		
2	D	1	Total	C	N	O	0	0
			27	16	9	2		

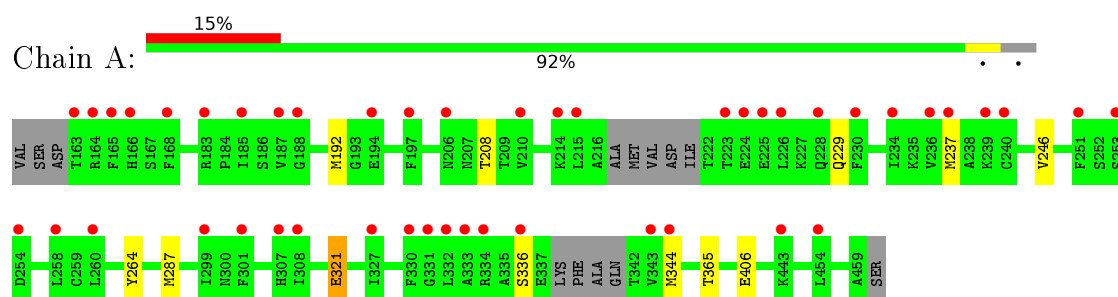
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	5	Total	O	0	0
			5	5		
3	B	5	Total	O	0	0
			5	5		
3	C	9	Total	O	0	0
			9	9		
3	D	8	Total	O	0	0
			8	8		

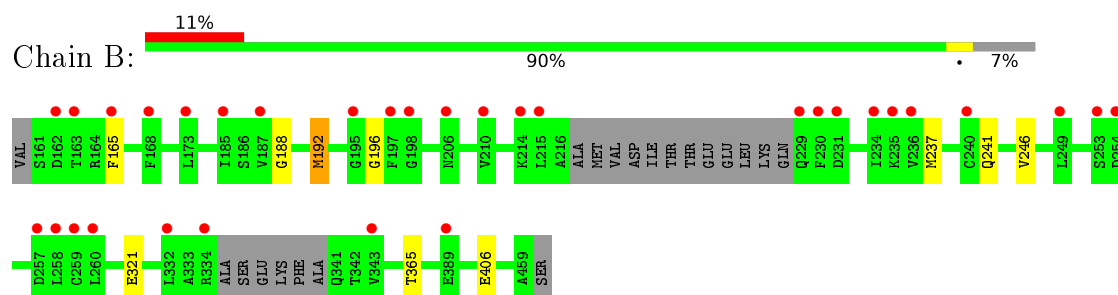
3 Residue-property plots [i](#)

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.

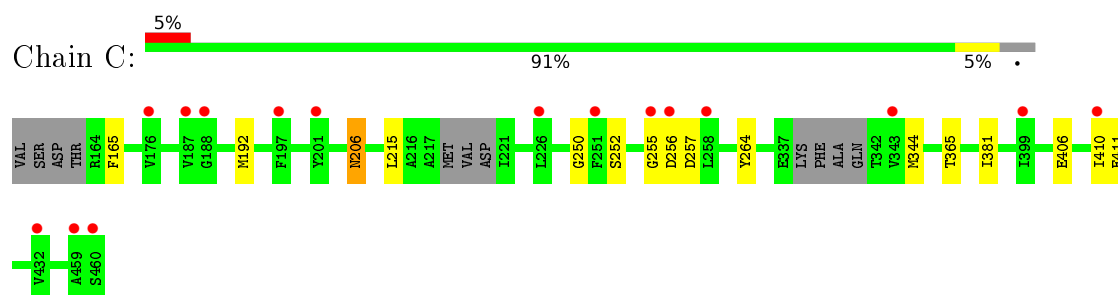
- Molecule 1: Interleukin-1 receptor-associated kinase 4



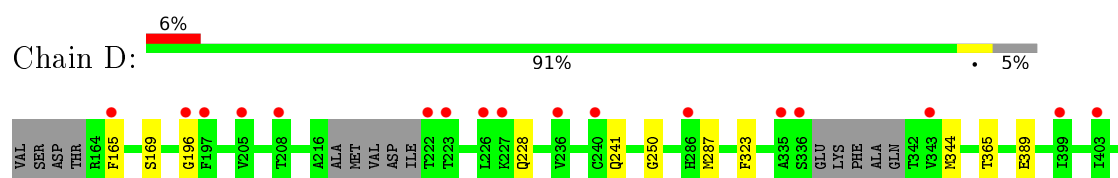
- Molecule 1: Interleukin-1 receptor-associated kinase 4

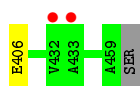


- Molecule 1: Interleukin-1 receptor-associated kinase 4



- Molecule 1: Interleukin-1 receptor-associated kinase 4





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	142.70Å 139.88Å 87.44Å 90.00° 125.25° 90.00°	Depositor
Resolution (Å)	45.00 – 2.67 45.00 – 2.67	Depositor EDS
% Data completeness (in resolution range)	99.6 (45.00-2.67) 87.8 (45.00-2.67)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.41 (at 2.69Å)	Xtriage
Refinement program	BUSTER 2.11.2	Depositor
R, R_{free}	0.204 , 0.233 0.210 , 0.236	Depositor DCC
R_{free} test set	2015 reflections (5.36%)	DCC
Wilson B-factor (Å ²)	62.4	Xtriage
Anisotropy	0.501	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 57.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.186 for -h-2*k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9115	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 20.14 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 9.2729e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: TPO, SEP, 6YE

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	0.51	0/2266	0.61	0/3053
1	B	0.51	0/2207	0.63	0/2972
1	C	0.51	0/2264	0.63	0/3051
1	D	0.53	0/2258	0.62	0/3042
All	All	0.51	0/8995	0.62	0/12118

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	2262	0	2221	2	0
1	B	2204	0	2154	2	0
1	C	2260	0	2212	3	0
1	D	2254	0	2216	3	0
2	A	27	0	0	0	0
2	B	27	0	0	1	0
2	C	27	0	0	0	0
2	D	27	0	0	0	0
3	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	5	0	0	0	0
3	C	9	0	0	0	0
3	D	8	0	0	0	0
All	All	9115	0	8803	10	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 1.

All (10) 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:287:MET:HE2	1:D:323:PHE:HB2	1.86	0.56
1:B:192:MET:HG2	2:B:501:6YE:C20	2.36	0.56
1:A:237:MET:HE1	1:A:246:VAL:HG23	1.92	0.50
1:D:287:MET:CE	1:D:323:PHE:HB2	2.40	0.50
1:B:237:MET:CE	1:B:246:VAL:HG23	2.46	0.45
1:C:165:PHE:HB3	1:C:250:GLY:HA2	2.00	0.43
1:C:381:ILE:HG21	1:C:410:ILE:HD11	2.01	0.43
1:A:192:MET:HE2	1:A:264:TYR:HE1	1.83	0.41
1:C:192:MET:HE2	1:C:264:TYR:HE1	1.85	0.41
1:D:165:PHE:HB3	1:D:250:GLY:HA2	2.04	0.40

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	280/301 (93%)	266 (95%)	12 (4%)	2 (1%)	26	53
1	B	272/301 (90%)	253 (93%)	15 (6%)	4 (2%)	13	30
1	C	282/301 (94%)	265 (94%)	14 (5%)	3 (1%)	17	40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	278/301 (92%)	265 (95%)	11 (4%)	2 (1%)	26	53
All	All	1112/1204 (92%)	1049 (94%)	52 (5%)	11 (1%)	19	42

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	406	GLU
1	B	406	GLU
1	C	406	GLU
1	D	406	GLU
1	B	321	GLU
1	C	206	ASN
1	C	255	GLY
1	D	196	GLY
1	A	321	GLU
1	B	196	GLY
1	B	188	GLY

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	247/259 (95%)	240 (97%)	7 (3%)	51	79
1	B	240/259 (93%)	236 (98%)	4 (2%)	68	89
1	C	245/259 (95%)	237 (97%)	8 (3%)	45	74
1	D	246/259 (95%)	240 (98%)	6 (2%)	57	83
All	All	978/1036 (94%)	953 (97%)	25 (3%)	54	81

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	208	THR
1	A	229	GLN
1	A	287	MET

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Mol	Chain	Res	Type
1	A	321	GLU
1	A	336	SER
1	A	344	MET
1	A	365	THR
1	B	165	PHE
1	B	192	MET
1	B	241	GLN
1	B	365	THR
1	C	206	ASN
1	C	215	LEU
1	C	252	SER
1	C	256	ASP
1	C	257	ASP
1	C	344	MET
1	C	365	THR
1	C	411	GLU
1	D	169	SER
1	D	228	GLN
1	D	241	GLN
1	D	344	MET
1	D	365	THR
1	D	389	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	229	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

12 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	TPO	A	342	1	7,10,11	0.75	0	10,14,16	1.25	1 (10%)
1	TPO	A	345	1	7,10,11	0.83	0	10,14,16	1.26	1 (10%)
1	SEP	A	346	1	7,9,10	0.95	0	8,12,14	1.22	1 (12%)
1	TPO	B	342	1	7,10,11	0.67	0	10,14,16	1.28	1 (10%)
1	TPO	B	345	1	7,10,11	0.91	0	10,14,16	1.32	1 (10%)
1	SEP	B	346	1	7,9,10	0.73	0	8,12,14	1.10	1 (12%)
1	TPO	C	342	1	7,10,11	0.74	0	10,14,16	1.29	1 (10%)
1	TPO	C	345	1	7,10,11	0.94	0	10,14,16	1.46	1 (10%)
1	SEP	C	346	1	7,9,10	1.10	0	8,12,14	0.97	0
1	TPO	D	342	1	7,10,11	0.72	0	10,14,16	1.30	2 (20%)
1	TPO	D	345	1	7,10,11	1.01	0	10,14,16	1.44	1 (10%)
1	SEP	D	346	1	7,9,10	1.14	1 (14%)	8,12,14	0.93	1 (12%)

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
1	TPO	A	342	1	-	0/8/11/13	0/0/0/0
1	TPO	A	345	1	-	1/8/11/13	0/0/0/0
1	SEP	A	346	1	-	0/5/8/10	0/0/0/0
1	TPO	B	342	1	-	0/8/11/13	0/0/0/0
1	TPO	B	345	1	-	1/8/11/13	0/0/0/0
1	SEP	B	346	1	-	0/5/8/10	0/0/0/0
1	TPO	C	342	1	-	0/8/11/13	0/0/0/0
1	TPO	C	345	1	-	1/8/11/13	0/0/0/0
1	SEP	C	346	1	-	0/5/8/10	0/0/0/0
1	TPO	D	342	1	-	0/8/11/13	0/0/0/0
1	TPO	D	345	1	-	1/8/11/13	0/0/0/0
1	SEP	D	346	1	-	0/5/8/10	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	346	SEP	P-O1P	2.10	1.57	1.50

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	346	SEP	O-C-CA	-2.50	119.01	125.72
1	D	342	TPO	O-C-CA	-2.01	120.18	125.69
1	D	346	SEP	O-C-CA	-2.01	120.32	125.72
1	A	342	TPO	O3P-P-OG1	2.27	113.42	106.62
1	D	342	TPO	O2P-P-OG1	2.28	113.44	106.62
1	B	345	TPO	O3P-P-OG1	2.29	113.47	106.62
1	B	342	TPO	O2P-P-OG1	2.29	113.47	106.62
1	A	345	TPO	O3P-P-OG1	2.33	113.60	106.62
1	A	346	SEP	OG-CB-CA	2.34	110.30	108.26
1	C	342	TPO	O3P-P-OG1	2.41	113.82	106.62
1	D	345	TPO	O3P-P-OG1	2.47	114.00	106.62
1	C	345	TPO	OG1-P-O1P	2.92	114.45	107.48

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	345	TPO	OG1-CB-CA-N
1	B	345	TPO	OG1-CB-CA-N
1	C	345	TPO	OG1-CB-CA-N
1	D	345	TPO	OG1-CB-CA-N

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

4 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	6YE	A	501	-	23,30,30	1.53	2 (8%)	23,43,43	2.35	1 (4%)
2	6YE	B	501	-	23,30,30	1.25	2 (8%)	23,43,43	1.40	5 (21%)
2	6YE	C	501	-	23,30,30	1.44	2 (8%)	23,43,43	1.34	1 (4%)
2	6YE	D	501	-	23,30,30	1.24	2 (8%)	23,43,43	2.12	3 (13%)

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	6YE	A	501	-	-	0/8/24/24	0/4/4/4
2	6YE	B	501	-	-	0/8/24/24	0/4/4/4
2	6YE	C	501	-	-	0/8/24/24	0/4/4/4
2	6YE	D	501	-	-	0/8/24/24	0/4/4/4

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	6YE	C04-C02	-2.38	1.46	1.50
2	C	501	6YE	C23-C19	2.11	1.41	1.37
2	B	501	6YE	C23-C19	2.80	1.42	1.37
2	B	501	6YE	C10-N09	3.41	1.37	1.32
2	D	501	6YE	C10-N09	3.51	1.37	1.32
2	A	501	6YE	C23-C19	4.13	1.44	1.37
2	A	501	6YE	C10-N09	4.40	1.39	1.32
2	C	501	6YE	C10-N09	5.44	1.40	1.32

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	6YE	O03-C02-C04	-3.03	117.45	121.76
2	B	501	6YE	N09-C10-N13	-2.32	114.06	116.82
2	B	501	6YE	C18-N13-C10	-2.16	115.45	120.45
2	B	501	6YE	C04-C02-N01	2.43	118.35	114.51
2	B	501	6YE	C12-C11-C10	2.49	118.40	117.42
2	B	501	6YE	C17-C18-N13	2.74	118.12	110.74
2	D	501	6YE	C04-C02-N01	3.19	119.54	114.51
2	C	501	6YE	C12-C11-C10	4.72	119.27	117.42
2	D	501	6YE	C12-C11-C10	8.23	120.65	117.42
2	A	501	6YE	C12-C11-C10	10.41	121.51	117.42

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	6YE	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	285/301 (94%)	1.07	46 (16%) 3 2	45, 86, 132, 144	0
1	B	278/301 (92%)	1.03	32 (11%) 6 5	45, 80, 137, 165	0
1	C	287/301 (95%)	0.60	16 (5%) 28 25	42, 73, 112, 123	0
1	D	283/301 (94%)	0.58	19 (6%) 21 19	43, 68, 107, 141	0
All	All	1133/1204 (94%)	0.82	113 (9%) 9 6	42, 75, 128, 165	0

All (113) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	197	PHE	13.6
1	A	240	CYS	11.6
1	B	240	CYS	10.8
1	B	230	PHE	8.8
1	A	226	LEU	7.3
1	B	236	VAL	6.2
1	C	460	SER	5.6
1	B	163	THR	5.4
1	B	215	LEU	5.4
1	B	334	ARG	5.4
1	A	185	ILE	5.3
1	A	253	SER	4.9
1	C	255	GLY	4.9
1	A	223	THR	4.7
1	C	197	PHE	4.5
1	A	332	LEU	4.5
1	A	343	VAL	4.5
1	B	332	LEU	4.4
1	D	197	PHE	4.4
1	A	164	ARG	4.3
1	B	168	PHE	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	236	VAL	4.0
1	A	188	GLY	4.0
1	B	165	PHE	3.9
1	A	230	PHE	3.8
1	B	198	GLY	3.8
1	B	343	VAL	3.7
1	C	187	VAL	3.7
1	C	343	VAL	3.7
1	A	215	LEU	3.5
1	A	254	ASP	3.5
1	A	166	HIS	3.5
1	D	165	PHE	3.5
1	B	253	SER	3.4
1	A	260	LEU	3.4
1	B	234	ILE	3.4
1	C	256	ASP	3.4
1	D	226	LEU	3.4
1	A	334	ARG	3.3
1	B	214	LYS	3.3
1	A	336	SER	3.2
1	A	299	ILE	3.2
1	B	260	LEU	3.2
1	A	251	PHE	3.2
1	A	258	LEU	3.2
1	A	197	PHE	3.2
1	B	249	LEU	3.1
1	B	195	GLY	3.1
1	B	173	LEU	3.1
1	A	234	ILE	3.0
1	B	258	LEU	3.0
1	B	257	ASP	2.9
1	A	165	PHE	2.9
1	A	239	LYS	2.9
1	D	240	CYS	2.9
1	C	251	PHE	2.8
1	D	223	THR	2.8
1	A	187	VAL	2.8
1	B	187	VAL	2.8
1	C	410	ILE	2.8
1	A	168	PHE	2.7
1	A	163	THR	2.7
1	C	188	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	206	ASN	2.7
1	C	459	ALA	2.6
1	A	210	VAL	2.6
1	A	333	ALA	2.6
1	A	301	PHE	2.6
1	D	399	ILE	2.6
1	A	237	MET	2.5
1	B	206	ASN	2.5
1	A	308	ILE	2.5
1	B	185	ILE	2.5
1	C	226	LEU	2.5
1	C	176	VAL	2.4
1	A	454	LEU	2.4
1	D	343	VAL	2.4
1	A	214	LYS	2.4
1	B	162	ASP	2.4
1	D	196	GLY	2.4
1	B	259	CYS	2.3
1	D	286	HIS	2.3
1	B	235	LYS	2.3
1	A	331	GLY	2.3
1	C	399	ILE	2.3
1	A	443	LYS	2.3
1	A	327	ILE	2.2
1	B	254	ASP	2.2
1	D	336	SER	2.2
1	A	224	GLU	2.2
1	D	433	ALA	2.1
1	B	229	GLN	2.1
1	A	194	GLU	2.1
1	B	389	GLU	2.1
1	A	330	PHE	2.1
1	B	210	VAL	2.1
1	D	403	ILE	2.1
1	C	258	LEU	2.1
1	A	228	GLN	2.1
1	D	227	LYS	2.1
1	D	335	ALA	2.1
1	A	183	ARG	2.0
1	D	208	THR	2.0
1	A	307	HIS	2.0
1	C	432	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	236	VAL	2.0
1	C	201	TYR	2.0
1	D	222	THR	2.0
1	A	344	MET	2.0
1	D	432	VAL	2.0
1	B	231	ASP	2.0
1	A	225	GLU	2.0
1	D	205	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	SEP	A	346	10/11	0.74	0.16	-	120,124,129,129	0
1	TPO	B	342	11/12	0.89	0.19	-	123,125,129,129	0
1	SEP	B	346	10/11	0.73	0.18	-	124,127,133,133	0
1	TPO	D	342	11/12	0.76	0.18	-	113,118,127,128	0
1	TPO	B	345	11/12	0.89	0.17	-	120,124,126,127	0
1	TPO	D	345	11/12	0.93	0.13	-	104,106,108,109	0
1	SEP	C	346	10/11	0.77	0.14	-	101,109,120,120	0
1	TPO	A	342	11/12	0.75	0.25	-	124,125,130,131	0
1	TPO	A	345	11/12	0.90	0.16	-	118,121,123,123	0
1	TPO	C	342	11/12	0.83	0.17	-	109,112,120,121	0
1	TPO	C	345	11/12	0.91	0.19	-	96,98,102,103	0
1	SEP	D	346	10/11	0.72	0.17	-	108,113,119,120	0

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	6YE	C	501	27/27	0.97	0.20	0.11	44,53,57,59	0
2	6YE	D	501	27/27	0.97	0.19	-0.06	34,47,55,57	0
2	6YE	B	501	27/27	0.95	0.20	-0.44	57,62,75,77	0
2	6YE	A	501	27/27	0.95	0.19	-0.50	56,66,80,82	0

6.5 Other polymers [i](#)

There are no such residues in this entry.