



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:46 PM GMT

PDB ID : 4MMS  
Title : Crystal Structure of Prefusion-stabilized RSV F Variant Cav1 at pH 5.5  
Authors : Mclellan, J.S.; Joyce, M.G.; Stewart-Jones, G.B.E.; Sastry, M.; Yang, Y.;  
Graham, B.S.; Kwong, P.D.  
Deposited on : 2013-09-09  
Resolution : 2.40 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 (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

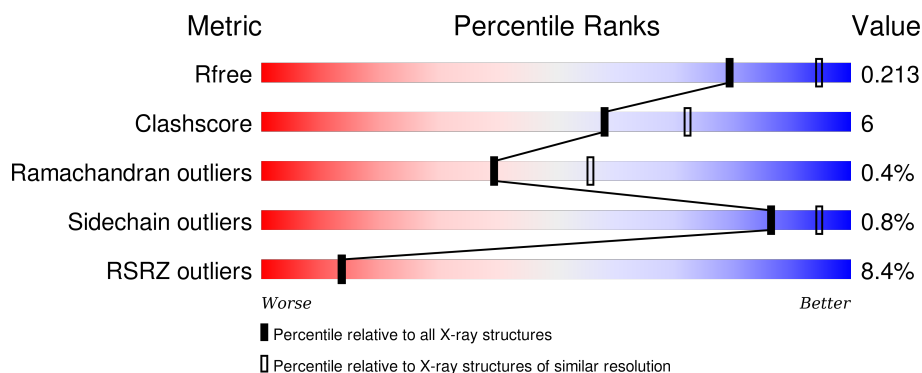
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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	82	<div> <div>15%</div> <div>89%</div> <div>10%</div> <div>.</div> </div>
1	C	82	<div> <div>15%</div> <div>80%</div> <div>13%</div> <div>6%</div> </div>
1	E	82	<div> <div>17%</div> <div>77%</div> <div>21%</div> <div>..</div> </div>
2	B	414	<div> <div>6%</div> <div>78%</div> <div>11%</div> <div>11%</div> </div>
2	D	414	<div> <div>7%</div> <div>76%</div> <div>13%</div> <div>11%</div> </div>

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Mol	Chain	Length	Quality of chain
2	F	414	

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
3	SO4	D	602	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11013 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 Fusion glycoprotein F2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	81	Total	C	N	O	S	0	0	0
			635	397	107	128	3			
1	C	77	Total	C	N	O	S	0	0	0
			603	380	98	122	3			
1	E	81	Total	C	N	O	S	0	0	0
			635	397	107	128	3			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	102	ALA	PRO	engineered mutation	UNP P03420
C	102	ALA	PRO	engineered mutation	UNP P03420
E	102	ALA	PRO	engineered mutation	UNP P03420

- Molecule 2 is a protein called Fusion glycoprotein F1 fused with Fibrin trimerization domain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	370	Total	C	N	O	S	0	0	0
			2852	1805	469	560	18			
2	D	370	Total	C	N	O	S	0	0	0
			2852	1805	469	560	18			
2	F	369	Total	C	N	O	S	0	0	0
			2844	1799	468	559	18			

There are 45 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	190	PHE	SER	engineered mutation	UNP P03420
B	207	LEU	VAL	engineered mutation	UNP P03420
B	379	VAL	ILE	engineered mutation	UNP P03420
B	447	VAL	MET	engineered mutation	UNP P03420

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Chain	Residue	Modelled	Actual	Comment	Reference
B	514	SER	-	LINKER	UNP P03420
B	515	ALA	-	LINKER	UNP P03420
B	516	ILE	-	LINKER	UNP P03420
B	517	GLY	-	LINKER	UNP P03420
B	539	LEU	PHE	VIRIANT	UNP P10104
B	545	GLY	-	EXPRESSION TAG	UNP P10104
B	546	GLY	-	EXPRESSION TAG	UNP P10104
B	547	LEU	-	EXPRESSION TAG	UNP P10104
B	548	VAL	-	EXPRESSION TAG	UNP P10104
B	549	PRO	-	EXPRESSION TAG	UNP P10104
B	550	ARG	-	EXPRESSION TAG	UNP P10104
D	190	PHE	SER	engineered mutation	UNP P03420
D	207	LEU	VAL	engineered mutation	UNP P03420
D	379	VAL	ILE	engineered mutation	UNP P03420
D	447	VAL	MET	engineered mutation	UNP P03420
D	514	SER	-	LINKER	UNP P03420
D	515	ALA	-	LINKER	UNP P03420
D	516	ILE	-	LINKER	UNP P03420
D	517	GLY	-	LINKER	UNP P03420
D	539	LEU	PHE	VIRIANT	UNP P10104
D	545	GLY	-	EXPRESSION TAG	UNP P10104
D	546	GLY	-	EXPRESSION TAG	UNP P10104
D	547	LEU	-	EXPRESSION TAG	UNP P10104
D	548	VAL	-	EXPRESSION TAG	UNP P10104
D	549	PRO	-	EXPRESSION TAG	UNP P10104
D	550	ARG	-	EXPRESSION TAG	UNP P10104
F	190	PHE	SER	engineered mutation	UNP P03420
F	207	LEU	VAL	engineered mutation	UNP P03420
F	379	VAL	ILE	engineered mutation	UNP P03420
F	447	VAL	MET	engineered mutation	UNP P03420
F	514	SER	-	LINKER	UNP P03420
F	515	ALA	-	LINKER	UNP P03420
F	516	ILE	-	LINKER	UNP P03420
F	517	GLY	-	LINKER	UNP P03420
F	539	LEU	PHE	VIRIANT	UNP P10104
F	545	GLY	-	EXPRESSION TAG	UNP P10104
F	546	GLY	-	EXPRESSION TAG	UNP P10104
F	547	LEU	-	EXPRESSION TAG	UNP P10104
F	548	VAL	-	EXPRESSION TAG	UNP P10104
F	549	PRO	-	EXPRESSION TAG	UNP P10104
F	550	ARG	-	EXPRESSION TAG	UNP P10104

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



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

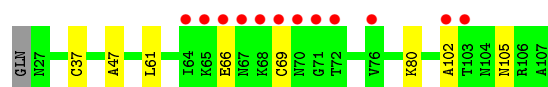
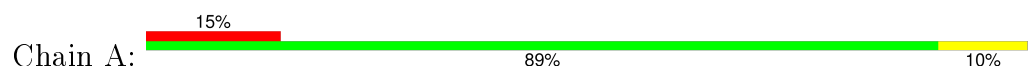
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	21	Total 21	O 21	0	0
4	B	157	Total 157	O 157	0	0
4	C	11	Total 11	O 11	0	0
4	D	161	Total 161	O 161	0	0
4	E	20	Total 20	O 20	0	0
4	F	152	Total 152	O 152	0	0

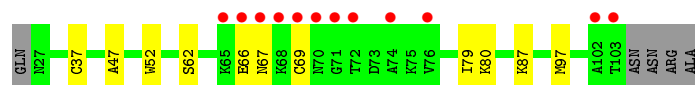
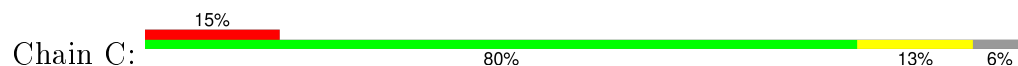
### 3 Residue-property plots [i](#)

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.

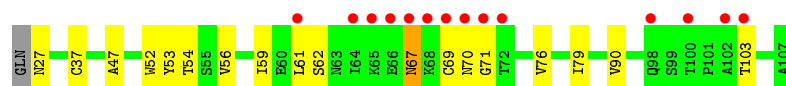
- Molecule 1: Fusion glycoprotein F2



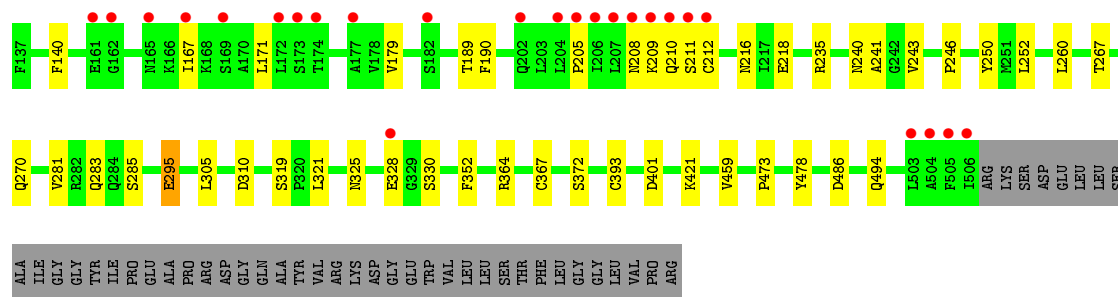
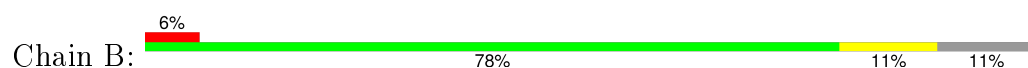
- Molecule 1: Fusion glycoprotein F2



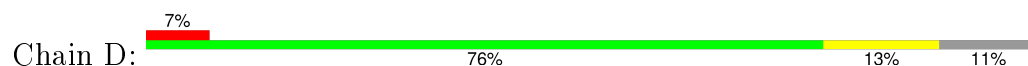
- Molecule 1: Fusion glycoprotein F2



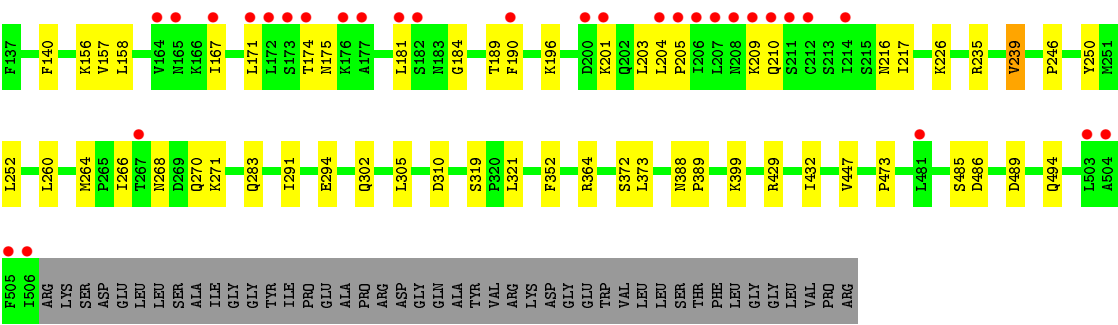
- Molecule 2: Fusion glycoprotein F1 fused with Fibrin trimerization domain



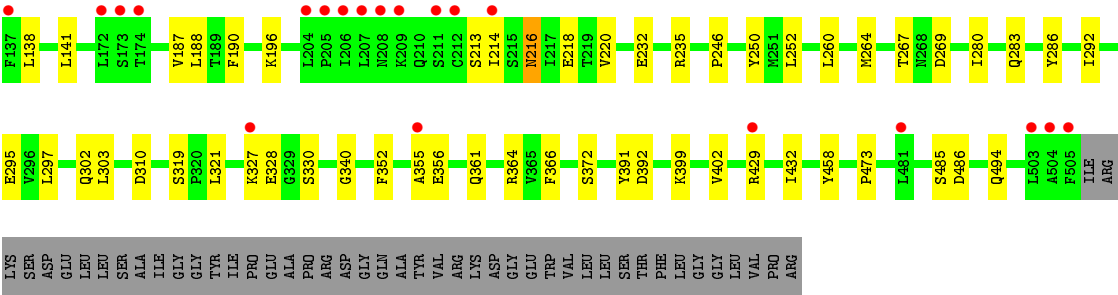
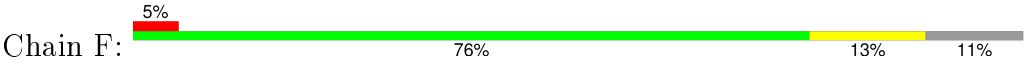
- Molecule 2: Fusion glycoprotein F1 fused with Fibrin trimerization domain







- Molecule 2: Fusion glycoprotein F1 fused with Fibrin trimerization domain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	170.75Å 170.75Å 163.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.86 – 2.40 37.86 – 2.40	Depositor EDS
% Data completeness (in resolution range)	95.5 (37.86-2.40) 95.6 (37.86-2.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.73 (at 2.39Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, $R_{free}$	0.187 , 0.214 0.185 , 0.213	Depositor DCC
$R_{free}$ test set	4593 reflections (5.06%)	DCC
Wilson B-factor (Å <sup>2</sup> )	48.8	Xtriage
Anisotropy	0.122	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 53.2	EDS
Estimated twinning fraction	0.012 for -h,-l,-k 0.005 for l,-k,h	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 90789 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	11013	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.70% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: 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	0.23	0/642	0.48	0/867
1	C	0.26	0/610	0.48	0/824
1	E	0.25	0/642	0.49	0/867
2	B	0.24	0/2896	0.45	0/3929
2	D	0.23	0/2896	0.45	0/3929
2	F	0.24	0/2888	0.47	0/3918
All	All	0.24	0/10574	0.46	0/14334

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	635	0	642	6	0
1	C	603	0	612	8	0
1	E	635	0	642	18	0
2	B	2852	0	2884	36	0
2	D	2852	0	2884	41	0
2	F	2844	0	2873	50	0
3	B	25	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	25	0	0	0	0
3	F	20	0	0	0	0
4	A	21	0	0	2	0
4	B	157	0	0	7	1
4	C	11	0	0	0	0
4	D	161	0	0	11	0
4	E	20	0	0	2	0
4	F	152	0	0	7	1
All	All	11013	0	10537	125	1

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 6.

All (125) 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)
2:F:216:ASN:ND2	2:F:218:GLU:OE2	1.95	1.00
2:F:286:TYR:OH	4:F:765:HOH:O	1.83	0.94
2:D:184:GLY:O	4:D:854:HOH:O	1.95	0.82
2:F:246:PRO:HB3	2:F:283:GLN:HA	1.62	0.81
2:B:246:PRO:HB3	2:B:283:GLN:HA	1.62	0.81
2:B:478:TYR:O	4:B:749:HOH:O	1.99	0.79
2:D:246:PRO:HB3	2:D:283:GLN:HA	1.69	0.75
2:D:264:MET:O	4:D:831:HOH:O	2.05	0.74
2:F:213:SER:OG	4:F:771:HOH:O	2.07	0.72
1:E:70:ASN:OD1	1:E:71:GLY:N	2.22	0.71
2:B:140:PHE:O	4:B:763:HOH:O	2.09	0.70
2:D:266:ILE:O	4:D:831:HOH:O	2.12	0.67
2:F:429:ARG:HG3	2:F:429:ARG:HH11	1.60	0.67
2:F:458:TYR:OH	4:F:716:HOH:O	2.12	0.66
2:B:250:TYR:OH	2:F:235:ARG:NH1	2.29	0.65
3:B:604:SO4:O4	4:B:840:HOH:O	2.15	0.64
2:D:399:LYS:HG3	2:D:485:SER:HB2	1.80	0.63
1:E:56:VAL:HG23	2:F:187:VAL:HG21	1.80	0.62
2:F:328:GLU:OE1	4:F:825:HOH:O	2.16	0.61
2:D:201:LYS:NZ	4:D:821:HOH:O	2.16	0.60
1:A:69:CYS:SG	2:B:212:CYS:N	2.75	0.60
4:A:214:HOH:O	2:B:305:LEU:HD11	2.00	0.59
2:D:271:LYS:NZ	4:D:851:HOH:O	2.33	0.59
2:B:330:SER:O	4:B:816:HOH:O	2.17	0.58
2:F:429:ARG:HH21	2:F:432:ILE:HG21	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:76:VAL:HG22	2:F:214:ILE:HG12	1.86	0.57
2:D:140:PHE:O	4:D:756:HOH:O	2.17	0.57
1:C:62:SER:HB3	2:D:196:LYS:HA	1.86	0.56
2:D:226:LYS:NZ	4:D:819:HOH:O	2.39	0.56
2:B:209:LYS:HB3	2:B:210:GLN:C	2.26	0.56
2:B:401:ASP:OD2	4:B:825:HOH:O	2.18	0.56
1:E:27:ASN:ND2	4:E:211:HOH:O	2.33	0.56
2:F:232:GLU:HG2	2:F:250:TYR:CE2	2.41	0.56
1:A:61:LEU:O	2:B:295:GLU:HB2	2.06	0.55
2:F:429:ARG:NH2	2:F:432:ILE:HG21	2.22	0.54
2:D:310:ASP:OD1	2:D:364:ARG:NH1	2.38	0.54
1:C:79:ILE:HD13	2:D:203:LEU:HD11	1.89	0.54
2:B:235:ARG:NH1	2:D:250:TYR:OH	2.41	0.54
2:B:209:LYS:HG2	2:B:211:SER:O	2.08	0.53
2:F:310:ASP:OD1	2:F:364:ARG:NH1	2.37	0.53
2:B:310:ASP:OD1	2:B:364:ARG:NH1	2.35	0.53
2:D:239:VAL:HG22	2:F:246:PRO:HG2	1.90	0.53
2:B:252:LEU:HD21	2:B:260:LEU:HD12	1.90	0.53
2:F:252:LEU:HD21	2:F:260:LEU:HD12	1.91	0.52
2:D:321:LEU:HD11	2:D:473:PRO:HB3	1.92	0.52
2:F:267:THR:HG22	2:F:269:ASP:H	1.74	0.52
2:D:156:LYS:O	4:D:771:HOH:O	2.19	0.51
1:A:47:ALA:HB2	2:B:364:ARG:HD2	1.92	0.51
2:B:328:GLU:OE1	2:F:391:TYR:HA	2.11	0.51
2:D:432:ILE:HD11	2:D:447:VAL:HG22	1.93	0.51
2:F:399:LYS:HG3	2:F:485:SER:HB2	1.92	0.50
2:D:167:ILE:HG23	2:D:189:THR:HG21	1.92	0.50
1:C:37:CYS:SG	2:D:319:SER:HB3	2.51	0.49
2:D:235:ARG:HD3	2:F:250:TYR:CE2	2.47	0.49
1:E:47:ALA:HB2	2:F:364:ARG:HD2	1.94	0.49
2:D:352:PHE:CE2	2:D:372:SER:HB3	2.47	0.49
1:A:102:ALA:HB2	2:B:241:ALA:HB3	1.93	0.49
2:B:167:ILE:HD13	2:B:179:VAL:HG21	1.95	0.49
2:B:281:VAL:O	2:B:285:SER:OG	2.24	0.49
2:F:429:ARG:HG3	2:F:429:ARG:NH1	2.27	0.49
2:D:252:LEU:HD21	2:D:260:LEU:HD12	1.95	0.48
2:B:209:LYS:HA	2:B:210:GLN:HB2	1.96	0.48
2:B:267:THR:H	2:B:270:GLN:HE21	1.62	0.47
2:B:352:PHE:CE2	2:B:372:SER:HB3	2.49	0.47
2:B:421:LYS:HE2	4:B:853:HOH:O	2.14	0.47
2:F:310:ASP:OD2	4:F:799:HOH:O	2.21	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:67:ASN:HD21	1:C:80:LYS:HD3	1.79	0.47
1:C:47:ALA:HB2	2:D:364:ARG:HD2	1.97	0.47
1:E:70:ASN:ND2	4:E:218:HOH:O	2.47	0.46
1:E:37:CYS:SG	2:F:319:SER:HB3	2.56	0.46
2:F:321:LEU:HD11	2:F:473:PRO:HB3	1.97	0.46
2:B:328:GLU:CD	2:F:392:ASP:H	2.18	0.46
1:E:61:LEU:O	2:F:295:GLU:HB3	2.16	0.46
2:D:184:GLY:C	4:D:854:HOH:O	2.48	0.46
2:B:321:LEU:HD11	2:B:473:PRO:HB3	1.98	0.46
2:F:352:PHE:CE2	2:F:372:SER:HB3	2.51	0.46
2:D:489:ASP:OD2	4:D:840:HOH:O	2.20	0.45
2:D:266:ILE:HD13	2:D:270:GLN:HB2	1.96	0.45
1:E:62:SER:HB3	2:F:196:LYS:HA	1.98	0.45
2:F:327:LYS:HG2	4:F:840:HOH:O	2.16	0.45
1:E:59:ILE:HD12	2:F:297:LEU:HD23	1.99	0.45
2:D:373:LEU:HD13	2:F:402:VAL:HG21	1.99	0.45
2:F:264:MET:CE	2:F:303:LEU:HD12	2.46	0.45
1:E:79:ILE:HD11	2:F:220:VAL:HA	1.98	0.45
1:E:53:TYR:OH	2:F:188:LEU:HB2	2.18	0.44
2:D:217:ILE:HD13	2:F:218:GLU:OE1	2.17	0.44
2:D:204:LEU:N	2:D:205:PRO:HD2	2.33	0.44
1:C:66:GLU:HA	1:C:87:LYS:NZ	2.33	0.43
2:F:327:LYS:HE3	2:F:330:SER:HB2	2.00	0.43
2:F:327:LYS:NZ	4:F:840:HOH:O	2.29	0.43
1:A:80:LYS:NZ	4:A:215:HOH:O	2.37	0.43
1:E:67:ASN:ND2	1:E:67:ASN:O	2.51	0.43
2:B:171:LEU:HD11	2:B:189:THR:HG22	2.00	0.43
2:B:486:ASP:HB2	2:F:494:GLN:NE2	2.33	0.43
2:D:494:GLN:NE2	2:F:486:ASP:HB2	2.34	0.42
2:F:356:GLU:H	2:F:356:GLU:CD	2.22	0.42
2:B:205:PRO:HA	2:B:208:ASN:ND2	2.34	0.42
2:B:216:ASN:HB3	2:B:218:GLU:OE1	2.20	0.42
1:E:90:VAL:HG13	2:F:292:ILE:HD11	2.02	0.42
1:E:52:TRP:CE3	2:F:302:GLN:HG2	2.55	0.42
1:A:37:CYS:SG	2:B:319:SER:HB3	2.59	0.42
2:D:157:VAL:HG11	2:D:181:LEU:HB3	2.01	0.42
2:D:171:LEU:HD11	2:D:189:THR:HG22	2.00	0.42
2:B:393:CYS:HB3	4:B:713:HOH:O	2.19	0.42
2:F:340:GLY:HA2	2:F:355:ALA:HB2	2.00	0.42
2:F:280:ILE:HG21	2:F:366:PHE:CG	2.55	0.42
2:D:266:ILE:HG21	2:D:305:LEU:HD22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:69:CYS:SG	1:E:70:ASN:N	2.93	0.42
2:B:352:PHE:CE2	2:B:367:CYS:HB3	2.55	0.42
2:D:388:ASN:HA	2:D:389:PRO:HD3	1.88	0.41
2:D:209:LYS:HB3	2:D:210:GLN:C	2.40	0.41
2:B:325:ASN:HB3	3:B:605:SO4:O3	2.21	0.41
2:B:267:THR:HB	2:B:270:GLN:HG3	2.02	0.41
1:C:52:TRP:CE3	2:D:302:GLN:HG2	2.55	0.41
2:F:138:LEU:HB3	2:F:141:LEU:HD12	2.01	0.41
2:B:240:ASN:HB3	2:B:243:VAL:O	2.21	0.41
2:F:232:GLU:HG2	2:F:250:TYR:CZ	2.56	0.41
2:F:280:ILE:HD11	2:F:361:GLN:HE21	1.85	0.41
1:E:61:LEU:O	2:F:196:LYS:HB2	2.22	0.40
2:D:268:ASN:OD1	4:D:833:HOH:O	2.22	0.40
2:D:174:THR:OG1	2:D:175:ASN:N	2.54	0.40
2:B:494:GLN:OE1	2:D:486:ASP:HB2	2.21	0.40
1:C:97:MET:HG3	2:D:291:ILE:HA	2.02	0.40
1:E:54:THR:O	2:F:187:VAL:HG23	2.22	0.40
2:D:158:LEU:HB3	2:D:291:ILE:HD13	2.02	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:779:HOH:O	4:F:762:HOH:O[7_555]	2.12	0.08

## 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	79/82 (96%)	72 (91%)	6 (8%)	1 (1%)	15	21
1	C	75/82 (92%)	69 (92%)	6 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	79/82 (96%)	71 (90%)	7 (9%)	1 (1%)	15	21
2	B	368/414 (89%)	352 (96%)	15 (4%)	1 (0%)	46	63
2	D	368/414 (89%)	354 (96%)	12 (3%)	2 (0%)	34	48
2	F	367/414 (89%)	353 (96%)	14 (4%)	0	100	100
All	All	1336/1488 (90%)	1271 (95%)	60 (4%)	5 (0%)	39	56

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	66	GLU
2	D	216	ASN
1	E	103	THR
2	B	295	GLU
2	D	294	GLU

### 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	72/73 (99%)	71 (99%)	1 (1%)	74	88
1	C	69/73 (94%)	68 (99%)	1 (1%)	74	88
1	E	72/73 (99%)	71 (99%)	1 (1%)	74	88
2	B	338/373 (91%)	336 (99%)	2 (1%)	90	96
2	D	338/373 (91%)	335 (99%)	3 (1%)	84	93
2	F	337/373 (90%)	335 (99%)	2 (1%)	90	96
All	All	1226/1338 (92%)	1216 (99%)	10 (1%)	86	94

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	105	ASN
2	B	190	PHE

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Mol	Chain	Res	Type
2	B	459	VAL
1	C	69	CYS
2	D	190	PHE
2	D	239	VAL
2	D	429	ARG
1	E	67	ASN
2	F	190	PHE
2	F	216	ASN

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

Mol	Chain	Res	Type
2	B	270	GLN
2	B	494	GLN
1	E	67	ASN
2	F	317	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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](#)

14 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
3	SO4	B	601	-	4,4,4	0.21	0	6,6,6	0.07	0
3	SO4	B	602	-	4,4,4	0.24	0	6,6,6	0.08	0
3	SO4	B	603	-	4,4,4	0.24	0	6,6,6	0.08	0
3	SO4	B	604	-	4,4,4	0.21	0	6,6,6	0.16	0
3	SO4	B	605	-	4,4,4	0.31	0	6,6,6	0.13	0
3	SO4	D	601	-	4,4,4	0.21	0	6,6,6	0.07	0
3	SO4	D	602	-	4,4,4	0.23	0	6,6,6	0.08	0
3	SO4	D	603	-	4,4,4	0.23	0	6,6,6	0.08	0
3	SO4	D	604	-	4,4,4	0.21	0	6,6,6	0.08	0
3	SO4	D	605	-	4,4,4	0.21	0	6,6,6	0.09	0
3	SO4	F	601	-	4,4,4	0.23	0	6,6,6	0.09	0
3	SO4	F	602	-	4,4,4	0.24	0	6,6,6	0.09	0
3	SO4	F	603	-	4,4,4	0.24	0	6,6,6	0.08	0
3	SO4	F	604	-	4,4,4	0.23	0	6,6,6	0.09	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
3	SO4	B	601	-	-	0/0/0/0	0/0/0/0
3	SO4	B	602	-	-	0/0/0/0	0/0/0/0
3	SO4	B	603	-	-	0/0/0/0	0/0/0/0
3	SO4	B	604	-	-	0/0/0/0	0/0/0/0
3	SO4	B	605	-	-	0/0/0/0	0/0/0/0
3	SO4	D	601	-	-	0/0/0/0	0/0/0/0
3	SO4	D	602	-	-	0/0/0/0	0/0/0/0
3	SO4	D	603	-	-	0/0/0/0	0/0/0/0
3	SO4	D	604	-	-	0/0/0/0	0/0/0/0
3	SO4	D	605	-	-	0/0/0/0	0/0/0/0
3	SO4	F	601	-	-	0/0/0/0	0/0/0/0
3	SO4	F	602	-	-	0/0/0/0	0/0/0/0
3	SO4	F	603	-	-	0/0/0/0	0/0/0/0
3	SO4	F	604	-	-	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 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	604	SO4	1	0
3	B	605	SO4	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	81/82 (98%)	0.61	12 (14%)	3 3	24, 56, 139, 171	0
1	C	77/82 (93%)	0.65	12 (15%)	3 3	23, 58, 157, 173	0
1	E	81/82 (98%)	0.55	14 (17%)	2 2	23, 52, 130, 151	0
2	B	370/414 (89%)	0.24	25 (6%)	20 20	22, 42, 108, 156	0
2	D	370/414 (89%)	0.35	30 (8%)	15 14	21, 46, 124, 152	0
2	F	369/414 (89%)	0.10	20 (5%)	29 30	23, 43, 97, 143	0
All	All	1348/1488 (90%)	0.30	113 (8%)	14 13	21, 46, 121, 173	0

All (113) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	68	LYS	11.8
2	D	172	LEU	9.9
2	F	505	PHE	8.8
2	B	210	GLN	7.8
2	D	505	PHE	7.7
2	D	214	ILE	7.5
1	E	71	GLY	7.1
2	B	211	SER	6.9
2	B	172	LEU	6.9
1	C	72	THR	6.9
2	B	207	LEU	6.9
1	A	66	GLU	6.8
2	D	211	SER	6.7
1	A	70	ASN	6.5
2	B	212	CYS	6.4
1	C	67	ASN	6.4
2	F	504	ALA	6.2
2	D	208	ASN	6.1
1	C	65	LYS	6.1

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Mol	Chain	Res	Type	RSRZ
1	E	66	GLU	6.1
2	D	209	LYS	6.1
2	B	505	PHE	5.9
2	B	208	ASN	5.9
2	D	503	LEU	5.9
1	E	68	LYS	5.8
2	D	173	SER	5.7
1	C	70	ASN	5.6
1	C	66	GLU	5.5
2	D	506	ILE	5.3
1	C	69	CYS	5.3
2	F	481	LEU	5.2
1	C	68	LYS	5.1
2	D	171	LEU	5.1
2	F	207	LEU	5.1
2	B	506	ILE	5.0
1	E	103	THR	4.9
2	D	204	LEU	4.8
2	D	205	PRO	4.8
1	C	71	GLY	4.8
2	D	212	CYS	4.7
2	F	211	SER	4.7
1	E	65	LYS	4.6
1	A	67	ASN	4.5
2	D	210	GLN	4.4
2	D	206	ILE	4.4
2	F	172	LEU	4.3
1	A	71	GLY	4.3
2	B	209	LYS	4.3
2	F	208	ASN	4.3
2	D	207	LEU	4.3
2	D	481	LEU	4.2
1	E	70	ASN	4.1
1	C	76	VAL	4.1
1	A	65	LYS	4.0
1	E	72	THR	4.0
2	D	182	SER	4.0
1	A	72	THR	3.9
2	B	174	THR	3.9
1	A	76	VAL	3.9
2	D	181	LEU	3.9
2	B	206	ILE	3.8

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Mol	Chain	Res	Type	RSRZ
2	F	327	LYS	3.6
2	B	161	GLU	3.6
2	B	503	LEU	3.6
2	F	355	ALA	3.5
1	E	100	THR	3.5
2	D	174	THR	3.5
2	B	205	PRO	3.4
2	D	267	THR	3.4
1	A	102	ALA	3.4
2	B	204	LEU	3.3
2	B	173	SER	3.3
2	D	504	ALA	3.3
2	F	429	ARG	3.2
1	A	69	CYS	3.1
1	A	64	ILE	3.1
1	C	102	ALA	3.1
1	E	102	ALA	3.1
2	B	162	GLY	3.1
2	D	164	VAL	3.1
2	D	190	PHE	3.0
2	F	503	LEU	3.0
1	E	98	GLN	2.9
1	E	69	CYS	2.9
2	D	201	LYS	2.9
2	F	174	THR	2.8
2	D	177	ALA	2.8
2	B	504	ALA	2.8
2	D	165	ASN	2.8
2	B	177	ALA	2.7
2	D	200	ASP	2.7
2	F	204	LEU	2.6
2	F	205	PRO	2.6
2	B	328	GLU	2.5
2	B	167	ILE	2.5
1	A	103	THR	2.5
1	E	67	ASN	2.4
1	C	74	ALA	2.4
2	B	202	GLN	2.4
2	F	173	SER	2.4
2	F	209	LYS	2.3
2	B	182	SER	2.3
2	F	212	CYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	64	ILE	2.2
2	D	167	ILE	2.2
1	C	103	THR	2.1
2	F	214	ILE	2.1
2	B	169	SER	2.1
2	F	206	ILE	2.1
2	D	176	LYS	2.1
1	E	61	LEU	2.1
2	B	165	ASN	2.1
2	F	137	PHE	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
3	SO4	D	602	5/5	0.94	0.22	3.54	76,84,97,104	0
3	SO4	B	602	5/5	0.98	0.24	1.48	72,73,77,97	0
3	SO4	F	601	5/5	0.96	0.21	0.83	79,90,99,102	0
3	SO4	B	603	5/5	0.90	0.19	0.57	104,104,109,109	0
3	SO4	D	604	5/5	0.92	0.11	-0.04	92,114,119,122	0
3	SO4	B	604	5/5	0.90	0.13	-0.56	62,68,100,104	0
3	SO4	F	604	5/5	0.94	0.10	-0.58	93,115,119,122	0
3	SO4	D	605	5/5	0.89	0.12	-1.09	138,138,142,144	0
3	SO4	B	601	5/5	0.99	0.09	-1.33	36,38,42,43	0
3	SO4	D	601	5/5	0.98	0.08	-2.12	48,51,56,63	0
3	SO4	F	602	5/5	0.95	0.13	-	90,100,103,109	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	SO4	F	603	5/5	0.94	0.23	-	126,131,132,133	0
3	SO4	B	605	5/5	0.73	0.18	-	144,151,158,161	0
3	SO4	D	603	5/5	0.92	0.19	-	113,116,116,119	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.