



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 20, 2016 – 05:55 PM EST

PDB ID : 4J97  
Title : Crystal Structure of FGF Receptor 2 (FGFR2) Kinase Domain Harboring the Pathogenic Gain-of-Function K659E Mutation Identified in Endometrial Cancer.  
Authors : Chen, H.; Mohammadi, M.  
Deposited on : 2013-02-15  
Resolution : 2.55 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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20028442  
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-20028442

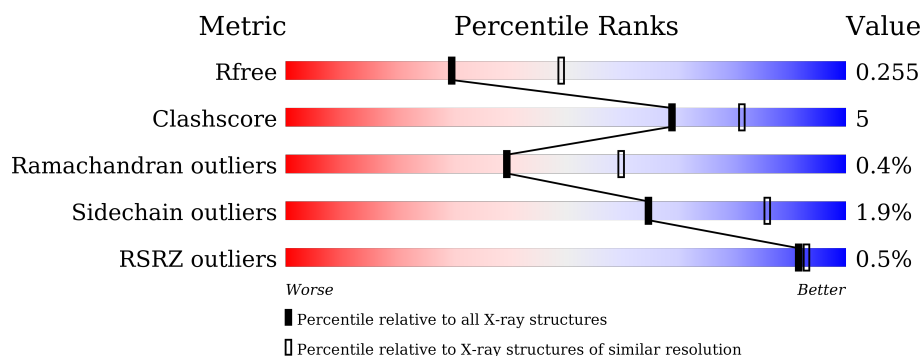
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.55 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	4549 (2.58-2.50)
Clashscore	102246	5292 (2.58-2.50)
Ramachandran outliers	100387	5194 (2.58-2.50)
Sidechain outliers	100360	5196 (2.58-2.50)
RSRZ outliers	91569	4561 (2.58-2.50)

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>75%</div> <div>12%</div> <div>13%</div> </div>
1	B	324	<div> <div>76%</div> <div>11%</div> <div>•</div> <div>13%</div> </div>
1	C	324	<div> <div>%</div> <div>78%</div> <div>9%</div> <div>•</div> <div>13%</div> </div>
1	D	324	<div> <div>%</div> <div>74%</div> <div>14%</div> <div>•</div> <div>12%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9286 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 Fibroblast growth factor receptor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	282	Total	C	N	O	S	0	2	0
			2248	1431	380	415	22			
1	B	283	Total	C	N	O	S	0	2	0
			2245	1429	380	414	22			
1	C	283	Total	C	N	O	S	0	1	0
			2245	1428	382	414	21			
1	D	285	Total	C	N	O	S	0	1	0
			2278	1451	385	420	22			

There are 60 discrepancies between the modelled and reference sequences:

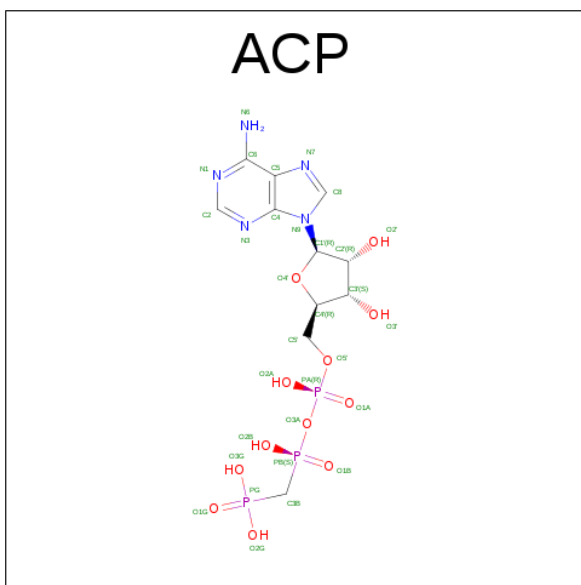
Chain	Residue	Modelled	Actual	Comment	Reference
A	445	MET	-	EXPRESSION TAG	UNP P21802
A	446	GLY	-	EXPRESSION TAG	UNP P21802
A	447	SER	-	EXPRESSION TAG	UNP P21802
A	448	SER	-	EXPRESSION TAG	UNP P21802
A	449	HIS	-	EXPRESSION TAG	UNP P21802
A	450	HIS	-	EXPRESSION TAG	UNP P21802
A	451	HIS	-	EXPRESSION TAG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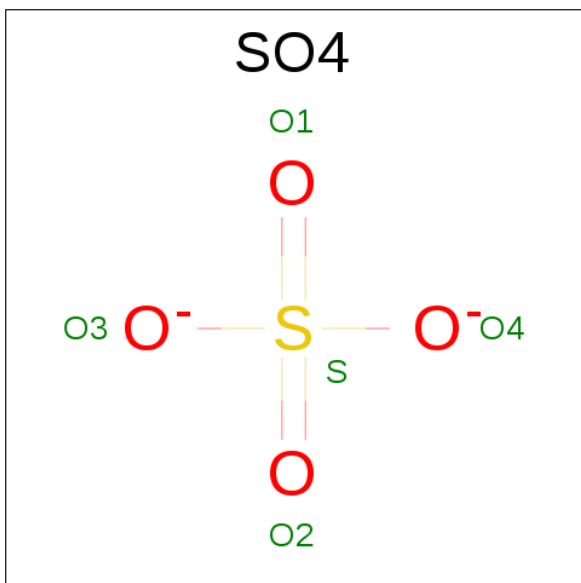
Chain	Residue	Modelled	Actual	Comment	Reference
B	451	HIS	-	EXPRESSION TAG	UNP P21802
B	452	HIS	-	EXPRESSION TAG	UNP P21802
B	453	HIS	-	EXPRESSION TAG	UNP P21802
B	454	HIS	-	EXPRESSION TAG	UNP P21802
B	455	SER	-	EXPRESSION TAG	UNP P21802
B	456	GLN	-	EXPRESSION TAG	UNP P21802
B	457	ASP	-	EXPRESSION TAG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

- Molecule 2 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
2	A	1	Total 23	C 10	N 5	O 7	P 1	0	0
2	B	1	Total 31	C 11	N 5	O 12	P 3	0	0
2	C	1	Total 31	C 11	N 5	O 12	P 3	0	0
2	D	1	Total 31	C 11	N 5	O 12	P 3	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

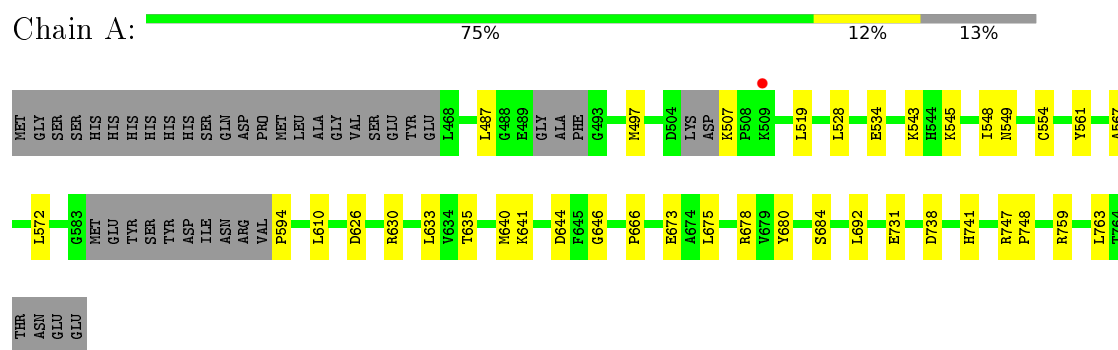
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	30	Total O 30 30	0	0
4	B	37	Total O 37 37	0	0
4	C	31	Total O 31 31	0	0
4	D	31	Total O 31 31	0	0

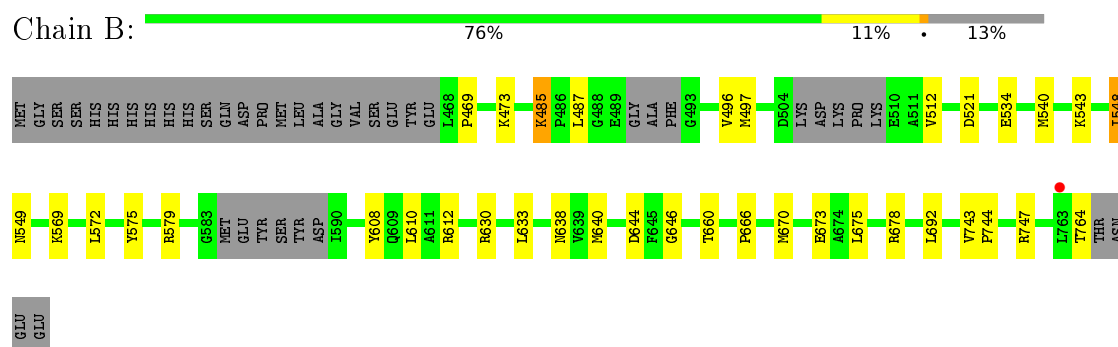
### 3 Residue-property plots [i](#)

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.

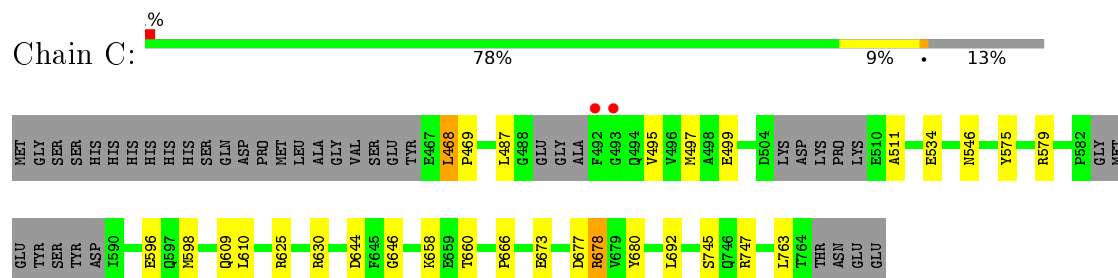
- Molecule 1: Fibroblast growth factor receptor 2



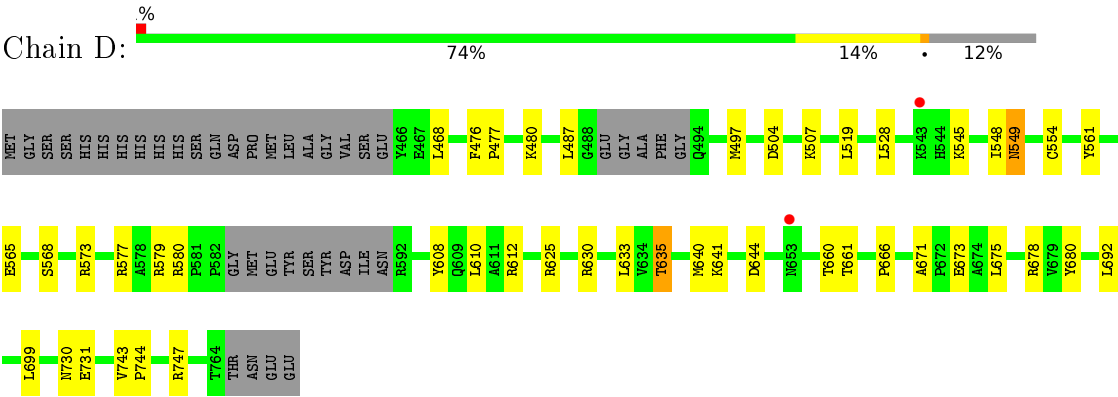
- Molecule 1: Fibroblast growth factor receptor 2



- Molecule 1: Fibroblast growth factor receptor 2



- Molecule 1: Fibroblast growth factor receptor 2





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	70.58 Å 70.28 Å 85.50 Å 92.39° 112.19° 115.98°	Depositor
Resolution (Å)	41.35 – 2.55 42.27 – 2.55	Depositor EDS
% Data completeness (in resolution range)	96.4 (41.35-2.55) 86.1 (42.27-2.55)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.06 (at 2.54 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, $R_{free}$	0.200 , 0.257 0.199 , 0.255	Depositor DCC
$R_{free}$ test set	1931 reflections (4.81%)	DCC
Wilson B-factor (Å <sup>2</sup> )	34.5	Xtriage
Anisotropy	0.730	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 34.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.068 for k,h,-h-k-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	9286	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.20% 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: 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	0.22	0/2300	0.39	0/3108
1	B	0.22	0/2296	0.40	0/3105
1	C	0.21	0/2293	0.40	0/3102
1	D	0.21	0/2331	0.41	0/3152
All	All	0.22	0/9220	0.40	0/12467

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	2248	0	2246	20	0
1	B	2245	0	2234	19	0
1	C	2245	0	2228	18	0
1	D	2278	0	2281	29	0
2	A	23	0	12	0	0
2	B	31	0	14	0	0
2	C	31	0	14	1	0
2	D	31	0	14	1	0
3	A	10	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	5	0	0	0	0
3	D	5	0	0	0	0
4	A	30	0	0	0	0
4	B	37	0	0	2	0
4	C	31	0	0	0	0
4	D	31	0	0	1	0
All	All	9286	0	9043	83	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 5.

All (83) 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:673:GLU:OE2	1:D:747:ARG:NH2	2.16	0.79
1:B:670:MET:SD	4:B:934:HOH:O	2.50	0.70
1:B:572:LEU:HD13	1:B:640:MET:HE1	1.74	0.68
1:A:731:GLU:OE2	1:A:759:ARG:NH1	2.27	0.67
1:C:630:ARG:HH22	1:C:666:PRO:HG2	1.60	0.66
1:D:573:ARG:NH1	4:D:930:HOH:O	2.26	0.66
1:C:673:GLU:OE2	1:C:747:ARG:NH2	2.26	0.66
1:C:579:ARG:HB2	1:C:598:MET:HG2	1.79	0.64
1:A:572:LEU:HD13	1:A:640:MET:HE1	1.79	0.64
1:D:675:LEU:HD12	1:D:678:ARG:HH12	1.61	0.64
1:D:568:SER:H	1:D:635:THR:HG23	1.63	0.63
1:B:630:ARG:HH22	1:B:666:PRO:HG2	1.63	0.63
1:D:630:ARG:HH22	1:D:666:PRO:HG2	1.63	0.63
1:B:569:LYS:NZ	1:B:638:ASN:OD1	2.28	0.62
1:A:675:LEU:O	1:A:678:ARG:NH2	2.33	0.61
1:C:610:LEU:HD13	1:C:692:LEU:HD21	1.83	0.61
1:A:630:ARG:HH22	1:A:666:PRO:HG2	1.65	0.61
1:A:567:ALA:HA	1:A:635:THR:HG22	1.85	0.58
1:A:626:ASP:OD1	1:A:630:ARG:NH2	2.36	0.58
1:D:630:ARG:NH2	1:D:666:PRO:HG2	2.19	0.58
1:B:673:GLU:OE2	1:B:747:ARG:NH2	2.27	0.57
1:D:487:LEU:HD21	1:D:497:MET:HB2	1.86	0.57
1:D:610:LEU:HD13	1:D:692:LEU:HD21	1.87	0.57
1:D:675:LEU:HA	1:D:678:ARG:NH1	2.20	0.57
1:D:548:ILE:HG13	1:D:633:LEU:HD12	1.87	0.56
1:A:594:PRO:HB3	1:B:485:LYS:HG3	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:545:LYS:O	1:D:641:LYS:NZ	2.38	0.55
1:D:580:ARG:NH1	1:D:699:LEU:O	2.36	0.55
1:B:660:THR:O	1:B:678:ARG:NE	2.40	0.55
1:A:610:LEU:HD13	1:A:692:LEU:HD21	1.89	0.55
1:A:487:LEU:HD21	1:A:497:MET:HB2	1.89	0.54
1:A:630:ARG:NH2	1:A:666:PRO:HG2	2.23	0.53
1:D:675:LEU:HD12	1:D:678:ARG:NH1	2.24	0.53
1:D:549:ASN:ND2	1:D:565:GLU:OE1	2.41	0.52
1:D:565:GLU:OE2	1:D:641:LYS:HE3	2.09	0.52
1:D:608:TYR:CZ	1:D:612:ARG:HD2	2.44	0.52
1:D:661:THR:O	1:D:678:ARG:NH2	2.44	0.51
1:C:658:LYS:HE2	1:C:678:ARG:HB3	1.91	0.51
1:C:534:GLU:HB2	1:C:646:GLY:HA2	1.93	0.51
1:B:548:ILE:HG13	1:B:633:LEU:HD12	1.92	0.50
1:A:545:LYS:O	1:A:641:LYS:NZ	2.43	0.50
1:D:579:ARG:HG3	1:D:579:ARG:HH11	1.77	0.50
1:C:630:ARG:NH2	1:C:666:PRO:HG2	2.24	0.50
1:D:673:GLU:HG2	1:D:744:PRO:HG3	1.93	0.50
1:C:575:TYR:O	1:C:579:ARG:HG2	2.12	0.49
1:D:504:ASP:OD2	1:D:507:LYS:HD3	2.14	0.47
1:B:575:TYR:O	1:B:579:ARG:HD3	2.14	0.47
1:B:675:LEU:HD13	4:B:934:HOH:O	2.15	0.46
1:C:499:GLU:HG2	1:C:511:ALA:HB1	1.98	0.46
2:D:801:ACP:H5'2	2:D:801:ACP:H8	1.97	0.46
1:A:594:PRO:HG2	1:B:487:LEU:HD23	1.97	0.46
1:C:487:LEU:HD21	1:C:497:MET:HB2	1.97	0.46
1:D:477:PRO:HG2	1:D:480:LYS:HB2	1.97	0.46
1:B:473:LYS:HD2	1:C:677:ASP:OD2	2.16	0.46
1:A:534:GLU:HB2	1:A:646:GLY:HA2	1.98	0.46
1:C:579:ARG:HE	1:C:596:GLU:HB2	1.81	0.45
1:D:577:ARG:HA	1:D:580:ARG:HD2	1.98	0.45
1:A:543:LYS:HE3	1:A:549:ASN:HD21	1.81	0.45
1:A:519:LEU:HD11	1:A:528:LEU:HD13	1.99	0.45
1:A:673:GLU:OE2	1:A:747:ARG:NH2	2.37	0.45
1:B:610:LEU:HD13	1:B:692:LEU:HD21	1.99	0.45
1:D:671:ALA:HB1	1:D:673:GLU:OE2	2.16	0.45
1:C:625:ARG:HA	1:C:680:TYR:CZ	2.53	0.44
1:D:554:CYS:HB2	1:D:561:TYR:HB2	1.98	0.44
1:B:534:GLU:HB2	1:B:646:GLY:HA2	2.00	0.44
1:B:487:LEU:HD21	1:B:497:MET:HB2	1.99	0.44
1:C:546:ASN:ND2	1:C:609:GLN:HB3	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:644:ASP:OD2	2:C:801:ACP:H3B2	2.18	0.44
1:A:554:CYS:HB2	1:A:561:TYR:HB2	2.00	0.43
1:B:543:LYS:HD2	1:B:549:ASN:OD1	2.18	0.43
1:D:519:LEU:HD11	1:D:528:LEU:HD13	2.01	0.42
1:D:640:MET:HE2	1:D:640:MET:HB3	1.92	0.42
1:B:469:PRO:HG2	1:C:745:SER:HA	2.01	0.42
1:B:608:TYR:CZ	1:B:612:ARG:HD2	2.54	0.41
1:C:487:LEU:HD12	1:C:495:VAL:HG12	2.00	0.41
1:A:548:ILE:HG13	1:A:633:LEU:HD12	2.03	0.41
1:D:476:PHE:CD1	1:D:477:PRO:HD2	2.56	0.41
1:A:680:TYR:CE1	1:A:684:SER:HB2	2.56	0.41
1:C:468:LEU:HA	1:C:469:PRO:HD2	2.00	0.41
1:A:738:ASP:HB3	1:A:748:PRO:HD3	2.03	0.40
1:D:625:ARG:HA	1:D:680:TYR:CZ	2.56	0.40
1:D:743:VAL:HA	1:D:744:PRO:HD3	1.97	0.40
1:B:743:VAL:HA	1:B:744:PRO:HD3	1.95	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%)	269 (98%)	6 (2%)	1 (0%)	39	60
1	B	277/324 (86%)	270 (98%)	7 (2%)	0	100	100
1	C	276/324 (85%)	267 (97%)	7 (2%)	2 (1%)	26	44
1	D	281/324 (87%)	271 (96%)	9 (3%)	1 (0%)	39	60
All	All	1110/1296 (86%)	1077 (97%)	29 (3%)	4 (0%)	39	60

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	763	LEU
1	A	763	LEU
1	D	731	GLU
1	C	468	LEU

### 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	246/284 (87%)	243 (99%)	3 (1%)	78	92
1	B	244/284 (86%)	236 (97%)	8 (3%)	45	71
1	C	243/284 (86%)	241 (99%)	2 (1%)	86	96
1	D	250/284 (88%)	244 (98%)	6 (2%)	57	81
All	All	983/1136 (86%)	964 (98%)	19 (2%)	65	86

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	507	LYS
1	A	644	ASP
1	A	741	HIS
1	B	485	LYS
1	B	496	VAL
1	B	512	VAL
1	B	521	ASP
1	B	540	MET
1	B	548	ILE
1	B	644	ASP
1	B	764	THR
1	C	660	THR
1	C	678	ARG
1	D	468	LEU
1	D	549	ASN
1	D	635	THR
1	D	644	ASP
1	D	660	THR

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Mol	Chain	Res	Type
1	D	730	ASN

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 ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

9 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	ACP	A	801	-	22,25,33	2.16	6 (27%)	22,38,52	2.80	3 (13%)
3	SO4	A	802	-	4,4,4	0.26	0	6,6,6	0.06	0
3	SO4	A	803	-	4,4,4	0.23	0	6,6,6	0.06	0
2	ACP	B	801	-	29,33,33	2.22	8 (27%)	29,52,52	2.49	2 (6%)
3	SO4	B	802	-	4,4,4	0.23	0	6,6,6	0.07	0
2	ACP	C	801	-	29,33,33	2.26	8 (27%)	29,52,52	2.46	3 (10%)
3	SO4	C	802	-	4,4,4	0.25	0	6,6,6	0.05	0
2	ACP	D	801	-	29,33,33	2.25	8 (27%)	29,52,52	2.42	3 (10%)
3	SO4	D	802	-	4,4,4	0.24	0	6,6,6	0.07	0

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	ACP	A	801	-	-	0/6/26/38	0/3/3/3
3	SO4	A	802	-	-	0/0/0/0	0/0/0/0
3	SO4	A	803	-	-	0/0/0/0	0/0/0/0
2	ACP	B	801	-	-	0/15/38/38	0/3/3/3
3	SO4	B	802	-	-	0/0/0/0	0/0/0/0
2	ACP	C	801	-	-	0/15/38/38	0/3/3/3
3	SO4	C	802	-	-	0/0/0/0	0/0/0/0
2	ACP	D	801	-	-	0/15/38/38	0/3/3/3
3	SO4	D	802	-	-	0/0/0/0	0/0/0/0

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	ACP	C2'-C1'	-5.14	1.45	1.53
2	D	801	ACP	C2'-C1'	-5.10	1.45	1.53
2	B	801	ACP	C2'-C1'	-5.08	1.45	1.53
2	C	801	ACP	C2'-C1'	-5.06	1.45	1.53
2	B	801	ACP	C2'-C3'	-3.88	1.42	1.53
2	D	801	ACP	C2'-C3'	-3.85	1.43	1.53
2	A	801	ACP	C2'-C3'	-3.84	1.43	1.53
2	C	801	ACP	C2'-C3'	-3.81	1.43	1.53
2	B	801	ACP	C3'-C4'	-2.75	1.45	1.53
2	C	801	ACP	C3'-C4'	-2.65	1.45	1.53
2	D	801	ACP	C3'-C4'	-2.60	1.46	1.53
2	A	801	ACP	C3'-C4'	-2.59	1.46	1.53
2	A	801	ACP	C2-N3	2.46	1.36	1.32
2	B	801	ACP	C2-N3	2.50	1.36	1.32
2	D	801	ACP	C2-N3	2.56	1.36	1.32
2	C	801	ACP	C2-N3	2.57	1.36	1.32
2	C	801	ACP	C6-N6	2.82	1.45	1.34
2	A	801	ACP	C6-N6	2.83	1.45	1.34
2	B	801	ACP	C6-N6	2.83	1.45	1.34
2	D	801	ACP	C6-N6	2.88	1.45	1.34
2	B	801	ACP	PG-C3B	4.19	1.84	1.80
2	B	801	ACP	PB-C3B	4.38	1.84	1.80
2	D	801	ACP	PG-C3B	4.42	1.84	1.80
2	C	801	ACP	PG-C3B	4.47	1.84	1.80
2	D	801	ACP	PB-C3B	4.75	1.85	1.80
2	C	801	ACP	PB-C3B	4.79	1.85	1.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	ACP	O4'-C1'	5.38	1.48	1.41
2	C	801	ACP	O4'-C1'	5.44	1.49	1.41
2	D	801	ACP	O4'-C1'	5.45	1.49	1.41
2	B	801	ACP	O4'-C1'	5.50	1.49	1.41

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	ACP	N3-C2-N1	-11.29	120.00	128.87
2	B	801	ACP	N3-C2-N1	-11.11	120.15	128.87
2	D	801	ACP	N3-C2-N1	-11.10	120.15	128.87
2	C	801	ACP	N3-C2-N1	-10.82	120.37	128.87
2	B	801	ACP	C4'-O4'-C1'	-6.02	103.27	109.64
2	C	801	ACP	C4'-O4'-C1'	-5.56	103.74	109.64
2	D	801	ACP	C4'-O4'-C1'	-4.49	104.89	109.64
2	A	801	ACP	C4'-O4'-C1'	-4.40	104.98	109.64
2	C	801	ACP	C2'-C3'-C4'	2.64	108.03	102.64
2	D	801	ACP	C2'-C3'-C4'	2.83	108.43	102.64
2	A	801	ACP	C2'-C3'-C4'	2.84	108.44	102.64

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	801	ACP	1	0
2	D	801	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	282/324 (87%)	-0.21	1 (0%) 93 94	12, 21, 40, 72	0
1	B	283/324 (87%)	-0.27	1 (0%) 93 94	12, 21, 41, 60	0
1	C	283/324 (87%)	-0.24	2 (0%) 89 91	13, 22, 46, 62	0
1	D	285/324 (87%)	-0.18	2 (0%) 89 91	15, 25, 47, 67	0
All	All	1133/1296 (87%)	-0.23	6 (0%) 91 93	12, 22, 45, 72	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	509	LYS	4.4
1	C	492	PHE	2.3
1	D	653	ASN	2.2
1	B	763	LEU	2.2
1	C	493	GLY	2.1
1	D	543	LYS	2.1

### 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	ACP	B	801	31/31	0.84	0.19	0.80	21,42,156,163	0
2	ACP	D	801	31/31	0.82	0.17	0.68	28,49,146,162	0
2	ACP	C	801	31/31	0.83	0.18	0.61	18,54,150,153	0
2	ACP	A	801	23/31	0.88	0.15	-0.45	14,41,103,105	0
3	SO4	A	802	5/5	0.98	0.14	-0.83	14,31,35,39	0
3	SO4	C	802	5/5	0.99	0.10	-1.43	26,26,28,30	0
3	SO4	B	802	5/5	0.99	0.12	-1.57	31,31,33,35	0
3	SO4	D	802	5/5	0.99	0.09	-1.73	30,30,32,32	0
3	SO4	A	803	5/5	0.86	0.14	-	81,82,83,84	0

## 6.5 Other polymers

There are no such residues in this entry.