



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 10:30 pm GMT

PDB ID : 4J99  
Title : Crystal Structure of FGF Receptor 2 (FGFR2) Kinase Domain Harboring the Gain-of-Function K659T Mutation.  
Authors : Chen, H.; Mohammadi, M.  
Deposited on : 2013-02-15  
Resolution : 1.85 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](mailto: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.

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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 : trunk28620  
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) : recalc28949

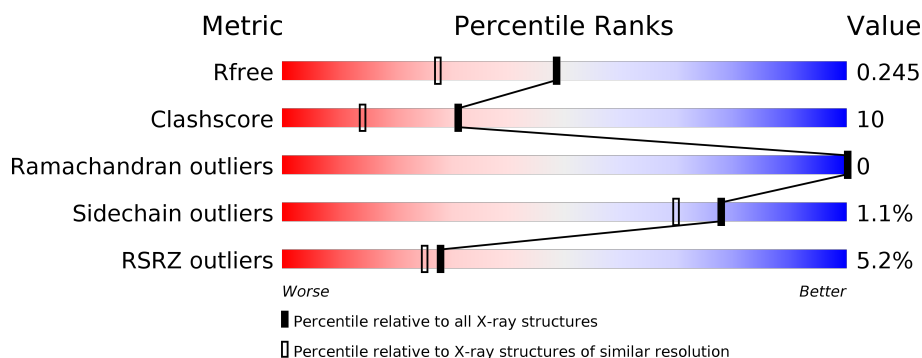
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.85 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	2964 (1.86-1.82)
Clashscore	112137	3197 (1.86-1.82)
Ramachandran outliers	110173	3164 (1.86-1.82)
Sidechain outliers	110143	3165 (1.86-1.82)
RSRZ outliers	101464	2973 (1.86-1.82)

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  $\geq 3$ , 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	324	<div> <div>3%</div> <div> <div></div> <div>75%</div> <div>11%</div> <div>14%</div> </div> </div>
1	B	324	<div> <div>3%</div> <div> <div></div> <div>77%</div> <div>12%</div> <div>10%</div> </div> </div>
1	C	324	<div> <div>7%</div> <div> <div></div> <div>80%</div> <div>9%</div> <div>10%</div> </div> </div>
1	D	324	<div> <div>6%</div> <div> <div></div> <div>71%</div> <div>15%</div> <div>13%</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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	C	804	-	-	-	X
4	MG	C	803	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9814 atoms, of which 68 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 Fibroblast growth factor receptor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	280	Total	C	N	O	S	0	4	0
			2241	1434	374	412	21			
1	B	291	Total	C	N	O	S	0	5	0
			2320	1481	385	431	23			
1	C	291	Total	C	N	O	S	0	5	0
			2309	1473	384	429	23			
1	D	281	Total	C	N	O	S	0	2	0
			2229	1425	373	410	21			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	445	MET	-	EXPRESSION TAG	UNP P21802
A	446	GLY	-	EXPRESSION TAG	UNP P21802
A	447	SER	-	EXPRESSION TAG	UNP P21802
A	448	SER	-	EXPRESSION TAG	UNP P21802
A	449	HIS	-	EXPRESSION TAG	UNP P21802
A	450	HIS	-	EXPRESSION TAG	UNP P21802
A	451	HIS	-	EXPRESSION TAG	UNP P21802
A	452	HIS	-	EXPRESSION TAG	UNP P21802
A	453	HIS	-	EXPRESSION TAG	UNP P21802
A	454	HIS	-	EXPRESSION TAG	UNP P21802
A	455	SER	-	EXPRESSION TAG	UNP P21802
A	456	GLN	-	EXPRESSION TAG	UNP P21802
A	457	ASP	-	EXPRESSION TAG	UNP P21802
A	491	ALA	CYS	ENGINEERED MUTATION	UNP P21802
A	659	THR	LYS	ENGINEERED MUTATION	UNP P21802
B	445	MET	-	EXPRESSION TAG	UNP P21802
B	446	GLY	-	EXPRESSION TAG	UNP P21802
B	447	SER	-	EXPRESSION TAG	UNP P21802
B	448	SER	-	EXPRESSION TAG	UNP P21802
B	449	HIS	-	EXPRESSION TAG	UNP P21802
B	450	HIS	-	EXPRESSION TAG	UNP P21802

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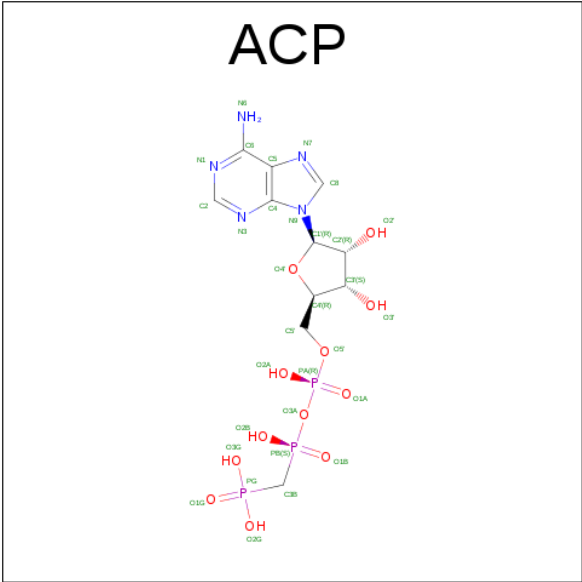
Chain	Residue	Modelled	Actual	Comment	Reference
B	451	HIS	-	EXPRESSION TAG	UNP P21802
B	452	HIS	-	EXPRESSION TAG	UNP P21802
B	453	HIS	-	EXPRESSION TAG	UNP P21802
B	454	HIS	-	EXPRESSION TAG	UNP P21802
B	455	SER	-	EXPRESSION TAG	UNP P21802
B	456	GLN	-	EXPRESSION TAG	UNP P21802
B	457	ASP	-	EXPRESSION TAG	UNP P21802
B	491	ALA	CYS	ENGINEERED MUTATION	UNP P21802
B	659	THR	LYS	ENGINEERED MUTATION	UNP P21802
C	445	MET	-	EXPRESSION TAG	UNP P21802
C	446	GLY	-	EXPRESSION TAG	UNP P21802
C	447	SER	-	EXPRESSION TAG	UNP P21802
C	448	SER	-	EXPRESSION TAG	UNP P21802
C	449	HIS	-	EXPRESSION TAG	UNP P21802
C	450	HIS	-	EXPRESSION TAG	UNP P21802
C	451	HIS	-	EXPRESSION TAG	UNP P21802
C	452	HIS	-	EXPRESSION TAG	UNP P21802
C	453	HIS	-	EXPRESSION TAG	UNP P21802
C	454	HIS	-	EXPRESSION TAG	UNP P21802
C	455	SER	-	EXPRESSION TAG	UNP P21802
C	456	GLN	-	EXPRESSION TAG	UNP P21802
C	457	ASP	-	EXPRESSION TAG	UNP P21802
C	491	ALA	CYS	ENGINEERED MUTATION	UNP P21802
C	659	THR	LYS	ENGINEERED MUTATION	UNP P21802
D	445	MET	-	EXPRESSION TAG	UNP P21802
D	446	GLY	-	EXPRESSION TAG	UNP P21802
D	447	SER	-	EXPRESSION TAG	UNP P21802
D	448	SER	-	EXPRESSION TAG	UNP P21802
D	449	HIS	-	EXPRESSION TAG	UNP P21802
D	450	HIS	-	EXPRESSION TAG	UNP P21802
D	451	HIS	-	EXPRESSION TAG	UNP P21802
D	452	HIS	-	EXPRESSION TAG	UNP P21802
D	453	HIS	-	EXPRESSION TAG	UNP P21802
D	454	HIS	-	EXPRESSION TAG	UNP P21802
D	455	SER	-	EXPRESSION TAG	UNP P21802
D	456	GLN	-	EXPRESSION TAG	UNP P21802
D	457	ASP	-	EXPRESSION TAG	UNP P21802
D	491	ALA	CYS	ENGINEERED MUTATION	UNP P21802
D	659	THR	LYS	ENGINEERED MUTATION	UNP P21802

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula:  $C_{11}H_{18}N_5O_{12}P_3$ ).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	P	0	0
			48	11	17	5	12	3		
3	B	1	Total	C	H	N	O	P	0	0
			48	11	17	5	12	3		
3	C	1	Total	C	H	N	O	P	0	0
			48	11	17	5	12	3		
3	D	1	Total	C	H	N	O	P	0	0
			48	11	17	5	12	3		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	2	Total	Mg	0	0
			2	2		
4	C	1	Total	Mg	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	116	Total	O	0	0
			116	116		
5	B	168	Total	O	0	0
			168	168		
5	C	117	Total	O	0	0
			117	117		

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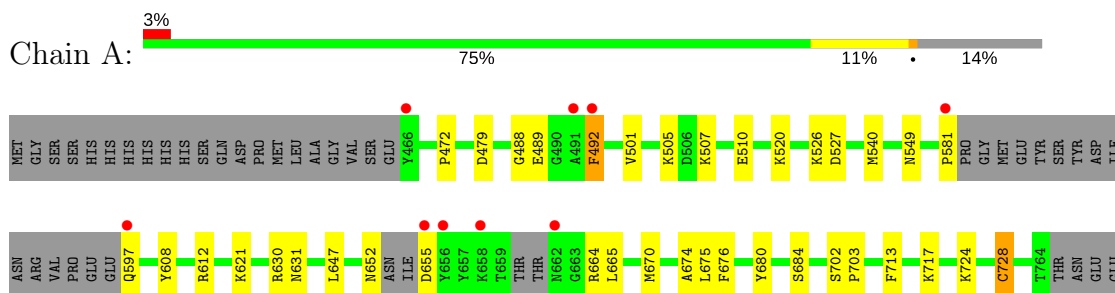
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	84	Total	O	0	0
			84	84		



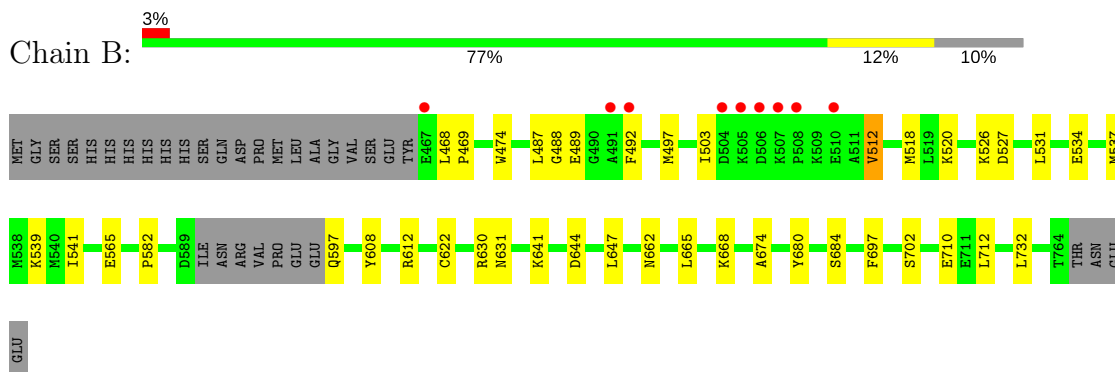
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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 ( $RSRZ > 2$ ). 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.

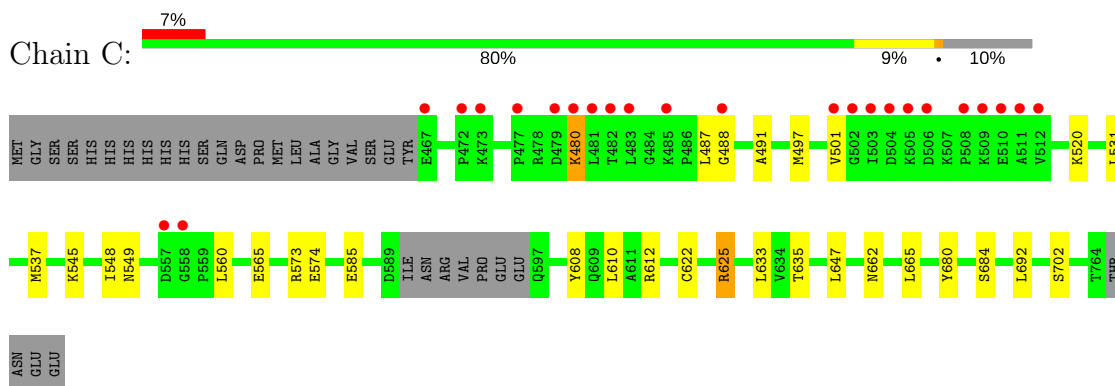
#### • Molecule 1: Fibroblast growth factor receptor 2



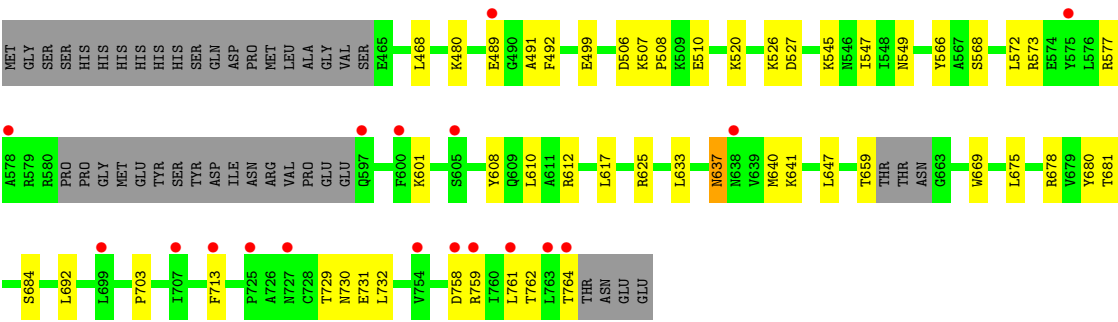
#### • Molecule 1: Fibroblast growth factor receptor 2



#### • Molecule 1: Fibroblast growth factor receptor 2



#### • Molecule 1: Fibroblast growth factor receptor 2



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	278.51Å 78.39Å 73.20Å 90.00° 101.02° 90.00°	Depositor
Resolution (Å)	42.31 – 1.85 42.31 – 1.85	Depositor EDS
% Data completeness (in resolution range)	96.3 (42.31-1.85) 93.1 (42.31-1.85)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.03	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.81 (at 1.84Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, $R_{free}$	0.206 , 0.240 0.209 , 0.245	Depositor DCC
$R_{free}$ test set	1993 reflections (1.64%)	DCC
Wilson B-factor (Å <sup>2</sup> )	27.7	Xtriage
Anisotropy	0.176	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 51.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	9814	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.72% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>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: MG, ACP, SO4

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	0.50	1/2297 (0.0%)	0.63	0/3104
1	B	0.49	0/2386	0.64	0/3232
1	C	0.43	0/2374	0.61	3/3216 (0.1%)
1	D	0.34	0/2281	0.56	0/3083
All	All	0.45	1/9338 (0.0%)	0.61	3/12635 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	728	CYS	CB-SG	-7.20	1.70	1.82

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	480	LYS	CD-CE-NZ	-7.50	94.44	111.70
1	C	625	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	C	480	LYS	CG-CD-CE	-5.24	96.19	111.90

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	2241	0	2229	53	0
1	B	2320	0	2295	63	0
1	C	2309	0	2278	35	0
1	D	2229	0	2214	45	0
2	A	10	0	0	0	0
2	B	10	0	0	0	0
2	C	10	0	0	1	0
2	D	5	0	0	0	0
3	A	31	17	14	5	0
3	B	31	17	14	7	0
3	C	31	17	14	4	0
3	D	31	17	14	1	0
4	C	1	0	0	0	0
4	D	2	0	0	0	0
5	A	116	0	0	6	0
5	B	168	0	0	9	0
5	C	117	0	0	6	0
5	D	84	0	0	4	0
All	All	9746	68	9072	189	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 10.

All (189) 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:480:LYS:HE2	1:C:501:VAL:CB	1.69	1.21
1:C:480:LYS:HE2	1:C:501:VAL:HB	1.16	1.13
1:A:665:LEU:HD13	1:A:680[C]:TYR:OH	1.52	1.10
1:C:480:LYS:CE	1:C:501:VAL:HB	1.82	1.10
1:B:665:LEU:HD13	1:B:680[A]:TYR:OH	1.51	1.07
1:A:492:PHE:CD1	1:A:492:PHE:O	2.09	1.05
1:C:480:LYS:HE2	1:C:501:VAL:CG1	1.88	1.01
1:B:597:GLN:NE2	5:B:1021:HOH:O	1.91	1.01
1:A:631:ASN:OD1	3:A:802:ACP:O3G	1.79	0.99
1:A:492:PHE:O	1:A:492:PHE:HD1	1.41	0.99
1:A:675:LEU:HD11	1:A:713:PHE:CE1	2.03	0.94
1:B:630:ARG:NE	5:B:1058:HOH:O	1.84	0.93
1:A:621:LYS:HD2	1:A:652:ASN:HD22	1.35	0.92
1:A:664:ARG:CZ	1:B:526:LYS:HD3	2.00	0.90
1:A:675:LEU:HD11	1:A:713:PHE:HE1	1.35	0.89
3:C:802:ACP:O1B	5:C:959:HOH:O	1.90	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:608:TYR:CZ	1:B:612:ARG:HD2	2.07	0.88
1:C:545:LYS:HD2	5:C:967:HOH:O	1.73	0.87
1:C:491:ALA:HB2	5:D:978:HOH:O	1.74	0.85
1:D:729:THR:HG23	1:D:732:LEU:H	1.41	0.84
1:A:540:MET:HG3	5:A:979:HOH:O	1.79	0.83
3:A:802:ACP:O3G	5:A:970:HOH:O	1.95	0.82
1:C:488:GLY:HA3	3:C:802:ACP:H4'	1.61	0.82
1:C:585:GLU:OE1	5:C:902:HOH:O	2.00	0.79
1:D:761:LEU:O	1:D:764:THR:HG22	1.80	0.79
1:A:492:PHE:HB2	1:A:527:ASP:OD1	1.82	0.79
1:B:488:GLY:HA3	3:B:802:ACP:H4'	1.64	0.79
1:A:505:LYS:HE3	5:A:940:HOH:O	1.83	0.79
1:A:526:LYS:HD3	1:B:662:ASN:HB3	1.64	0.77
1:B:665:LEU:CD1	1:B:680[A]:TYR:OH	2.33	0.77
1:A:581:PRO:HG3	1:A:597:GLN:NE2	2.00	0.76
1:A:526:LYS:NZ	1:B:662:ASN:HD22	1.84	0.76
1:C:480:LYS:HE2	1:C:501:VAL:HG12	1.66	0.76
1:B:630:ARG:NH2	5:B:1032:HOH:O	2.16	0.75
1:D:659:THR:CG2	1:D:678:ARG:HB3	2.17	0.74
1:C:537:MET:CE	1:C:622[A]:CYS:SG	2.76	0.74
1:A:621:LYS:HD2	1:A:652:ASN:ND2	2.02	0.74
1:B:492:PHE:CE2	5:B:1016:HOH:O	2.41	0.73
1:B:468:LEU:HD12	1:B:469:PRO:HD2	1.71	0.73
1:A:549:ASN:OD1	5:A:990:HOH:O	2.06	0.73
1:C:480:LYS:CE	1:C:501:VAL:CB	2.52	0.72
1:A:665:LEU:HD13	1:A:680[C]:TYR:CZ	2.23	0.72
1:D:489:GLU:HG3	1:D:520:LYS:HD3	1.69	0.72
1:C:635:THR:OG1	2:C:804:SO4:O2	2.02	0.71
1:D:608:TYR:CZ	1:D:612:ARG:HD2	2.25	0.71
1:C:537:MET:HE2	1:C:622[A]:CYS:SG	2.31	0.71
1:A:676:PHE:CE1	1:A:717:LYS:HE3	2.25	0.70
1:B:582:PRO:O	5:B:1020:HOH:O	2.09	0.70
1:B:503:ILE:HG22	1:B:512:VAL:CG1	2.21	0.70
1:B:665:LEU:HD13	1:B:680[A]:TYR:CZ	2.26	0.70
1:C:487:LEU:HD21	1:C:497:MET:HE2	1.73	0.69
1:C:662:ASN:O	5:C:1012:HOH:O	2.11	0.67
1:A:724:LYS:HE2	1:A:728:CYS:O	1.94	0.67
1:D:637:ASN:N	1:D:637:ASN:OD1	2.25	0.66
1:D:659:THR:HG23	1:D:678:ARG:HB3	1.77	0.66
1:B:630:ARG:NH1	5:B:1058:HOH:O	2.29	0.65
1:B:565:GLU:OE2	1:B:641:LYS:HE3	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:802:ACP:O1A	3:B:802:ACP:H3B1	1.96	0.65
1:C:520:LYS:NZ	5:C:1015:HOH:O	2.21	0.65
1:B:608:TYR:OH	1:B:612:ARG:HD2	1.98	0.64
1:B:630:ARG:CZ	5:B:1058:HOH:O	2.35	0.63
1:A:608:TYR:CZ	1:A:612:ARG:HD2	2.33	0.63
1:D:731:GLU:OE2	1:D:759:ARG:NH1	2.32	0.62
1:A:664:ARG:NH2	1:B:526:LYS:HD3	2.13	0.62
1:A:526:LYS:HZ2	1:B:662:ASN:HD22	1.48	0.62
1:B:518:MET:HB2	5:B:1023:HOH:O	1.99	0.62
1:A:664:ARG:CZ	1:B:526:LYS:CD	2.76	0.61
1:A:492:PHE:C	1:A:492:PHE:CD1	2.74	0.59
1:B:612:ARG:HD3	5:B:937:HOH:O	2.02	0.59
1:D:729:THR:HG22	1:D:732:LEU:HD12	1.84	0.59
1:C:625:ARG:HD3	1:C:647:LEU:O	2.02	0.59
1:B:680[B]:TYR:CE1	1:B:684:SER:HB2	2.38	0.59
1:B:492:PHE:CD1	1:B:492:PHE:O	2.56	0.59
1:A:489:GLU:HG3	1:A:520:LYS:HD3	1.85	0.58
1:A:655:ASP:N	1:A:655:ASP:OD1	2.35	0.58
1:B:647:LEU:HD13	1:B:665:LEU:HD23	1.85	0.58
1:A:680[A]:TYR:CE1	1:A:684:SER:HB2	2.37	0.58
1:B:537:MET:HE1	1:B:622[B]:CYS:SG	2.44	0.58
1:A:664:ARG:NH1	1:B:526:LYS:CE	2.67	0.57
3:C:802:ACP:H3B2	3:C:802:ACP:O2A	2.04	0.57
1:B:631:ASN:OD1	3:B:802:ACP:PG	2.63	0.57
1:C:608:TYR:OH	1:C:612:ARG:HD2	2.04	0.57
1:A:665:LEU:CD1	1:A:680[C]:TYR:CE2	2.87	0.57
1:A:675:LEU:HD11	1:A:713:PHE:CD1	2.40	0.57
3:A:802:ACP:O2'	5:A:972:HOH:O	2.15	0.57
1:A:488:GLY:HA3	3:A:802:ACP:H4'	1.87	0.56
1:B:503:ILE:HG22	1:B:512:VAL:HG13	1.88	0.56
1:C:549:ASN:HD22	1:C:565:GLU:CD	2.09	0.56
1:D:491:ALA:N	3:D:802:ACP:O2G	2.38	0.56
1:C:480:LYS:O	1:C:480:LYS:HG3	2.04	0.56
1:D:659:THR:CG2	1:D:678:ARG:CB	2.84	0.56
1:D:669:TRP:CZ2	1:D:703:PRO:HG2	2.41	0.56
1:B:644:ASP:OD2	3:B:802:ACP:O2G	2.24	0.55
1:C:537:MET:HE1	1:C:622[A]:CYS:SG	2.45	0.55
1:D:573:ARG:NH2	1:D:577:ARG:NH2	2.55	0.55
1:A:526:LYS:NZ	1:B:662:ASN:ND2	2.52	0.54
1:B:487:LEU:HD21	1:B:497:MET:HG3	1.90	0.54
1:B:537:MET:HE3	1:B:541:ILE:HG13	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:491:ALA:HB3	1:D:492:PHE:CE2	2.42	0.53
1:A:664:ARG:NH1	1:B:526:LYS:HE3	2.23	0.53
1:C:573:ARG:NH1	1:C:574:GLU:OE2	2.42	0.53
1:D:758:ASP:O	1:D:762:THR:HG23	2.09	0.53
1:A:676:PHE:CZ	1:A:717:LYS:HG3	2.43	0.53
1:D:573:ARG:NH2	1:D:577:ARG:HH22	2.06	0.53
1:D:601:LYS:HG3	1:D:764:THR:HG23	1.90	0.53
1:D:659:THR:HG22	1:D:678:ARG:CA	2.40	0.52
1:C:665:LEU:HD22	1:C:680[B]:TYR:OH	2.09	0.52
1:C:480:LYS:CD	1:C:501:VAL:HB	2.38	0.52
1:B:474:TRP:CD1	1:B:539:LYS:HE2	2.45	0.52
1:C:610:LEU:HD13	1:C:692:LEU:HD21	1.92	0.51
3:A:802:ACP:O2B	3:A:802:ACP:O1G	2.29	0.51
1:D:608:TYR:OH	1:D:612:ARG:HD2	2.10	0.51
1:D:659:THR:HG22	1:D:678:ARG:HB3	1.91	0.51
1:D:675:LEU:HD11	1:D:713:PHE:CE1	2.46	0.51
1:C:680[A]:TYR:CE1	1:C:684:SER:HB2	2.46	0.51
1:D:680:TYR:CE1	1:D:684:SER:HB2	2.45	0.50
1:A:674:ALA:HB1	1:A:680[C]:TYR:CE2	2.46	0.50
1:D:675:LEU:HD11	1:D:713:PHE:HE1	1.76	0.50
1:D:547:ILE:O	1:D:549:ASN:ND2	2.45	0.50
1:D:491:ALA:HB3	1:D:492:PHE:CD2	2.47	0.49
1:D:492:PHE:HB3	1:D:527:ASP:OD1	2.12	0.49
1:D:566:TYR:CZ	1:D:568:SER:HA	2.46	0.49
1:C:625:ARG:HA	1:C:680[A]:TYR:OH	2.13	0.49
1:B:674:ALA:HB1	1:B:680[A]:TYR:CE2	2.47	0.49
1:B:665:LEU:CD1	1:B:680[A]:TYR:CZ	2.93	0.49
1:A:665:LEU:CD1	1:A:680[C]:TYR:CZ	2.96	0.48
1:D:659:THR:HG22	1:D:678:ARG:C	2.33	0.48
1:B:492:PHE:HD1	1:B:492:PHE:O	1.95	0.48
1:B:503:ILE:HG22	1:B:512:VAL:HG11	1.96	0.48
1:B:487:LEU:HD21	1:B:497:MET:CG	2.44	0.47
1:D:610:LEU:HD13	1:D:692:LEU:HD21	1.96	0.47
1:A:472:PRO:HD2	5:A:916:HOH:O	2.14	0.47
1:D:681:THR:HB	5:D:926:HOH:O	2.14	0.47
1:C:480:LYS:CE	1:C:501:VAL:HG12	2.40	0.47
1:B:644:ASP:OD2	3:B:802:ACP:PG	2.73	0.47
1:A:507:LYS:HD2	1:A:510:GLU:OE2	2.15	0.46
1:B:489:GLU:HG3	1:B:520:LYS:HE3	1.98	0.46
1:B:631:ASN:OD1	3:B:802:ACP:O2G	2.34	0.46
1:A:665:LEU:HD12	1:A:670:MET:HE3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:489:GLU:CG	1:B:520:LYS:NZ	2.79	0.46
1:B:492:PHE:HB2	1:B:527:ASP:OD1	2.15	0.46
1:B:665:LEU:CD1	1:B:680[A]:TYR:CE2	2.99	0.45
1:A:647:LEU:HD13	1:A:665:LEU:HD23	1.98	0.45
3:C:802:ACP:C3B	3:C:802:ACP:O2A	2.64	0.45
1:D:507:LYS:HD2	1:D:510:GLU:OE1	2.17	0.45
1:A:676:PHE:CZ	1:A:717:LYS:HE3	2.52	0.45
1:C:480:LYS:HG2	1:C:480:LYS:HZ3	1.27	0.45
1:A:675:LEU:HD21	1:A:713:PHE:HD1	1.81	0.45
1:C:625:ARG:HA	1:C:680[A]:TYR:CZ	2.52	0.45
1:D:659:THR:HG22	1:D:678:ARG:O	2.17	0.45
1:A:675:LEU:HD23	1:A:676:PHE:CZ	2.52	0.45
1:D:572:LEU:HD13	1:D:640:MET:SD	2.57	0.45
1:A:675:LEU:HD21	1:A:713:PHE:CD1	2.52	0.45
1:A:526:LYS:HZ3	1:B:662:ASN:HD22	1.62	0.45
1:B:608:TYR:CE2	1:B:612:ARG:HD2	2.49	0.44
1:A:608:TYR:OH	1:A:612:ARG:HD2	2.18	0.44
1:D:480:LYS:NZ	5:D:951:HOH:O	2.49	0.44
1:D:625:ARG:HD3	1:D:647:LEU:O	2.18	0.44
1:C:480:LYS:HZ2	1:C:501:VAL:N	2.06	0.43
1:A:501:VAL:HG21	1:D:499:GLU:OE2	2.18	0.43
1:D:507:LYS:N	1:D:508:PRO:HD3	2.33	0.43
1:A:581:PRO:CG	1:A:597:GLN:NE2	2.76	0.43
1:D:491:ALA:HA	5:D:978:HOH:O	2.18	0.43
1:D:489:GLU:CG	1:D:520:LYS:HD3	2.45	0.43
1:B:492:PHE:HE1	1:B:531:LEU:HB2	1.83	0.43
1:B:503:ILE:CG2	1:B:512:VAL:CG1	2.95	0.43
1:A:526:LYS:HZ2	1:B:662:ASN:ND2	2.13	0.43
1:B:668:LYS:HG2	1:B:712:LEU:HD22	2.01	0.43
1:A:526:LYS:HZ3	1:B:662:ASN:ND2	2.15	0.42
1:C:491:ALA:N	5:C:959:HOH:O	1.99	0.42
1:D:545:LYS:O	1:D:641:LYS:HE2	2.20	0.42
1:B:489:GLU:HG2	1:B:520:LYS:HZ2	1.85	0.42
1:C:548:ILE:HG13	1:C:633:LEU:HD12	2.01	0.42
1:B:492:PHE:HZ	1:B:534:GLU:OE1	2.02	0.42
1:B:680[B]:TYR:CD1	1:B:684:SER:HB2	2.55	0.42
1:C:531:LEU:HD23	1:C:560:LEU:HD23	2.02	0.42
1:B:697:PHE:CZ	1:B:732:LEU:HD13	2.55	0.41
1:B:537:MET:CE	1:B:622[B]:CYS:SG	3.09	0.41
1:A:676:PHE:CE2	1:A:717:LYS:HG2	2.56	0.41
1:B:487:LEU:CD2	1:B:497:MET:HG3	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:702[A]:SER:HA	1:A:703:PRO:HD3	1.91	0.41
1:C:662:ASN:CB	1:D:526:LYS:HD3	2.51	0.41
1:B:489:GLU:CD	1:B:520:LYS:HZ1	2.19	0.41
1:A:665:LEU:CD1	1:A:680[C]:TYR:OH	2.44	0.40
1:B:631:ASN:OD1	3:B:802:ACP:O1G	2.39	0.40
1:D:506:ASP:C	1:D:508:PRO:HD3	2.42	0.40
1:D:659:THR:CG2	1:D:678:ARG:CA	2.99	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	276/324 (85%)	274 (99%)	2 (1%)	0	100	100
1	B	292/324 (90%)	289 (99%)	3 (1%)	0	100	100
1	C	292/324 (90%)	287 (98%)	5 (2%)	0	100	100
1	D	277/324 (86%)	273 (99%)	4 (1%)	0	100	100
All	All	1137/1296 (88%)	1123 (99%)	14 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 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	242/284 (85%)	239 (99%)	3 (1%)	75	67
1	B	252/284 (89%)	248 (98%)	4 (2%)	68	55
1	C	249/284 (88%)	248 (100%)	1 (0%)	93	91
1	D	239/284 (84%)	235 (98%)	4 (2%)	66	52
All	All	982/1136 (86%)	970 (99%)	12 (1%)	78	67

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	479	ASP
1	A	492	PHE
1	A	630	ARG
1	B	512	VAL
1	B	702[A]	SER
1	B	702[B]	SER
1	B	710	GLU
1	C	702	SER
1	D	468	LEU
1	D	633	LEU
1	D	637	ASN
1	D	730	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	549	ASN
1	A	652	ASN
1	B	662	ASN
1	D	546	ASN

### 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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 3 are monoatomic - leaving 11 for Mogul analysis.

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	SO4	A	801	-	4,4,4	0.14	0	6,6,6	0.13	0
3	ACP	A	802	-	27,33,33	2.09	8 (29%)	30,52,52	1.90	5 (16%)
2	SO4	A	803	-	4,4,4	0.20	0	6,6,6	0.13	0
2	SO4	B	801	-	4,4,4	0.15	0	6,6,6	0.31	0
3	ACP	B	802	-	27,33,33	2.06	6 (22%)	30,52,52	2.25	6 (20%)
2	SO4	B	803	-	4,4,4	0.35	0	6,6,6	0.27	0
2	SO4	C	801	-	4,4,4	0.16	0	6,6,6	0.25	0
3	ACP	C	802	4	27,33,33	2.03	6 (22%)	30,52,52	2.23	3 (10%)
2	SO4	C	804	-	4,4,4	0.16	0	6,6,6	0.08	0
2	SO4	D	801	-	4,4,4	0.13	0	6,6,6	0.14	0
3	ACP	D	802	4	27,33,33	2.08	6 (22%)	30,52,52	2.24	4 (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	SO4	A	801	-	-	0/0/0/0	0/0/0/0
3	ACP	A	802	-	-	0/15/38/38	0/3/3/3
2	SO4	A	803	-	-	0/0/0/0	0/0/0/0
2	SO4	B	801	-	-	0/0/0/0	0/0/0/0
3	ACP	B	802	-	-	0/15/38/38	0/3/3/3
2	SO4	B	803	-	-	0/0/0/0	0/0/0/0
2	SO4	C	801	-	-	0/0/0/0	0/0/0/0
3	ACP	C	802	4	-	0/15/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	C	804	-	-	0/0/0/0	0/0/0/0
2	SO4	D	801	-	-	0/0/0/0	0/0/0/0
3	ACP	D	802	4	-	0/15/38/38	0/3/3/3

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	802	ACP	C2'-C1'	-5.44	1.45	1.53
3	A	802	ACP	C2'-C1'	-4.85	1.45	1.53
3	C	802	ACP	C2'-C1'	-4.85	1.45	1.53
3	B	802	ACP	C2'-C1'	-4.58	1.46	1.53
3	D	802	ACP	C2'-C3'	-4.35	1.41	1.53
3	C	802	ACP	C2'-C3'	-4.23	1.42	1.53
3	B	802	ACP	C2'-C3'	-3.77	1.43	1.53
3	A	802	ACP	C2'-C3'	-3.73	1.43	1.53
3	A	802	ACP	C3'-C4'	-2.77	1.45	1.53
3	C	802	ACP	C3'-C4'	-2.62	1.46	1.53
3	D	802	ACP	C3'-C4'	-2.59	1.46	1.53
3	B	802	ACP	C3'-C4'	-2.48	1.46	1.53
3	A	802	ACP	PG-O2G	2.00	1.59	1.54
3	B	802	ACP	C2-N3	2.29	1.36	1.32
3	D	802	ACP	C2-N3	2.47	1.36	1.32
3	C	802	ACP	C6-N6	2.71	1.45	1.34
3	A	802	ACP	C6-N6	2.72	1.45	1.34
3	B	802	ACP	C6-N6	2.79	1.45	1.34
3	C	802	ACP	C2-N3	2.81	1.36	1.32
3	D	802	ACP	C6-N6	2.84	1.45	1.34
3	A	802	ACP	PB-O3A	2.91	1.61	1.58
3	A	802	ACP	C2-N3	3.22	1.37	1.32
3	A	802	ACP	O4'-C1'	5.33	1.48	1.41
3	C	802	ACP	O4'-C1'	5.68	1.49	1.41
3	D	802	ACP	O4'-C1'	5.75	1.49	1.41
3	B	802	ACP	O4'-C1'	6.42	1.50	1.41

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	802	ACP	N3-C2-N1	-9.72	120.39	128.86
3	D	802	ACP	N3-C2-N1	-9.22	120.83	128.86
3	C	802	ACP	N3-C2-N1	-9.16	120.88	128.86
3	A	802	ACP	N3-C2-N1	-7.83	122.04	128.86
3	D	802	ACP	C4'-O4'-C1'	-6.42	102.94	109.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	802	ACP	C4'-O4'-C1'	-5.90	103.49	109.77
3	B	802	ACP	C4'-O4'-C1'	-3.53	106.02	109.77
3	C	802	ACP	PA-O3A-PB	-3.19	122.11	132.39
3	B	802	ACP	O1G-PG-C3B	-3.17	104.22	111.22
3	A	802	ACP	C4'-O4'-C1'	-2.69	106.90	109.77
3	B	802	ACP	C4-C5-N7	-2.59	106.91	109.41
3	A	802	ACP	O3G-PG-C3B	-2.58	100.14	106.40
3	D	802	ACP	C4-C5-N7	-2.41	107.08	109.41
3	D	802	ACP	PA-O3A-PB	-2.33	124.89	132.39
3	B	802	ACP	PA-O3A-PB	-2.00	125.93	132.39
3	A	802	ACP	O2G-PG-C3B	2.13	111.58	106.40
3	A	802	ACP	C2'-C3'-C4'	2.35	107.19	102.62
3	B	802	ACP	O3G-PG-C3B	2.99	113.66	106.40

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	802	ACP	5	0
3	B	802	ACP	7	0
3	C	802	ACP	4	0
2	C	804	SO4	1	0
3	D	802	ACP	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	280/324 (86%)	-0.03	9 (3%)	48	45	17, 30, 60, 88	0
1	B	291/324 (89%)	-0.08	9 (3%)	49	46	18, 28, 54, 83	0
1	C	291/324 (89%)	0.22	24 (8%)	12	11	21, 38, 76, 91	0
1	D	281/324 (86%)	0.33	18 (6%)	20	18	27, 46, 71, 90	0
All	All	1143/1296 (88%)	0.11	60 (5%)	28	25	17, 35, 68, 91	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	656	TYR	7.0
1	D	761	LEU	6.8
1	D	763	LEU	5.4
1	A	581	PRO	5.3
1	D	578	ALA	5.2
1	C	479	ASP	5.2
1	D	764	THR	5.1
1	C	488	GLY	4.6
1	C	480	LYS	4.5
1	C	511	ALA	4.3
1	C	508	PRO	4.3
1	C	504	ASP	4.1
1	C	485	LYS	4.1
1	B	506	ASP	3.9
1	C	510	GLU	3.9
1	C	506	ASP	3.7
1	D	727	ASN	3.6
1	C	501	VAL	3.6
1	C	503	ILE	3.5
1	C	477	PRO	3.4
1	D	597	GLN	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	512	VAL	3.3
1	A	491	ALA	3.3
1	A	662	ASN	3.2
1	D	600	PHE	3.2
1	A	658	LYS	3.1
1	C	557	ASP	3.1
1	A	655	ASP	3.0
1	B	492	PHE	3.0
1	B	507	LYS	3.0
1	B	467	GLU	3.0
1	C	472	PRO	3.0
1	B	508	PRO	2.9
1	C	467	GLU	2.9
1	A	466	TYR	2.8
1	C	502	GLY	2.8
1	A	597	GLN	2.6
1	C	558	GLY	2.6
1	D	699	LEU	2.6
1	C	481	LEU	2.5
1	D	754	VAL	2.5
1	D	638	ASN	2.5
1	D	605	SER	2.5
1	D	759	ARG	2.5
1	A	492	PHE	2.4
1	D	575	TYR	2.4
1	B	504	ASP	2.4
1	D	725	PRO	2.4
1	C	505	LYS	2.3
1	D	713	PHE	2.3
1	B	491	ALA	2.2
1	C	483	LEU	2.2
1	D	707	ILE	2.1
1	B	505	LYS	2.1
1	C	482	THR	2.1
1	C	509	LYS	2.1
1	D	758	ASP	2.1
1	C	473	LYS	2.1
1	B	510	GLU	2.0
1	D	489	GLU	2.0



## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	SO4	C	804	5/5	0.88	0.22	2.93	97,100,101,104	0
4	MG	C	803	1/1	0.62	0.14	2.88	65,65,65,65	0
2	SO4	B	803	5/5	0.98	0.09	0.55	28,33,34,39	0
3	ACP	A	802	31/31	0.87	0.12	0.35	23,43,64,93	0
3	ACP	C	802	31/31	0.86	0.13	0.03	31,69,109,120	0
3	ACP	B	802	31/31	0.86	0.12	0.02	25,47,64,93	0
2	SO4	D	801	5/5	0.89	0.13	-0.08	73,74,77,83	0
2	SO4	A	801	5/5	0.95	0.13	-0.29	49,55,61,72	0
3	ACP	D	802	31/31	0.91	0.11	-0.38	39,57,97,116	0
2	SO4	C	801	5/5	0.99	0.09	-1.09	33,36,39,40	0
2	SO4	B	801	5/5	0.98	0.09	-1.38	36,37,39,42	0
4	MG	D	803	1/1	0.92	0.07	-	51,51,51,51	0
2	SO4	A	803	5/5	0.85	0.15	-	66,71,80,81	0
4	MG	D	804	1/1	0.77	0.10	-	46,46,46,46	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.