



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2025 – 01:04 pm BST

PDB ID : 9FCM / pdb\_00009fcm  
Title : Single-domain antibody binding the SARS-COV2 S2  
Authors : Vann Molle, I.; Remaut, H.  
Deposited on : 2024-05-15  
Resolution : 1.94 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0rc1
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

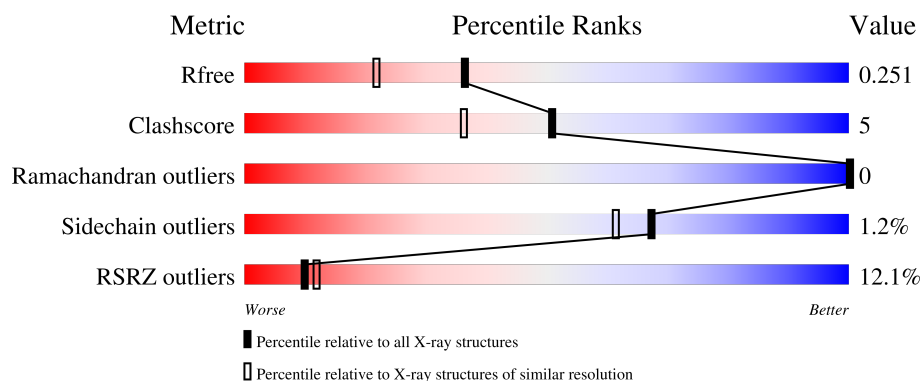
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.94 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))
$R_{free}$	164625	1306 (1.94-1.94)
Clashscore	180529	1400 (1.94-1.94)
Ramachandran outliers	177936	1387 (1.94-1.94)
Sidechain outliers	177891	1387 (1.94-1.94)
RSRZ outliers	164620	1306 (1.94-1.94)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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	149	<div> <div>19%</div> <div> <div>66%</div> <div>14%</div> <div>•</div> <div>18%</div> </div> </div>
1	B	149	<div> <div>5%</div> <div> <div>77%</div> <div>7%</div> <div>15%</div> </div> </div>
1	C	149	<div> <div>3%</div> <div> <div>77%</div> <div>9%</div> <div>•</div> <div>14%</div> </div> </div>
2	D	55	<div> <div>11%</div> <div> <div>71%</div> <div>11%</div> <div>18%</div> </div> </div>
2	E	55	<div> <div>9%</div> <div> <div>69%</div> <div>11%</div> <div>20%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	F	55	<div><div></div><div></div><div></div><div></div></div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4266 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 Single-domain antibody R3DC23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	122	Total	C	N	O	S	3	0	0
			959	603	166	186	4			
1	B	126	Total	C	N	O	S	4	0	0
			981	616	170	191	4			
1	C	128	Total	C	N	O	S	3	2	0
			1000	627	173	196	4			

- Molecule 2 is a protein called Spike protein S2'.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	45	Total	C	N	O	6	0	0
			357	222	60	75			
2	E	44	Total	C	N	O	2	1	0
			353	220	58	75			
2	F	41	Total	C	N	O	2	1	0
			338	210	59	69			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1157	GLY	-	expression tag	UNP P0DTC2
D	1158	PRO	-	expression tag	UNP P0DTC2
E	1157	GLY	-	expression tag	UNP P0DTC2
E	1158	PRO	-	expression tag	UNP P0DTC2
F	1157	GLY	-	expression tag	UNP P0DTC2
F	1158	PRO	-	expression tag	UNP P0DTC2

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		

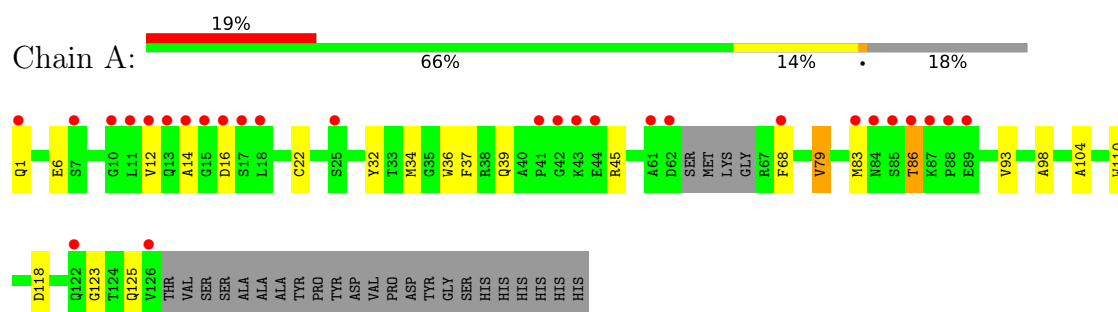
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	36	Total 36	O 36	0	0
4	B	88	Total 88	O 88	0	0
4	C	75	Total 75	O 75	0	0
4	D	28	Total 28	O 28	0	0
4	E	29	Total 29	O 29	0	0
4	F	21	Total 21	O 21	0	0

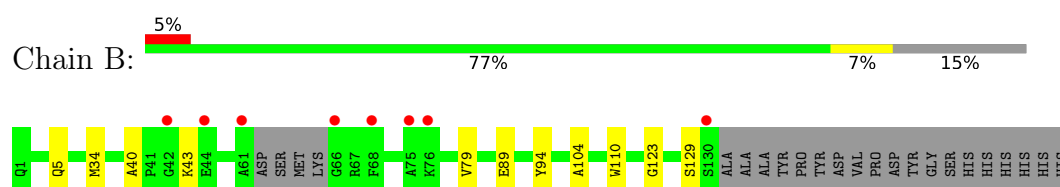
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

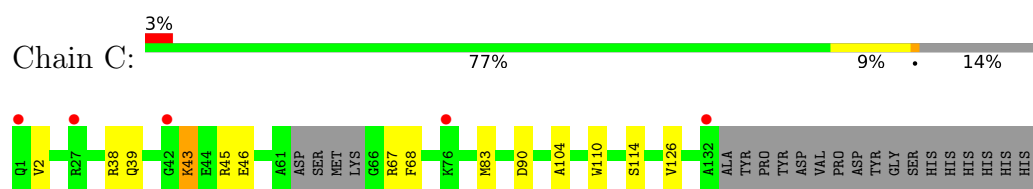
- Molecule 1: Single-domain antibody R3DC23



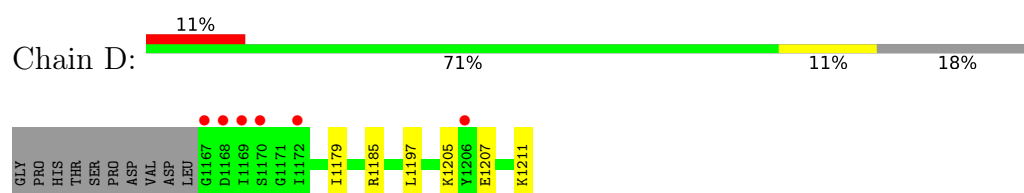
- Molecule 1: Single-domain antibody R3DC23



- Molecule 1: Single-domain antibody R3DC23



- Molecule 2: Spike protein S2'

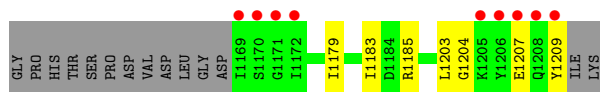


- Molecule 2: Spike protein S2'





- Molecule 2: Spike protein S2'



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.41Å 98.80Å 150.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	82.64 – 1.94 82.64 – 1.94	Depositor EDS
% Data completeness (in resolution range)	78.0 (82.64-1.94) 72.4 (82.64-1.94)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.72 (at 1.94Å)	Xtriage
Refinement program	PHENIX 1.21_5207	Depositor
R, $R_{free}$	0.200 , 0.247 0.201 , 0.251	Depositor DCC
$R_{free}$ test set	2500 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	14.8	Xtriage
Anisotropy	0.106	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 56.4	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	4266	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.69% 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

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	0.29	0/981	0.51	0/1328
1	B	0.35	0/1003	0.55	0/1358
1	C	0.34	0/1025	0.56	0/1388
2	D	0.36	0/358	0.58	0/479
2	E	0.34	0/357	0.53	0/480
2	F	0.35	0/339	0.55	0/455
All	All	0.33	0/4063	0.54	0/5488

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	959	0	902	13	0
1	B	981	0	927	6	0
1	C	1000	0	946	8	0
2	D	357	0	360	6	0
2	E	353	0	353	6	0
2	F	338	0	341	8	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	36	0	0	0	0
4	B	88	0	0	1	0
4	C	75	0	0	1	0
4	D	28	0	0	0	0
4	E	29	0	0	0	0
4	F	21	0	0	1	0
All	All	4266	0	3829	40	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 (40) 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:45:ARG:NH1	4:C:201:HOH:O	2.10	0.82
1:C:83:MET:HE1	1:C:126:VAL:HG21	1.66	0.78
1:C:67:ARG:NH1	1:C:90:ASP:OD2	2.26	0.67
1:C:39:GLN:NE2	1:C:43:LYS:O	2.28	0.67
1:A:1:GLN:NE2	1:A:32:TYR:OH	2.29	0.66
1:A:14:ALA:HA	1:A:86:THR:HG22	1.78	0.65
1:A:22:CYS:HB3	1:A:79:VAL:HG13	1.82	0.61
1:A:34:MET:HE1	1:A:98:ALA:HB2	1.87	0.57
1:B:34:MET:HG2	1:B:79:VAL:HG21	1.87	0.56
2:E:1183:ILE:HD11	2:F:1179:ILE:HG23	1.89	0.54
1:A:93:VAL:HG22	1:A:125:GLN:HG2	1.89	0.54
1:C:68:PHE:CE1	1:C:83:MET:HG2	2.44	0.52
1:B:5:GLN:HG2	4:B:263:HOH:O	2.12	0.50
2:D:1185:ARG:HH11	2:D:1185:ARG:HG2	1.77	0.50
2:F:1185[B]:ARG:NH2	4:F:1301:HOH:O	2.45	0.49
1:A:36:TRP:HE1	1:A:79:VAL:HG22	1.78	0.49
2:D:1211:LYS:HG3	2:E:1206:TYR:CE1	2.48	0.49
1:B:104:ALA:HA	1:B:110:TRP:CD1	2.51	0.46
2:E:1175:SER:O	2:E:1179:ILE:HG12	2.15	0.46
1:A:37:PHE:HB3	1:A:45:ARG:HG2	1.97	0.46
2:F:1204:GLY:HA2	2:F:1207:GLU:HG3	1.98	0.46
1:B:89:GLU:H	1:B:89:GLU:CD	2.23	0.46
1:C:104:ALA:HA	1:C:110:TRP:CD1	2.50	0.45
2:F:1204:GLY:HA2	2:F:1207:GLU:CD	2.41	0.45
2:D:1179:ILE:HG23	2:F:1183:ILE:HD11	1.99	0.45
1:A:104:ALA:HA	1:A:110:TRP:CD1	2.51	0.44
1:C:45:ARG:HD3	1:C:114[A]:SER:OG	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:38:ARG:HD2	1:C:46:GLU:OE2	2.18	0.44
2:D:1207:GLU:HG2	2:F:1209:TYR:CE1	2.53	0.44
2:E:1183:ILE:CD1	2:F:1179:ILE:HG23	2.49	0.43
1:A:68:PHE:CE2	1:A:83:MET:HG2	2.54	0.43
2:D:1197:LEU:HD21	2:E:1196:SER:HB2	2.01	0.42
1:A:118:ASP:OD1	2:D:1205:LYS:HD3	2.19	0.42
1:A:12:VAL:HG22	1:A:16:ASP:HB2	2.00	0.42
2:F:1203:LEU:HA	2:F:1203:LEU:HD12	1.85	0.42
1:B:40:ALA:HB3	1:B:43:LYS:HD3	2.02	0.42
1:B:94:TYR:O	1:B:123:GLY:HA2	2.19	0.42
2:E:1203:LEU:HA	2:E:1203:LEU:HD23	1.83	0.41
1:A:39:GLN:NE2	1:A:45:ARG:HE	2.18	0.41
1:A:6:GLU:CD	1:A:123:GLY:H	2.29	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	118/149 (79%)	116 (98%)	2 (2%)	0	100	100
1	B	122/149 (82%)	120 (98%)	2 (2%)	0	100	100
1	C	126/149 (85%)	124 (98%)	2 (2%)	0	100	100
2	D	43/55 (78%)	42 (98%)	1 (2%)	0	100	100
2	E	43/55 (78%)	43 (100%)	0	0	100	100
2	F	40/55 (73%)	40 (100%)	0	0	100	100
All	All	492/612 (80%)	485 (99%)	7 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 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	97/119 (82%)	95 (98%)	2 (2%)	48	36
1	B	100/119 (84%)	99 (99%)	1 (1%)	73	68
1	C	102/119 (86%)	100 (98%)	2 (2%)	50	38
2	D	40/49 (82%)	40 (100%)	0	100	100
2	E	40/49 (82%)	40 (100%)	0	100	100
2	F	38/49 (78%)	38 (100%)	0	100	100
All	All	417/504 (83%)	412 (99%)	5 (1%)	67	61

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	79	VAL
1	A	86	THR
1	B	129	SER
1	C	2	VAL
1	C	43	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1	GLN
1	A	3	GLN
1	A	39	GLN
1	A	82	GLN
1	A	84	ASN
1	B	5	GLN
1	B	39	GLN
1	C	82	GLN
1	C	84	ASN
2	D	1178	ASN
2	D	1180	GLN

### 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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

## 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	122/149 (81%)	1.12	28 (22%) 2 2	13, 34, 68, 85	11 (9%)
1	B	126/149 (84%)	0.29	8 (6%) 27 30	11, 23, 44, 62	7 (5%)
1	C	128/149 (85%)	0.21	5 (3%) 44 48	8, 24, 38, 49	8 (6%)
2	D	45/55 (81%)	0.50	6 (13%) 8 10	12, 20, 62, 87	6 (13%)
2	E	44/55 (80%)	0.43	5 (11%) 11 13	10, 22, 50, 64	3 (6%)
2	F	41/55 (74%)	0.74	9 (21%) 3 2	10, 21, 53, 65	6 (14%)
All	All	506/612 (82%)	0.54	61 (12%) 10 12	8, 25, 55, 87	41 (8%)

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	1169	ILE	7.7
2	E	1166	LEU	7.5
2	E	1209	TYR	6.4
2	D	1167	GLY	5.6
1	A	12	VAL	5.4
1	A	13	GLN	5.1
1	A	10	GLY	5.0
1	A	84	ASN	4.7
1	A	62	ASP	4.7
2	F	1169	ILE	4.6
1	A	1	GLN	4.5
1	A	86	THR	4.3
1	B	42	GLY	4.2
1	A	11	LEU	4.1
2	F	1206	TYR	4.1
2	F	1209	TYR	4.0
1	A	14	ALA	3.8
1	C	42	GLY	3.6
1	A	16	ASP	3.6

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Mol	Chain	Res	Type	RSRZ
2	D	1170	SER	3.5
2	F	1205	LYS	3.5
2	F	1207	GLU	3.4
1	A	43	LYS	3.3
2	F	1170	SER	3.3
1	A	41	PRO	3.3
1	A	68	PHE	3.3
1	B	130	SER	3.2
2	D	1168	ASP	3.2
1	A	42	GLY	3.2
1	A	89	GLU	3.1
1	A	88	PRO	2.9
1	A	85	SER	2.9
1	A	126	VAL	2.9
1	B	66	GLY	2.9
2	E	1168	ASP	2.9
1	C	132	ALA	2.8
1	C	1	GLN	2.8
1	B	68	PHE	2.7
2	D	1206	TYR	2.6
2	E	1173	ASN	2.6
2	F	1172	ILE	2.6
1	A	18	LEU	2.6
1	A	7	SER	2.5
2	F	1208	GLN	2.5
1	C	27	ARG	2.5
1	B	76	LYS	2.4
2	F	1171	GLY	2.4
2	D	1172	ILE	2.4
1	A	83	MET	2.4
1	B	61	ALA	2.3
1	A	87	LYS	2.3
1	A	44	GLU	2.3
1	B	75	ALA	2.2
1	A	61	ALA	2.2
1	C	76	LYS	2.2
1	A	15	GLY	2.1
1	B	44	GLU	2.1
1	A	17	SER	2.1
1	A	122	GLN	2.1
2	E	1170	SER	2.1
1	A	25	SER	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 monosaccharides 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. 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	B-factors( $\text{\AA}^2$ )	Q<0.9
3	CL	A	201	1/1	0.99	0.05	21,21,21,21	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.