Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 10:25 PM GMT

PDB ID	:	4XS2
Title	:	Irak4-inhibitor co-structure
Authors	:	Fischmann, T.O.
Deposited on	:	2015-01-21
Resolution	:	2.73 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 (i) symbol.

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

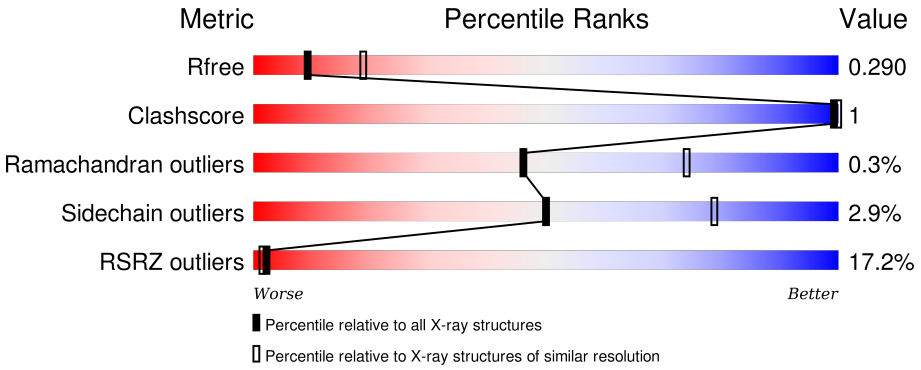
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.73 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	3050 (2.78-2.70)
Clashscore	102246	3424 (2.78-2.70)
Ramachandran outliers	100387	3367 (2.78-2.70)
Sidechain outliers	100360	3368 (2.78-2.70)
RSRZ outliers	91569	3055 (2.78-2.70)

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	301	18% 91% • 5%
1	B	301	18% 90% • 7%
1	C	301	15% 90% • 6%
1	D	301	14% 90% • 7%

2 Entry composition

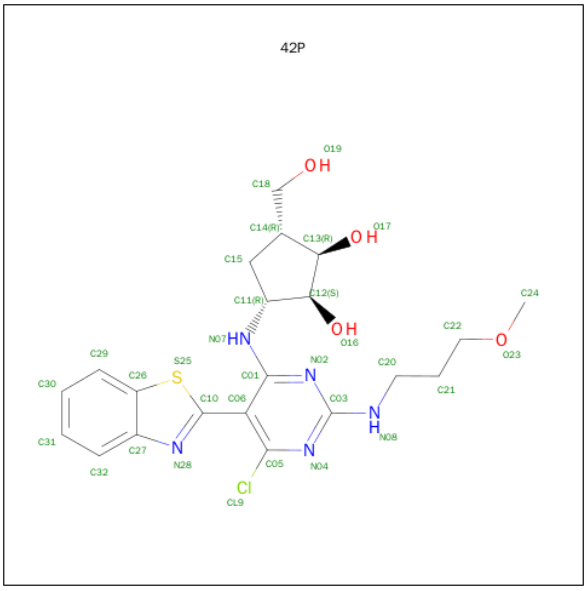
There are 3 unique types of molecules in this entry. The entry contains 9049 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	286	Total	C	N	O	P	S	0	0	4
			2244	1405	378	444	3	14			
1	B	281	Total	C	N	O	P	S	0	0	3
			2212	1387	373	435	3	14			
1	C	284	Total	C	N	O	P	S	0	0	2
			2223	1397	373	436	3	14			
1	D	280	Total	C	N	O	P	S	0	0	3
			2209	1383	374	435	3	14			

- Molecule 2 is (1R,2S,3R,5R)-3-({5-(1,3-benzothiazol-2-yl)-6-chloro-2-[(3-methoxypropyl)amino]pyrimidin-4-yl}amino)-5-(hydroxymethyl)cyclopentane-1,2-diol (three-letter code: 42P) (formula: $C_{21}H_{26}ClN_5O_4S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	S	0	0
			32	21	1	5	4	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	B	1	Total	C	Cl	N	O	S	0	0
			32	21	1	5	4	1		
2	C	1	Total	C	Cl	N	O	S	0	0
			32	21	1	5	4	1		
2	D	1	Total	C	Cl	N	O	S	0	0
			32	21	1	5	4	1		

- Molecule 3 is water.

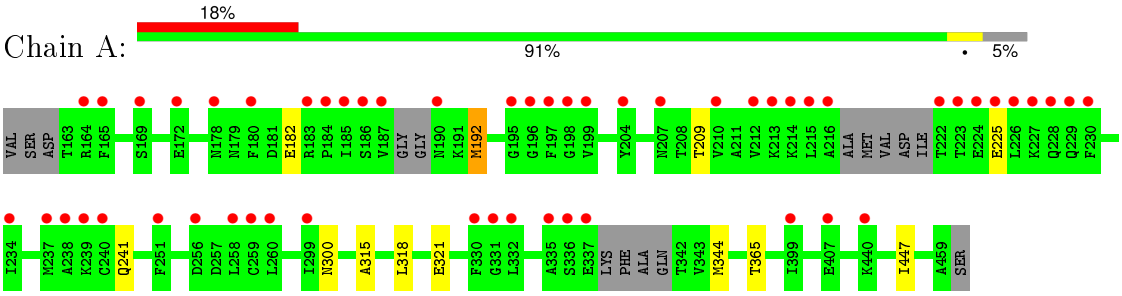
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	6	Total	O	0	0
			6	6		
3	B	7	Total	O	0	0
			7	7		
3	C	9	Total	O	0	0
			9	9		
3	D	11	Total	O	0	0
			11	11		

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.

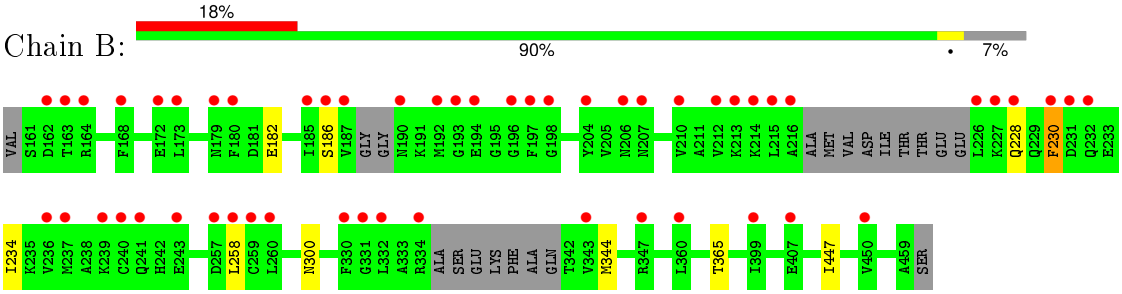
- Molecule 1: Interleukin-1 receptor-associated kinase 4

Chain A:



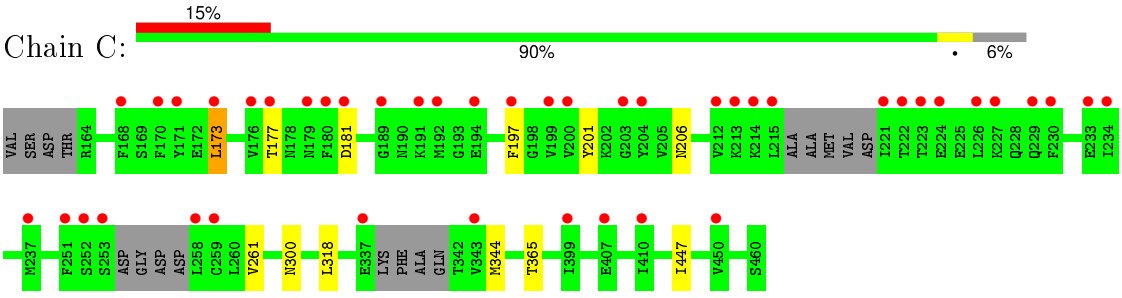
- Molecule 1: Interleukin-1 receptor-associated kinase 4

Chain B:



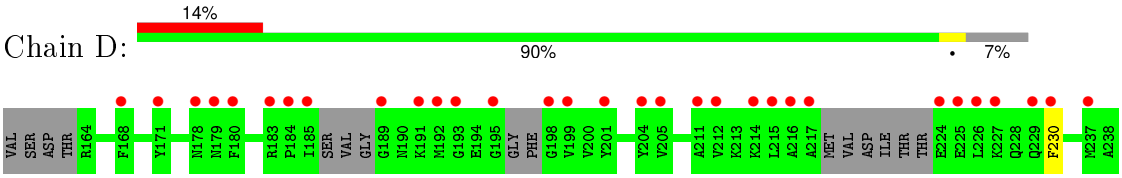
- Molecule 1: Interleukin-1 receptor-associated kinase 4

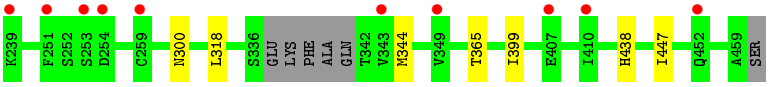
Chain C:



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

Chain D:




K239
F251
S252
S253
D254
C259
N300
L318
S336
GLU
LYS
PHE
ALA
GLN
T342
V343
M344
V349
T365
I399
E407
I410
H438
I447
Q452
A459
SER

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	143.97Å 139.99Å 87.62Å 90.00° 125.47° 90.00°	Depositor
Resolution (Å)	31.47 – 2.73 31.47 – 2.73	Depositor EDS
% Data completeness (in resolution range)	95.6 (31.47-2.73) 86.2 (31.47-2.73)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.37 (at 2.72Å)	Xtriage
Refinement program	BUSTER	Depositor
R, R_{free}	0.264 , 0.285 0.268 , 0.290	Depositor DCC
R_{free} test set	1817 reflections (5.34%)	DCC
Wilson B-factor (Å^2)	50.1	Xtriage
Anisotropy	0.539	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 38.3	EDS
Estimated twinning fraction	0.257 for -h-2*l,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Outliers	6 of 35871 reflections (0.017%)	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	9049	wwPDB-VP
Average B, all atoms (Å^2)	71.0	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 27.07 % 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 2.3486e-03.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: TPO, 42P, SEP

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	0.45	0/2247	0.56	0/3026
1	B	0.45	0/2215	0.57	0/2982
1	C	0.48	0/2226	0.58	0/2998
1	D	0.46	0/2210	0.57	0/2974
All	All	0.46	0/8898	0.57	0/11980

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

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	2244	0	2200	3	0
1	B	2212	0	2172	2	0
1	C	2223	0	2190	4	0
1	D	2209	0	2170	1	0
2	A	32	0	26	2	0
2	B	32	0	26	0	0
2	C	32	0	26	0	0
2	D	32	0	26	0	0
3	A	6	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	7	0	0	0	0
3	C	9	0	0	0	0
3	D	11	0	0	0	0
All	All	9049	0	8836	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:C:173:LEU:HD21	1:C:261:VAL:CG2	2.42	0.50
1:A:315:ALA:O	2:A:501:42P:H12	2.13	0.48
1:C:173:LEU:HD11	1:C:261:VAL:CG2	2.43	0.48
1:C:173:LEU:HD21	1:C:261:VAL:HG22	1.97	0.47
1:C:300:ASN:HA	1:C:447:ILE:HG21	1.97	0.46
1:B:230:PHE:CE1	1:B:234:ILE:HD11	2.51	0.46
1:D:300:ASN:HA	1:D:447:ILE:HG21	1.98	0.45
1:A:192:MET:HB3	2:A:501:42P:H3	1.98	0.45
1:A:300:ASN:HA	1:A:447:ILE:HG21	1.98	0.45
1:B:300:ASN:HA	1:B:447:ILE:HG21	1.97	0.44

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	276/301 (92%)	262 (95%)	14 (5%)	0	100	100
1	B	271/301 (90%)	260 (96%)	10 (4%)	1 (0%)	39	68
1	C	274/301 (91%)	258 (94%)	14 (5%)	2 (1%)	26	54

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	D	268/301 (89%)	255 (95%)	13 (5%)	0	100 100
All	All	1089/1204 (90%)	1035 (95%)	51 (5%)	3 (0%)	46 74

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	197	PHE
1	C	206	ASN
1	B	186	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	245/259 (95%)	236 (96%)	9 (4%)	41 71
1	B	242/259 (93%)	236 (98%)	6 (2%)	55 83
1	C	242/259 (93%)	235 (97%)	7 (3%)	50 79
1	D	241/259 (93%)	235 (98%)	6 (2%)	55 83
All	All	970/1036 (94%)	942 (97%)	28 (3%)	50 79

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	182	GLU
1	A	192	MET
1	A	209	THR
1	A	225	GLU
1	A	241	GLN
1	A	318	LEU
1	A	321	GLU
1	A	344	MET
1	A	365	THR
1	B	182	GLU
1	B	228	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	230	PHE
1	B	258	LEU
1	B	344	MET
1	B	365	THR
1	C	173	LEU
1	C	177	THR
1	C	181	ASP
1	C	201	TYR
1	C	318	LEU
1	C	344	MET
1	C	365	THR
1	D	230	PHE
1	D	318	LEU
1	D	344	MET
1	D	365	THR
1	D	399	ILE
1	D	438	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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	8,10,11	0.83	0	7,14,16	1.04	0
1	TPO	A	345	1	8,10,11	1.20	1 (12%)	7,14,16	1.14	0
1	SEP	A	346	1	8,9,10	0.70	0	8,12,14	1.63	3 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	TPO	B	342	1	8,10,11	0.73	0	7,14,16	0.92	0
1	TPO	B	345	1	8,10,11	1.31	1 (12%)	7,14,16	1.08	0
1	SEP	B	346	1	8,9,10	0.79	0	8,12,14	1.47	2 (25%)
1	TPO	C	342	1	8,10,11	0.78	0	7,14,16	1.01	1 (14%)
1	TPO	C	345	1	8,10,11	1.38	1 (12%)	7,14,16	1.11	0
1	SEP	C	346	1	8,9,10	0.73	0	8,12,14	1.32	1 (12%)
1	TPO	D	342	1	8,10,11	0.66	0	7,14,16	0.93	0
1	TPO	D	345	1	8,10,11	1.27	1 (12%)	7,14,16	1.43	1 (14%)
1	SEP	D	346	1	8,9,10	0.80	0	8,12,14	1.46	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	-	0/6/8/10	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	-	0/6/8/10	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	-	0/6/8/10	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	-	0/6/8/10	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	345	TPO	CB-CA	2.58	1.58	1.54
1	B	345	TPO	CB-CA	2.59	1.58	1.54
1	A	345	TPO	CB-CA	2.66	1.58	1.54
1	C	345	TPO	CB-CA	3.00	1.59	1.54

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	346	SEP	O-C-CA	-2.63	118.64	125.49
1	D	346	SEP	O-C-CA	-2.55	118.84	125.49
1	C	346	SEP	O-C-CA	-2.47	119.07	125.49
1	B	346	SEP	O-C-CA	-2.40	119.25	125.49
1	C	342	TPO	O-C-CA	-2.01	120.14	125.44
1	A	346	SEP	O3P-P-OG	2.12	112.67	106.56
1	B	346	SEP	OG-P-O1P	2.14	112.58	107.14
1	A	346	SEP	OG-CB-CA	2.23	110.17	108.27
1	D	345	TPO	OG1-P-O1P	2.79	114.07	107.11

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	345	TPO	OG1-CB-CA-N
1	C	345	TPO	OG1-CB-CA-N
1	A	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	42P	A	501	-	33,35,35	2.55	11 (33%)	31,49,49	3.21	10 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	42P	B	501	-	33,35,35	2.49	10 (30%)	31,49,49	2.73	10 (32%)
2	42P	C	501	-	33,35,35	1.96	8 (24%)	31,49,49	2.83	10 (32%)
2	42P	D	501	-	33,35,35	2.18	9 (27%)	31,49,49	2.65	9 (29%)

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	42P	A	501	-	-	0/12/32/32	0/4/4/4
2	42P	B	501	-	-	0/12/32/32	0/4/4/4
2	42P	C	501	-	-	0/12/32/32	0/4/4/4
2	42P	D	501	-	-	0/12/32/32	0/4/4/4

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	42P	C32-C27	2.08	1.45	1.41
2	B	501	42P	C01-N02	2.09	1.38	1.34
2	D	501	42P	C31-C30	2.10	1.43	1.38
2	D	501	42P	C01-N02	2.18	1.38	1.34
2	C	501	42P	C03-N08	2.22	1.38	1.34
2	D	501	42P	C31-C32	2.27	1.41	1.36
2	A	501	42P	C12-C11	2.30	1.55	1.53
2	D	501	42P	C03-N08	2.37	1.38	1.34
2	B	501	42P	C03-N08	2.37	1.38	1.34
2	B	501	42P	O17-C13	2.45	1.48	1.43
2	D	501	42P	C30-C29	2.47	1.42	1.36
2	A	501	42P	C06-C01	2.59	1.48	1.42
2	C	501	42P	C01-N02	2.66	1.39	1.34
2	B	501	42P	C10-N28	2.70	1.35	1.31
2	A	501	42P	C01-N02	2.70	1.39	1.34
2	C	501	42P	C31-C32	2.73	1.42	1.36
2	C	501	42P	C30-C29	2.76	1.43	1.36
2	B	501	42P	C12-C11	2.77	1.56	1.53
2	C	501	42P	C10-N28	2.81	1.35	1.31
2	D	501	42P	C10-S25	2.82	1.77	1.73
2	A	501	42P	C10-N28	2.94	1.35	1.31
2	B	501	42P	C29-C26	2.96	1.43	1.40
2	A	501	42P	C31-C32	3.05	1.43	1.36
2	D	501	42P	C10-N28	3.05	1.35	1.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	42P	C30-C29	3.13	1.43	1.36
2	B	501	42P	C30-C29	3.14	1.43	1.36
2	C	501	42P	C10-S25	3.22	1.78	1.73
2	C	501	42P	C05-N04	3.27	1.37	1.32
2	A	501	42P	C29-C26	3.30	1.43	1.40
2	A	501	42P	C05-N04	3.35	1.37	1.32
2	B	501	42P	C31-C32	3.39	1.44	1.36
2	A	501	42P	C10-S25	3.43	1.78	1.73
2	D	501	42P	C05-N04	3.66	1.38	1.32
2	B	501	42P	C05-N04	4.33	1.39	1.32
2	C	501	42P	C05-C06	7.33	1.45	1.39
2	D	501	42P	C05-C06	9.13	1.47	1.39
2	B	501	42P	C05-C06	10.33	1.48	1.39
2	A	501	42P	C05-C06	10.34	1.48	1.39

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501	42P	CL9-C05-N04	-4.12	108.15	115.45
2	C	501	42P	CL9-C05-N04	-3.91	108.54	115.45
2	B	501	42P	CL9-C05-N04	-3.49	109.28	115.45
2	D	501	42P	CL9-C05-N04	-3.33	109.56	115.45
2	B	501	42P	C05-C06-C01	-3.11	110.78	113.35
2	C	501	42P	C05-C06-C01	-3.10	110.79	113.35
2	D	501	42P	C15-C11-N07	-2.35	109.45	112.63
2	C	501	42P	C12-C11-N07	-2.14	108.27	112.57
2	D	501	42P	C05-C06-C01	-2.12	111.60	113.35
2	A	501	42P	C13-C12-C11	2.02	106.54	103.17
2	B	501	42P	C14-C15-C11	2.04	105.65	103.49
2	B	501	42P	C03-N02-C01	2.08	121.19	116.92
2	A	501	42P	C15-C14-C13	2.10	107.32	102.24
2	B	501	42P	C20-N08-C03	2.17	127.90	123.80
2	D	501	42P	C15-C14-C13	2.21	107.56	102.24
2	A	501	42P	C14-C13-C12	2.26	105.59	103.50
2	C	501	42P	C05-N04-C03	2.30	118.49	115.28
2	A	501	42P	C05-N04-C03	2.47	118.73	115.28
2	D	501	42P	C26-C27-N28	2.56	114.09	108.16
2	C	501	42P	C14-C15-C11	2.60	106.24	103.49
2	A	501	42P	C26-C27-N28	2.64	114.27	108.16
2	B	501	42P	C26-C27-N28	2.68	114.38	108.16
2	C	501	42P	C26-C27-N28	2.71	114.44	108.16
2	B	501	42P	C15-C14-C13	2.82	109.05	102.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	501	42P	C13-C12-C11	3.16	108.46	103.17
2	C	501	42P	C14-C13-C12	3.25	106.50	103.50
2	A	501	42P	C20-N08-C03	3.43	130.28	123.80
2	D	501	42P	C14-C15-C11	3.45	107.14	103.49
2	A	501	42P	C14-C15-C11	3.55	107.25	103.49
2	D	501	42P	C14-C13-C12	3.90	107.10	103.50
2	C	501	42P	C20-N08-C03	4.02	131.40	123.80
2	C	501	42P	C10-N28-C27	5.20	114.04	103.83
2	B	501	42P	C10-N28-C27	5.26	114.14	103.83
2	D	501	42P	C10-N28-C27	5.45	114.52	103.83
2	A	501	42P	C10-N28-C27	5.49	114.60	103.83
2	D	501	42P	C06-C05-CL9	10.44	126.29	119.31
2	B	501	42P	C06-C05-CL9	11.17	126.78	119.31
2	C	501	42P	C06-C05-CL9	11.54	127.03	119.31
2	A	501	42P	C06-C05-CL9	14.38	128.92	119.31

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	42P	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	283/301 (94%)	1.30	54 (19%)	2 1	31, 69, 135, 154	0
1	B	278/301 (92%)	1.15	53 (19%)	2 1	28, 61, 137, 166	0
1	C	281/301 (93%)	0.94	44 (15%)	3 2	27, 59, 115, 138	0
1	D	277/301 (92%)	0.89	41 (14%)	3 2	26, 58, 124, 142	0
All	All	1119/1204 (92%)	1.07	192 (17%)	2 1	26, 62, 129, 166	0

All (192) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	216	ALA	13.0
1	A	226	LEU	12.2
1	A	195	GLY	11.5
1	B	226	LEU	10.5
1	A	240	CYS	10.4
1	B	227	LYS	9.9
1	D	217	ALA	8.5
1	A	223	THR	8.2
1	B	230	PHE	8.2
1	B	237	MET	8.1
1	B	240	CYS	8.1
1	D	230	PHE	8.0
1	A	230	PHE	7.8
1	A	237	MET	7.0
1	A	215	LEU	6.7
1	B	197	PHE	6.7
1	A	197	PHE	6.3
1	A	204	TYR	6.2
1	C	223	THR	6.2
1	B	207	ASN	6.1
1	C	258	LEU	6.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	207	ASN	6.1
1	D	216	ALA	5.9
1	C	230	PHE	5.9
1	A	185	ILE	5.8
1	C	197	PHE	5.7
1	B	204	TYR	5.6
1	D	193	GLY	5.5
1	A	251	PHE	5.5
1	C	214	LYS	5.4
1	B	173	LEU	5.4
1	B	163	THR	5.4
1	C	215	LEU	5.2
1	C	180	PHE	5.2
1	A	336	SER	5.2
1	D	184	PRO	5.2
1	A	164	ARG	5.2
1	A	198	GLY	5.1
1	A	239	LYS	5.1
1	A	186	SER	5.1
1	B	215	LEU	5.1
1	A	337	GLU	5.1
1	B	185	ILE	5.0
1	B	330	PHE	5.0
1	A	229	GLN	5.0
1	D	168	PHE	5.0
1	D	224	GLU	4.9
1	A	225	GLU	4.8
1	C	213	LYS	4.8
1	C	221	ILE	4.8
1	C	194	GLU	4.7
1	A	187	VAL	4.7
1	B	216	ALA	4.5
1	B	260	LEU	4.5
1	A	228	GLN	4.4
1	C	259	CYS	4.4
1	B	164	ARG	4.4
1	D	227	LYS	4.4
1	B	214	LYS	4.4
1	B	334	ARG	4.3
1	D	189	GLY	4.3
1	A	165	PHE	4.3
1	A	180	PHE	4.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	198	GLY	4.1
1	C	203	GLY	4.1
1	C	181	ASP	4.1
1	B	187	VAL	4.0
1	D	192	MET	4.0
1	A	190	ASN	3.9
1	C	179	ASN	3.9
1	A	196	GLY	3.9
1	A	184	PRO	3.9
1	C	212	VAL	3.8
1	D	185	ILE	3.8
1	D	407	GLU	3.7
1	C	173	LEU	3.7
1	D	178	ASN	3.7
1	C	226	LEU	3.7
1	A	224	GLU	3.7
1	C	251	PHE	3.7
1	A	227	LYS	3.6
1	B	179	ASN	3.6
1	B	259	CYS	3.6
1	D	191	LYS	3.6
1	C	229	GLN	3.5
1	A	259	CYS	3.5
1	D	343	VAL	3.5
1	A	222	THR	3.5
1	B	347	ARG	3.4
1	D	215	LEU	3.4
1	B	407	GLU	3.4
1	C	176	VAL	3.4
1	B	186	SER	3.4
1	B	399	ILE	3.3
1	C	191	LYS	3.3
1	B	228	GLN	3.3
1	B	193	GLY	3.2
1	D	171	TYR	3.2
1	C	227	LYS	3.2
1	A	183	ARG	3.1
1	D	211	ALA	3.1
1	B	190	ASN	3.1
1	A	260	LEU	3.1
1	A	212	VAL	3.1
1	B	231	ASP	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	343	VAL	3.0
1	B	258	LEU	3.0
1	D	254	ASP	2.9
1	B	213	LYS	2.9
1	D	259	CYS	2.9
1	C	177	THR	2.9
1	D	239	LYS	2.9
1	B	212	VAL	2.9
1	D	183	ARG	2.9
1	C	222	THR	2.8
1	B	168	PHE	2.8
1	A	178	ASN	2.8
1	C	233	GLU	2.8
1	C	337	GLU	2.8
1	D	226	LEU	2.8
1	D	349	VAL	2.8
1	D	253	SER	2.7
1	A	399	ILE	2.7
1	A	234	ILE	2.7
1	C	171	TYR	2.7
1	D	229	GLN	2.7
1	B	450	VAL	2.7
1	C	200	VAL	2.7
1	B	239	LYS	2.7
1	C	253	SER	2.7
1	C	199	VAL	2.6
1	C	399	ILE	2.6
1	C	204	TYR	2.6
1	A	213	LYS	2.6
1	A	330	PHE	2.6
1	D	212	VAL	2.6
1	A	256	ASP	2.6
1	C	410	ILE	2.6
1	A	407	GLU	2.6
1	D	204	TYR	2.6
1	A	331	GLY	2.5
1	B	331	GLY	2.5
1	D	179	ASN	2.5
1	D	180	PHE	2.5
1	D	201	TYR	2.5
1	C	168	PHE	2.5
1	C	170	PHE	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	192	MET	2.5
1	C	252	SER	2.5
1	B	162	ASP	2.5
1	B	332	LEU	2.4
1	A	210	VAL	2.4
1	A	299	ILE	2.4
1	B	210	VAL	2.4
1	A	258	LEU	2.4
1	D	251	PHE	2.4
1	C	224	GLU	2.4
1	B	172	GLU	2.4
1	A	214	LYS	2.4
1	A	440	LYS	2.4
1	C	343	VAL	2.3
1	C	407	GLU	2.3
1	B	180	PHE	2.3
1	B	241	GLN	2.3
1	D	452	GLN	2.3
1	C	189	GLY	2.3
1	A	172	GLU	2.2
1	B	360	LEU	2.2
1	B	196	GLY	2.2
1	B	232	GLN	2.2
1	C	450	VAL	2.2
1	B	257	ASP	2.2
1	B	194	GLU	2.2
1	D	225	GLU	2.2
1	B	192	MET	2.2
1	D	214	LYS	2.1
1	D	199	VAL	2.1
1	B	236	VAL	2.1
1	D	195	GLY	2.1
1	C	234	ILE	2.1
1	C	237	MET	2.1
1	A	335	ALA	2.1
1	D	205	VAL	2.1
1	D	237	MET	2.1
1	A	169	SER	2.1
1	A	332	LEU	2.0
1	B	206	ASN	2.0
1	D	410	ILE	2.0
1	D	198	GLY	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	238	ALA	2.0
1	B	243	GLU	2.0
1	A	199	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, 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
1	SEP	A	346	10/11	0.77	0.16	-	100,102,106,107	0
1	TPO	C	342	11/12	0.70	0.23	-	99,100,105,105	0
1	TPO	B	342	11/12	0.81	0.21	-	98,100,102,102	0
1	SEP	D	346	10/11	0.81	0.17	-	87,91,97,97	0
1	TPO	D	342	11/12	0.70	0.22	-	94,96,101,101	0
1	TPO	C	345	11/12	0.88	0.19	-	89,90,93,94	0
1	SEP	B	346	10/11	0.77	0.18	-	98,100,104,104	0
1	TPO	A	345	11/12	0.77	0.16	-	100,101,102,103	0
1	TPO	D	345	11/12	0.89	0.16	-	87,88,91,91	0
1	TPO	B	345	11/12	0.79	0.20	-	96,99,100,100	0
1	SEP	C	346	10/11	0.68	0.23	-	91,94,99,100	0
1	TPO	A	342	11/12	0.76	0.23	-	109,111,113,113	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, 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
2	42P	C	501	32/32	0.81	0.30	0.57	99,108,112,114	0
2	42P	D	501	32/32	0.82	0.29	0.51	85,88,90,91	0
2	42P	A	501	32/32	0.76	0.31	0.19	94,98,101,102	0
2	42P	B	501	32/32	0.84	0.23	-0.14	69,73,82,85	0

6.5 Other polymers (i)

There are no such residues in this entry.