



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2016 – 10:08 PM EDT

PDB ID : 5FLF  
Title : DISEASE LINKED MUTATION IN FGFR  
Authors : Thiyagarajan, N.; Bunney, T.D.; Katan, M.  
Deposited on : 2015-10-26  
Resolution : 2.58 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-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

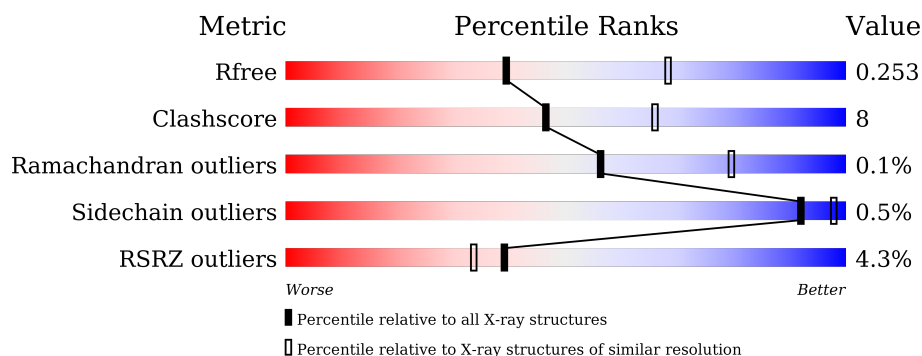
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.58 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	2636 (2.60-2.56)
Clashscore	102246	3003 (2.60-2.56)
Ramachandran outliers	100387	2956 (2.60-2.56)
Sidechain outliers	100360	2956 (2.60-2.56)
RSRZ outliers	91569	2642 (2.60-2.56)

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	310	<div> <div>3%</div> <div> <div></div> <div>82%</div> <div>12%</div> <div>• 5%</div> </div> </div>
1	B	310	<div> <div>%</div> <div> <div></div> <div>81%</div> <div>14%</div> <div>6%</div> </div> </div>
1	C	310	<div> <div>%</div> <div> <div></div> <div>75%</div> <div>16%</div> <div>9%</div> </div> </div>
1	D	310	<div> <div>2%</div> <div> <div></div> <div>79%</div> <div>15%</div> <div>6%</div> </div> </div>
1	E	310	<div> <div>13%</div> <div> <div></div> <div>69%</div> <div>14%</div> <div>17%</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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	D	1767	-	-	-	X
5	PGE	C	1765	-	-	-	X
5	PGE	D	1770	-	-	-	X
5	PGE	D	1771	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11786 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 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	296	Total	C	N	O	S	0	0	0
			2358	1501	402	438	17			
1	B	292	Total	C	N	O	S	0	4	0
			2350	1496	404	432	18			
1	C	283	Total	C	N	O	S	0	2	0
			2263	1440	391	414	18			
1	D	290	Total	C	N	O	S	0	1	0
			2312	1470	398	427	17			
1	E	258	Total	C	N	O	S	0	0	0
			2045	1304	353	371	17			

There are 25 discrepancies between the modelled and reference sequences:

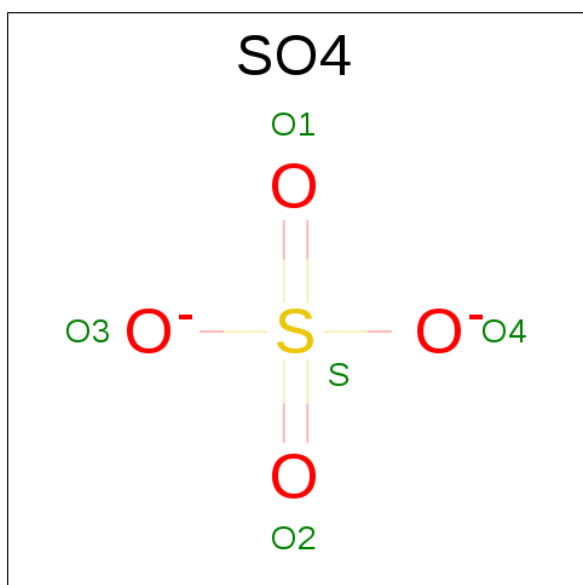
Chain	Residue	Modelled	Actual	Comment	Reference
A	456	MET	-	EXPRESSION TAG	UNP P11362
A	457	VAL	-	EXPRESSION TAG	UNP P11362
A	488	ALA	CYS	CONFLICT	UNP P11362
A	584	SER	CYS	CONFLICT	UNP P11362
A	675	GLY	ARG	ENGINEERED MUTATION	UNP P11362
B	456	MET	-	EXPRESSION TAG	UNP P11362
B	457	VAL	-	EXPRESSION TAG	UNP P11362
B	488	ALA	CYS	CONFLICT	UNP P11362
B	584	SER	CYS	CONFLICT	UNP P11362
B	675	GLY	ARG	ENGINEERED MUTATION	UNP P11362
C	456	MET	-	EXPRESSION TAG	UNP P11362
C	457	VAL	-	EXPRESSION TAG	UNP P11362
C	488	ALA	CYS	CONFLICT	UNP P11362
C	584	SER	CYS	CONFLICT	UNP P11362
C	675	GLY	ARG	ENGINEERED MUTATION	UNP P11362
D	456	MET	-	EXPRESSION TAG	UNP P11362
D	457	VAL	-	EXPRESSION TAG	UNP P11362
D	488	ALA	CYS	CONFLICT	UNP P11362
D	584	SER	CYS	CONFLICT	UNP P11362

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Chain	Residue	Modelled	Actual	Comment	Reference
D	675	GLY	ARG	ENGINEERED MUTATION	UNP P11362
E	456	MET	-	EXPRESSION TAG	UNP P11362
E	457	VAL	-	EXPRESSION TAG	UNP P11362
E	488	ALA	CYS	CONFLICT	UNP P11362
E	584	SER	CYS	CONFLICT	UNP P11362
E	675	GLY	ARG	ENGINEERED MUTATION	UNP P11362

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



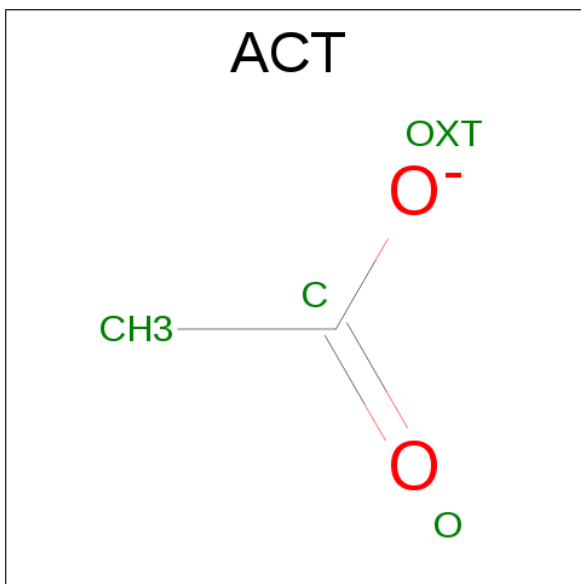
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	E	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).

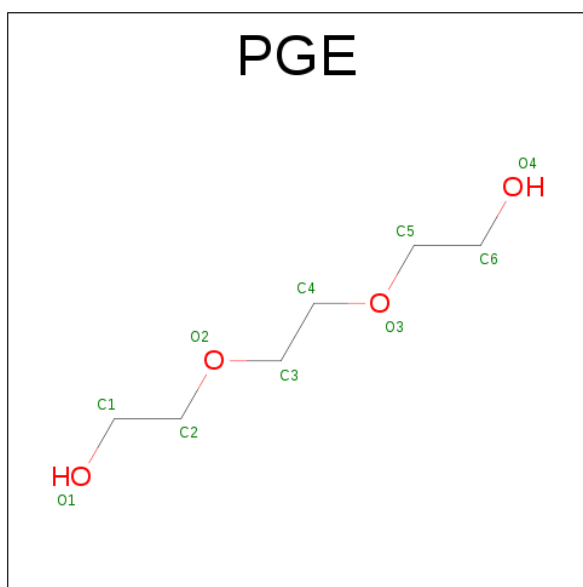


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Cl	0	0
			1	1		
4	D	3	Total	Cl	0	0
			3	3		
4	C	1	Total	Cl	0	0
			1	1		

- Molecule 5 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula:  $C_6H_{14}O_4$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			10	6	4		
5	D	1	Total	C	O	0	0
			10	6	4		
5	D	1	Total	C	O	0	0
			10	6	4		
5	D	1	Total	C	O	0	0
			10	6	4		

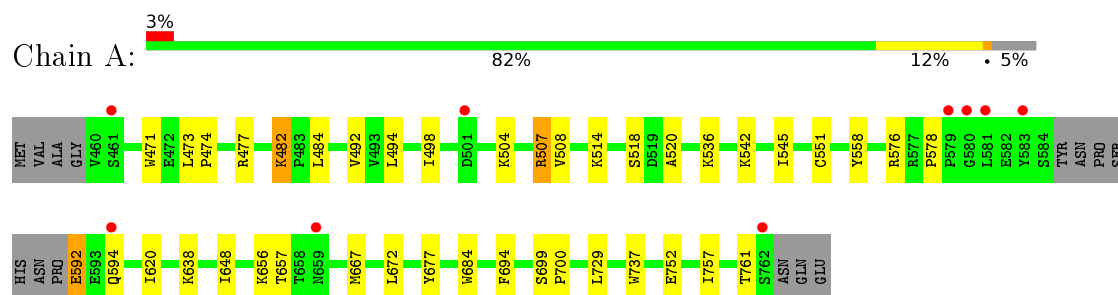
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	71	Total	O	0	0
			71	71		
6	B	101	Total	O	0	0
			101	101		
6	C	70	Total	O	0	0
			70	70		
6	D	94	Total	O	0	0
			94	94		
6	E	28	Total	O	0	0
			28	28		

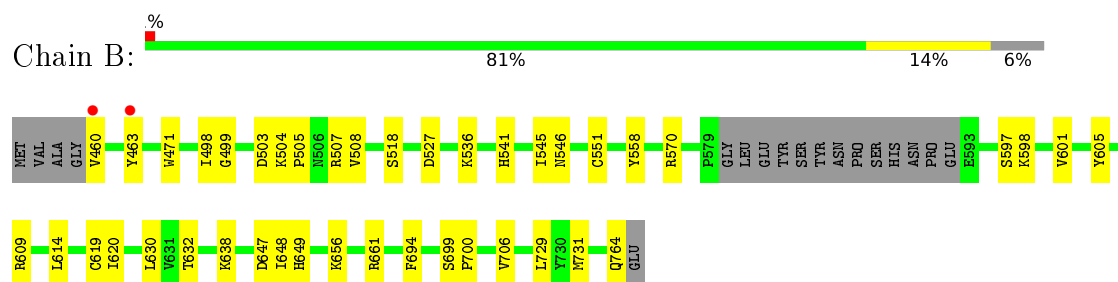
### 3 Residue-property plots

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.

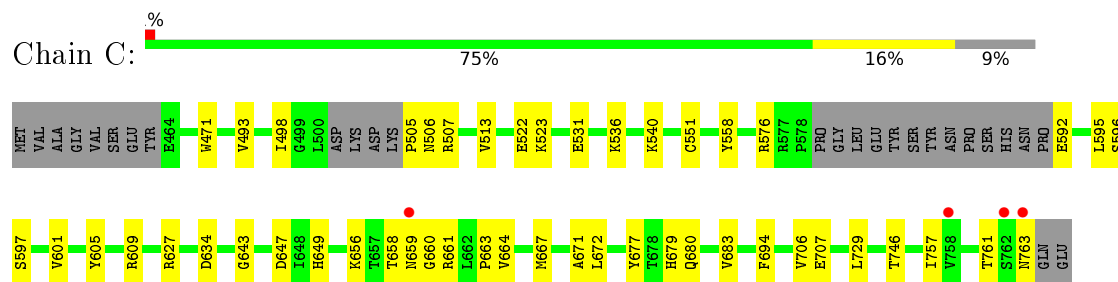
#### • Molecule 1: FIBROBLAST GROWTH FACTOR RECEPTOR 1



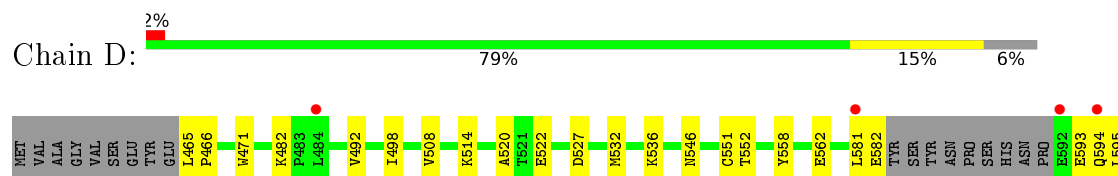
#### • Molecule 1: FIBROBLAST GROWTH FACTOR RECEPTOR 1



#### • Molecule 1: FIBROBLAST GROWTH FACTOR RECEPTOR 1

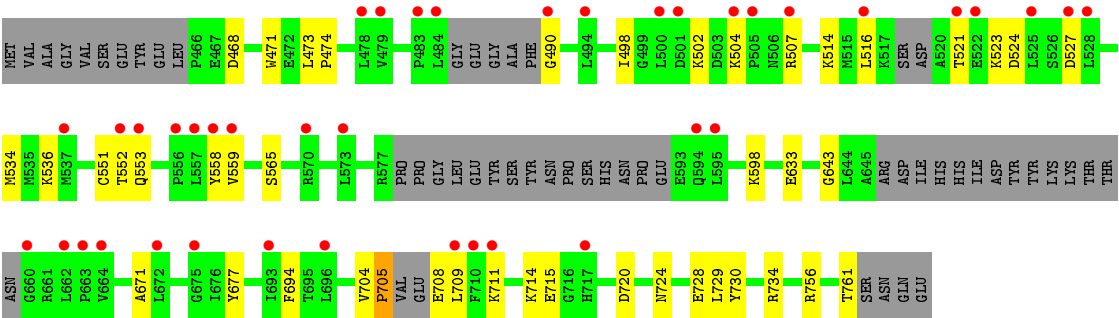


#### • Molecule 1: FIBROBLAST GROWTH FACTOR RECEPTOR 1





● Molecule 1: FIBROBLAST GROWTH FACTOR RECEPTOR 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	76.26Å 152.28Å 195.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	71.06 – 2.58 76.26 – 2.58	Depositor EDS
% Data completeness (in resolution range)	97.5 (71.06-2.58) 97.5 (76.26-2.58)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.79 (at 2.58Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.194 , 0.255 0.196 , 0.253	Depositor DCC
$R_{free}$ test set	3477 reflections (4.91%)	DCC
Wilson B-factor (Å <sup>2</sup> )	42.1	Xtriage
Anisotropy	0.457	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 56.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	11786	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.85% 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: CL, PGE, SO4, ACT

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	0.23	0/2408	0.42	0/3254
1	B	0.26	0/2409	0.44	0/3256
1	C	0.24	0/2315	0.42	0/3125
1	D	0.24	0/2360	0.42	0/3189
1	E	0.25	0/2083	0.48	0/2808
All	All	0.24	0/11575	0.43	0/15632

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	2358	0	2365	31	0
1	B	2350	0	2369	25	0
1	C	2263	0	2287	49	0
1	D	2312	0	2330	38	0
1	E	2045	0	2077	44	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	25	0	0	0	0
2	E	5	0	0	0	0
3	A	4	0	3	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	3	0	0	0	0
5	C	10	0	14	5	0
5	D	30	0	42	2	0
6	A	71	0	0	4	0
6	B	101	0	0	3	0
6	C	70	0	0	2	0
6	D	94	0	0	2	0
6	E	28	0	0	1	0
All	All	11786	0	11487	173	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 8.

All (173) 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:E:504:LYS:CD	1:E:507:ARG:NH1	1.76	1.48
1:E:504:LYS:HD3	1:E:507:ARG:NH1	1.05	1.36
1:E:504:LYS:HD3	1:E:507:ARG:CZ	1.60	1.30
1:C:659:ASN:ND2	1:D:522:GLU:OE1	1.65	1.29
1:E:504:LYS:NZ	1:E:507:ARG:HH12	1.31	1.28
1:C:659:ASN:OD1	1:D:522:GLU:HB2	1.31	1.27
1:E:504:LYS:CE	1:E:507:ARG:HH12	1.61	1.11
1:A:504:LYS:HD3	1:A:507:ARG:HD3	1.20	1.11
1:A:504:LYS:NZ	1:A:507:ARG:HH11	1.50	1.09
1:A:504:LYS:NZ	1:A:507:ARG:NH1	2.03	1.04
1:E:504:LYS:CE	1:E:507:ARG:NH1	2.19	0.98
1:E:504:LYS:HD3	1:E:507:ARG:HH11	1.25	0.95
1:A:504:LYS:HZ3	1:A:507:ARG:NH1	1.62	0.94
1:C:592:GLU:N	6:C:2031:HOH:O	1.99	0.93
1:E:504:LYS:NZ	1:E:507:ARG:NH1	2.17	0.93
1:A:504:LYS:HZ2	1:A:507:ARG:HH11	0.97	0.91
1:E:504:LYS:HZ3	1:E:507:ARG:HH12	1.15	0.89
1:C:659:ASN:OD1	1:D:522:GLU:CB	2.21	0.88
1:C:596:SER:HB2	1:C:763:ASN:HB3	1.54	0.88
1:A:504:LYS:CD	1:A:507:ARG:HD3	2.06	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:504:LYS:HD3	1:A:507:ARG:CD	2.05	0.84
1:C:596:SER:HB2	1:C:763:ASN:CB	2.12	0.80
1:C:596:SER:CB	1:C:763:ASN:HB3	2.19	0.72
1:E:504:LYS:CD	1:E:507:ARG:CZ	2.41	0.72
1:E:534:MET:HG2	1:E:643:GLY:HA2	1.73	0.70
1:C:659:ASN:CG	1:D:522:GLU:HB2	2.11	0.70
1:C:659:ASN:HD21	1:D:522:GLU:HB3	1.58	0.68
1:D:728:GLU:OE2	1:D:756:ARG:NH2	2.27	0.67
1:D:627:ARG:HH21	1:D:663:PRO:HG2	1.59	0.66
1:A:518:SER:O	6:A:2012:HOH:O	2.14	0.65
1:E:514:LYS:HB2	1:E:559:VAL:HB	1.79	0.64
1:E:728:GLU:OE2	1:E:756:ARG:NH2	2.31	0.64
1:A:492:VAL:HG22	1:A:514:LYS:HG2	1.80	0.63
1:D:664:VAL:HG12	1:D:709:LEU:HD23	1.81	0.63
1:D:647:ASP:OD1	1:D:649:HIS:ND1	2.27	0.62
1:C:659:ASN:CG	1:C:660:GLY:H	2.02	0.62
1:C:659:ASN:HD21	1:D:522:GLU:CB	2.13	0.61
1:B:731:MET:SD	6:B:2083:HOH:O	2.56	0.61
1:D:748:LYS:HD3	5:D:1770:PGE:H32	1.81	0.61
1:A:520:ALA:HB3	1:B:706:VAL:HG21	1.83	0.60
1:A:551:CYS:HB2	1:A:558:TYR:HB2	1.84	0.59
1:B:647:ASP:OD1	1:B:649[B]:HIS:ND1	2.31	0.59
1:E:704:VAL:O	1:E:708:GLU:N	2.35	0.59
1:C:659:ASN:CG	1:C:660:GLY:N	2.56	0.59
1:C:664:VAL:HG21	1:C:706:VAL:HG13	1.84	0.59
1:C:523:LYS:NZ	1:D:659:ASN:O	2.30	0.59
1:D:527:ASP:OD2	1:D:661:ARG:NH2	2.37	0.58
1:E:473:LEU:HD12	1:E:474:PRO:HD2	1.86	0.58
1:C:656:LYS:HB3	1:C:677:TYR:HE2	1.69	0.58
1:C:683:VAL:HG21	5:C:1765:PGE:H5	1.86	0.57
1:E:504:LYS:HZ3	1:E:507:ARG:NH1	1.89	0.56
1:E:724:ASN:OD1	1:E:724:ASN:N	2.37	0.56
1:D:492:VAL:HG22	1:D:514:LYS:HG2	1.86	0.56
1:E:504:LYS:CE	1:E:507:ARG:CZ	2.82	0.56
1:C:523:LYS:HE2	1:C:661:ARG:HD3	1.87	0.56
1:E:521:THR:HG22	1:E:523:LYS:H	1.71	0.55
1:A:542:LYS:NZ	6:A:2020:HOH:O	2.39	0.55
1:E:711:LYS:O	1:E:715:GLU:HB2	2.06	0.55
1:B:460:VAL:N	6:B:2001:HOH:O	2.40	0.55
1:A:620:ILE:HD11	1:A:648:ILE:HD13	1.89	0.54
1:A:545:ILE:HG12	1:A:638:LYS:HB3	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:659:ASN:ND2	1:D:522:GLU:CB	2.71	0.54
1:C:658:THR:HG22	1:C:659:ASN:N	2.23	0.54
1:D:609:ARG:NH2	6:D:2044:HOH:O	2.40	0.54
1:E:504:LYS:HE2	1:E:507:ARG:HH22	1.72	0.53
1:B:527:ASP:OD2	1:B:661:ARG:NH2	2.29	0.53
1:E:711:LYS:HA	1:E:714:LYS:HB2	1.89	0.53
1:C:634:ASP:N	1:C:634:ASP:OD1	2.42	0.53
1:C:576:ARG:HD3	1:C:595:LEU:HD21	1.90	0.53
1:C:659:ASN:ND2	1:D:522:GLU:HB3	2.23	0.53
1:B:598:LYS:HD3	1:B:764:GLN:HA	1.92	0.52
1:A:752:GLU:OE2	1:C:609:ARG:NH1	2.42	0.52
1:C:627[A]:ARG:HH21	1:C:663:PRO:HG2	1.74	0.52
1:B:620[A]:ILE:HD11	1:B:648:ILE:HD13	1.92	0.52
1:E:504:LYS:HE2	1:E:507:ARG:NH2	2.25	0.52
1:A:473:LEU:HD12	1:A:474:PRO:HD2	1.92	0.51
6:A:2013:HOH:O	1:B:570:ARG:NH1	2.43	0.51
1:D:546:ASN:HB3	1:D:562:GLU:HG3	1.92	0.51
1:E:551:CYS:HB2	1:E:558:TYR:HB2	1.91	0.51
1:B:498:ILE:HG12	1:B:508:VAL:HG12	1.92	0.51
1:C:707:GLU:N	1:C:707:GLU:OE1	2.32	0.51
1:C:551:CYS:HB2	1:C:558:TYR:HB2	1.93	0.51
1:A:656:LYS:HG3	1:A:657:THR:O	2.11	0.51
1:A:757:ILE:O	1:A:761:THR:OG1	2.24	0.51
1:E:468:ASP:OD1	1:E:468:ASP:N	2.44	0.50
1:A:667:MET:HE2	1:A:672:LEU:HA	1.94	0.49
1:E:490:GLY:HA2	1:E:516:LEU:HA	1.94	0.49
1:C:493:VAL:HG13	1:C:513:VAL:HB	1.95	0.49
1:D:749:GLN:HE21	5:D:1770:PGE:H52	1.78	0.49
1:B:541:HIS:H	1:B:546[B]:ASN:HD21	1.59	0.49
1:C:667:MET:HE2	1:C:672:LEU:HA	1.95	0.48
1:C:659:ASN:CG	1:D:522:GLU:CB	2.79	0.48
1:C:656:LYS:HB3	1:C:677:TYR:CE2	2.48	0.48
1:E:504:LYS:HZ2	1:E:507:ARG:HH12	1.49	0.48
1:A:656:LYS:HB3	1:A:677:TYR:HE2	1.79	0.48
1:D:609:ARG:NH1	6:D:2026:HOH:O	2.46	0.48
1:D:598:LYS:HG3	1:D:761[B]:THR:HG23	1.96	0.48
1:E:730:TYR:CZ	1:E:734:ARG:HD3	2.49	0.47
1:B:503:ASP:N	1:B:503:ASP:OD1	2.47	0.47
1:E:504:LYS:CD	1:E:507:ARG:HH11	1.97	0.47
1:E:714:LYS:HA	1:E:714:LYS:HD3	1.49	0.47
1:D:498:ILE:HG12	1:D:508:VAL:HG12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:498:ILE:O	1:E:507:ARG:O	2.33	0.47
1:D:465:LEU:HD12	1:D:466:PRO:HD2	1.97	0.47
1:D:551:CYS:HB2	1:D:558:TYR:HB2	1.95	0.47
1:C:706:VAL:HG21	1:D:520:ALA:HB3	1.97	0.47
1:C:746:THR:HA	5:C:1765:PGE:H52	1.97	0.47
1:A:578:PRO:HG3	1:A:594:GLN:HG2	1.96	0.46
1:A:477:ARG:HD3	1:A:477:ARG:HA	1.69	0.46
1:C:531:GLU:HB2	1:C:643:GLY:HA2	1.97	0.46
1:C:679:HIS:HB3	5:C:1765:PGE:H32	1.96	0.46
1:C:659:ASN:CG	1:D:522:GLU:OE1	2.47	0.46
1:E:552:THR:OG1	1:E:553:GLN:OE1	2.22	0.46
1:A:484:LEU:HD21	1:A:494:LEU:HB2	1.98	0.45
1:C:540:LYS:HE3	1:C:540:LYS:HB2	1.69	0.45
1:A:482:LYS:HE3	1:A:494:LEU:HD23	1.98	0.45
1:B:471:TRP:CD1	1:B:536:LYS:HE2	2.51	0.45
1:B:460:VAL:HG13	1:B:463:TYR:CD2	2.51	0.45
1:D:694:PHE:CZ	1:D:729:LEU:HD13	2.52	0.45
1:A:699:SER:HA	1:A:700:PRO:HD3	1.85	0.45
1:B:499:GLY:HA2	1:B:505:PRO:HA	1.99	0.45
1:B:694:PHE:CZ	1:B:729:LEU:HD13	2.52	0.45
1:A:594:GLN:H	1:A:594:GLN:CD	2.19	0.45
1:B:504:LYS:HD3	1:B:507:ARG:NH1	2.31	0.45
1:C:656:LYS:NZ	1:C:671:ALA:O	2.42	0.45
1:B:551:CYS:HB2	1:B:558:TYR:HB2	1.99	0.45
1:B:605:TYR:CZ	1:B:609:ARG:HD2	2.51	0.45
1:C:757:ILE:O	1:C:761:THR:OG1	2.29	0.45
1:C:746:THR:HG22	5:C:1765:PGE:H42	1.99	0.44
1:E:671:ALA:HB1	1:E:677:TYR:CE2	2.51	0.44
1:C:505:PRO:HB2	1:C:506:ASN:H	1.56	0.44
1:D:581:LEU:O	1:D:582:GLU:HB2	2.18	0.44
1:E:524:ASP:HA	1:E:527:ASP:HB2	1.99	0.44
1:B:545:ILE:HD11	1:B:630:LEU:HD12	1.98	0.44
6:A:2065:HOH:O	1:C:605:TYR:OH	2.21	0.44
1:C:694:PHE:CZ	1:C:729:LEU:HD13	2.53	0.44
1:A:471:TRP:CD1	1:A:536:LYS:HE2	2.53	0.43
1:B:656:LYS:HA	1:B:656:LYS:HD2	1.67	0.43
1:C:680:GLN:HA	5:C:1765:PGE:H6	1.99	0.43
1:E:705:PRO:C	1:E:709:LEU:H	2.21	0.43
1:E:720:ASP:N	1:E:720:ASP:OD1	2.47	0.43
1:D:597:SER:O	1:D:601:VAL:HG23	2.18	0.43
1:D:665:LYS:HG2	1:D:709:LEU:HD22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:523:LYS:O	1:E:523:LYS:HD2	2.18	0.43
1:A:498:ILE:HA	1:A:508:VAL:HG12	2.01	0.43
1:D:482:LYS:H	1:D:482:LYS:HG2	1.51	0.43
1:D:593:GLU:HA	1:D:593:GLU:OE1	2.18	0.43
1:C:597:SER:O	1:C:601:VAL:HG23	2.19	0.43
1:C:507:ARG:HB2	1:C:507:ARG:CZ	2.48	0.43
1:C:659:ASN:OD1	1:C:660:GLY:N	2.52	0.43
1:D:532:MET:HE1	1:D:552:THR:HG21	2.01	0.42
1:D:614:LEU:HD23	1:D:614:LEU:HA	1.86	0.42
1:E:565:SER:OG	1:E:633:GLU:HG3	2.19	0.42
1:A:684:TRP:CE3	1:A:737:TRP:HA	2.55	0.42
1:B:597:SER:O	1:B:601:VAL:HG23	2.20	0.42
1:E:471:TRP:CD1	1:E:536:LYS:HE2	2.55	0.42
1:A:694:PHE:CZ	1:A:729:LEU:HD13	2.54	0.41
1:B:699:SER:HA	1:B:700:PRO:HD3	1.83	0.41
1:D:684:TRP:CE3	1:D:737:TRP:HA	2.55	0.41
1:B:518:SER:O	6:B:2017:HOH:O	2.22	0.41
1:B:632:THR:HG21	1:B:638:LYS:HE2	2.02	0.41
1:D:594:GLN:HB2	1:D:595:LEU:H	1.71	0.41
1:D:471:TRP:CD1	1:D:536:LYS:HE2	2.56	0.41
1:E:730:TYR:O	1:E:734:ARG:HG2	2.20	0.41
1:E:705:PRO:O	6:E:2014:HOH:O	2.22	0.41
1:A:576:ARG:HG2	1:A:592:GLU:HB3	2.03	0.41
1:C:471:TRP:CD1	1:C:536:LYS:HE2	2.55	0.41
1:C:522:GLU:HG3	6:C:2015:HOH:O	2.21	0.40
1:C:647:ASP:OD1	1:C:649:HIS:ND1	2.37	0.40
1:E:694:PHE:CZ	1:E:729:LEU:HD13	2.55	0.40
1:B:614:LEU:HD23	1:B:614:LEU:HA	1.83	0.40
1:E:598:LYS:HD3	1:E:761:THR:OG1	2.21	0.40
1:E:504:LYS:CE	1:E:507:ARG:NH2	2.84	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	292/310 (94%)	275 (94%)	17 (6%)	0	100	100
1	B	292/310 (94%)	280 (96%)	12 (4%)	0	100	100
1	C	279/310 (90%)	265 (95%)	14 (5%)	0	100	100
1	D	287/310 (93%)	277 (96%)	10 (4%)	0	100	100
1	E	248/310 (80%)	223 (90%)	24 (10%)	1 (0%)	39	63
All	All	1398/1550 (90%)	1320 (94%)	77 (6%)	1 (0%)	56	79

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	705	PRO

### 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	258/270 (96%)	255 (99%)	3 (1%)	78	92
1	B	259/270 (96%)	257 (99%)	2 (1%)	86	95
1	C	248/270 (92%)	247 (100%)	1 (0%)	93	98
1	D	253/270 (94%)	253 (100%)	0	100	100
1	E	223/270 (83%)	222 (100%)	1 (0%)	93	98
All	All	1241/1350 (92%)	1234 (99%)	7 (1%)	92	97

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	482	LYS
1	A	507	ARG
1	A	592	GLU
1	B	619[A]	CYS

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Mol	Chain	Res	Type
1	B	619[B]	CYS
1	C	498	ILE
1	E	502	LYS

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 ⓘ

Of 19 ligands modelled in this entry, 5 are monoatomic - leaving 14 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	1763	-	4,4,4	0.25	0	6,6,6	0.06	0
3	ACT	A	1764	-	0,3,3	0.00	-	0,3,3	0.00	-
2	SO4	B	1765	-	4,4,4	0.24	0	6,6,6	0.07	0
2	SO4	C	1764	-	4,4,4	0.25	0	6,6,6	0.08	0
5	PGE	C	1765	-	9,9,9	0.34	0	8,8,8	0.33	0
2	SO4	D	1764	-	4,4,4	0.26	0	6,6,6	0.11	0
2	SO4	D	1765	-	4,4,4	0.25	0	6,6,6	0.06	0
2	SO4	D	1766	-	4,4,4	0.25	0	6,6,6	0.07	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SO4	D	1767	-	4,4,4	0.25	0	6,6,6	0.07	0
2	SO4	D	1768	-	4,4,4	0.35	0	6,6,6	0.57	0
5	PGE	D	1769	-	9,9,9	0.32	0	8,8,8	0.35	0
5	PGE	D	1770	-	9,9,9	0.33	0	8,8,8	0.29	0
5	PGE	D	1771	-	9,9,9	0.33	0	8,8,8	0.35	0
2	SO4	E	1762	-	4,4,4	0.24	0	6,6,6	0.08	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	SO4	A	1763	-	-	0/0/0/0	0/0/0/0
3	ACT	A	1764	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1765	-	-	0/0/0/0	0/0/0/0
2	SO4	C	1764	-	-	0/0/0/0	0/0/0/0
5	PGE	C	1765	-	-	0/7/7/7	0/0/0/0
2	SO4	D	1764	-	-	0/0/0/0	0/0/0/0
2	SO4	D	1765	-	-	0/0/0/0	0/0/0/0
2	SO4	D	1766	-	-	0/0/0/0	0/0/0/0
2	SO4	D	1767	-	-	0/0/0/0	0/0/0/0
2	SO4	D	1768	-	-	0/0/0/0	0/0/0/0
5	PGE	D	1769	-	-	0/7/7/7	0/0/0/0
5	PGE	D	1770	-	-	0/7/7/7	0/0/0/0
5	PGE	D	1771	-	-	0/7/7/7	0/0/0/0
2	SO4	E	1762	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1765	PGE	5	0
5	D	1770	PGE	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<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	296/310 (95%)	0.33	9 (3%) 54 49	27, 49, 97, 118	0
1	B	292/310 (94%)	0.27	2 (0%) 89 87	23, 39, 85, 106	0
1	C	283/310 (91%)	0.26	4 (1%) 78 75	29, 45, 81, 108	0
1	D	290/310 (93%)	0.19	6 (2%) 67 63	23, 40, 80, 113	0
1	E	258/310 (83%)	0.81	40 (15%) 3 2	33, 71, 108, 120	0
All	All	1419/1550 (91%)	0.36	61 (4%) 39 33	23, 46, 96, 120	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	460	VAL	5.8
1	E	553	GLN	4.5
1	E	557	LEU	4.4
1	C	659	ASN	4.1
1	E	500	LEU	3.9
1	E	709	LEU	3.8
1	E	516	LEU	3.7
1	A	579	PRO	3.6
1	E	552	THR	3.6
1	E	507	ARG	3.4
1	C	762	SER	3.2
1	E	558	TYR	3.2
1	E	696	LEU	3.2
1	E	711	LYS	3.1
1	E	484	LEU	3.0
1	E	528	LEU	3.0
1	E	478	LEU	2.9
1	E	660	GLY	2.8
1	E	494	LEU	2.8
1	E	505	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	594	GLN	2.7
1	A	581	LEU	2.7
1	E	522	GLU	2.7
1	E	664	VAL	2.6
1	A	583	TYR	2.6
1	D	581	LEU	2.6
1	E	556	PRO	2.5
1	E	537	MET	2.5
1	E	570	ARG	2.5
1	E	710	PHE	2.4
1	E	717	HIS	2.4
1	E	573	LEU	2.4
1	D	594	GLN	2.4
1	A	501	ASP	2.3
1	E	525	LEU	2.3
1	B	463	TYR	2.3
1	E	662	LEU	2.3
1	A	762	SER	2.3
1	E	675	GLY	2.3
1	E	521	THR	2.2
1	E	490	GLY	2.2
1	D	592	GLU	2.2
1	E	479	VAL	2.2
1	A	580	GLY	2.2
1	A	461	SER	2.2
1	E	501	ASP	2.2
1	C	763	ASN	2.2
1	E	672	LEU	2.1
1	E	594	GLN	2.1
1	E	663	PRO	2.1
1	D	763	ASN	2.1
1	C	758	VAL	2.1
1	E	504	LYS	2.1
1	A	659	ASN	2.1
1	D	484	LEU	2.0
1	D	759	ALA	2.0
1	E	595	LEU	2.0
1	E	693	ILE	2.0
1	E	527	ASP	2.0
1	E	559	VAL	2.0
1	E	483	PRO	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( $\text{\AA}^2$ )	Q<0.9
5	PGE	D	1770	10/10	0.69	0.36	10.80	34,73,81,84	0
2	SO4	D	1767	5/5	0.84	0.28	8.22	87,91,116,127	0
5	PGE	C	1765	10/10	0.86	0.35	6.19	42,54,59,61	0
5	PGE	D	1771	10/10	0.79	0.23	3.05	56,74,79,80	0
2	SO4	D	1764	5/5	0.99	0.17	0.34	35,37,53,64	0
2	SO4	A	1763	5/5	0.95	0.18	-0.49	67,76,109,115	0
2	SO4	C	1764	5/5	0.97	0.15	-0.55	57,66,73,82	0
5	PGE	D	1769	10/10	0.92	0.15	-1.07	48,66,79,81	0
4	CL	D	1774	1/1	0.96	0.12	-1.30	38,38,38,38	0
2	SO4	B	1765	5/5	0.94	0.15	-2.88	71,93,109,116	0
2	SO4	D	1766	5/5	0.97	0.14	-2.92	62,65,87,89	0
2	SO4	D	1768	5/5	0.74	0.33	-	104,112,115,137	0
4	CL	D	1773	1/1	0.14	0.36	-	96,96,96,96	0
4	CL	B	1766	1/1	1.00	0.13	-	35,35,35,35	0
2	SO4	D	1765	5/5	0.75	0.34	-	106,108,138,139	0
3	ACT	A	1764	4/4	0.76	0.25	-	56,69,70,77	0
2	SO4	E	1762	5/5	0.97	0.19	-	55,56,62,69	0
4	CL	D	1772	1/1	0.98	0.11	-	43,43,43,43	0
4	CL	C	1766	1/1	0.75	0.12	-	88,88,88,88	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.