



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 03:23 pm BST

PDB ID : 3ZHG  
Title : Crystallographic structure of the native mouse SIGN-R1 CRD domain  
Authors : Silva-Martin, N.; Bartual, S.G.; Hermoso, J.A.  
Deposited on : 2012-12-21  
Resolution : 1.87 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.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

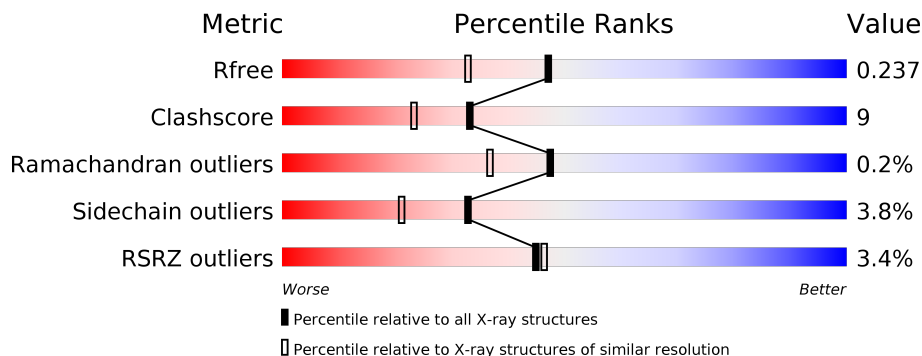
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.87 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))
$R_{free}$	130704	9470 (1.90-1.86)
Clashscore	141614	10282 (1.90-1.86)
Ramachandran outliers	138981	10152 (1.90-1.86)
Sidechain outliers	138945	10152 (1.90-1.86)
RSRZ outliers	127900	9303 (1.90-1.86)

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 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	158	
1	B	158	
1	C	158	
2	D	158	

## 2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 4819 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 CD209 ANTIGEN-LIKE PROTEIN B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	132	1081	689	183	200	9	0	1	0
1	B	132	1073	684	180	200	9	0	0	0
1	C	132	1081	689	183	200	9	0	1	0

There are 69 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	168	MET	-	expression tag	UNP Q8CJ91
A	169	SER	-	expression tag	UNP Q8CJ91
A	170	ALA	-	expression tag	UNP Q8CJ91
A	171	LEU	-	expression tag	UNP Q8CJ91
A	172	LEU	-	expression tag	UNP Q8CJ91
A	173	ILE	-	expression tag	UNP Q8CJ91
A	174	LEU	-	expression tag	UNP Q8CJ91
A	175	ALA	-	expression tag	UNP Q8CJ91
A	176	LEU	-	expression tag	UNP Q8CJ91
A	177	VAL	-	expression tag	UNP Q8CJ91
A	178	GLY	-	expression tag	UNP Q8CJ91
A	179	ALA	-	expression tag	UNP Q8CJ91
A	180	ALA	-	expression tag	UNP Q8CJ91
A	181	VAL	-	expression tag	UNP Q8CJ91
A	182	ALA	-	expression tag	UNP Q8CJ91
A	183	ASP	-	expression tag	UNP Q8CJ91
A	184	TYR	-	expression tag	UNP Q8CJ91
A	185	LYS	-	expression tag	UNP Q8CJ91
A	186	ASP	-	expression tag	UNP Q8CJ91
A	187	ASP	-	expression tag	UNP Q8CJ91
A	188	ASP	-	expression tag	UNP Q8CJ91
A	189	ASP	-	expression tag	UNP Q8CJ91
A	190	LYS	-	expression tag	UNP Q8CJ91

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Chain	Residue	Modelled	Actual	Comment	Reference
B	168	MET	-	expression tag	UNP Q8CJ91
B	169	SER	-	expression tag	UNP Q8CJ91
B	170	ALA	-	expression tag	UNP Q8CJ91
B	171	LEU	-	expression tag	UNP Q8CJ91
B	172	LEU	-	expression tag	UNP Q8CJ91
B	173	ILE	-	expression tag	UNP Q8CJ91
B	174	LEU	-	expression tag	UNP Q8CJ91
B	175	ALA	-	expression tag	UNP Q8CJ91
B	176	LEU	-	expression tag	UNP Q8CJ91
B	177	VAL	-	expression tag	UNP Q8CJ91
B	178	GLY	-	expression tag	UNP Q8CJ91
B	179	ALA	-	expression tag	UNP Q8CJ91
B	180	ALA	-	expression tag	UNP Q8CJ91
B	181	VAL	-	expression tag	UNP Q8CJ91
B	182	ALA	-	expression tag	UNP Q8CJ91
B	183	ASP	-	expression tag	UNP Q8CJ91
B	184	TYR	-	expression tag	UNP Q8CJ91
B	185	LYS	-	expression tag	UNP Q8CJ91
B	186	ASP	-	expression tag	UNP Q8CJ91
B	187	ASP	-	expression tag	UNP Q8CJ91
B	188	ASP	-	expression tag	UNP Q8CJ91
B	189	ASP	-	expression tag	UNP Q8CJ91
B	190	LYS	-	expression tag	UNP Q8CJ91
C	168	MET	-	expression tag	UNP Q8CJ91
C	169	SER	-	expression tag	UNP Q8CJ91
C	170	ALA	-	expression tag	UNP Q8CJ91
C	171	LEU	-	expression tag	UNP Q8CJ91
C	172	LEU	-	expression tag	UNP Q8CJ91
C	173	ILE	-	expression tag	UNP Q8CJ91
C	174	LEU	-	expression tag	UNP Q8CJ91
C	175	ALA	-	expression tag	UNP Q8CJ91
C	176	LEU	-	expression tag	UNP Q8CJ91
C	177	VAL	-	expression tag	UNP Q8CJ91
C	178	GLY	-	expression tag	UNP Q8CJ91
C	179	ALA	-	expression tag	UNP Q8CJ91
C	180	ALA	-	expression tag	UNP Q8CJ91
C	181	VAL	-	expression tag	UNP Q8CJ91
C	182	ALA	-	expression tag	UNP Q8CJ91
C	183	ASP	-	expression tag	UNP Q8CJ91
C	184	TYR	-	expression tag	UNP Q8CJ91
C	185	LYS	-	expression tag	UNP Q8CJ91
C	186	ASP	-	expression tag	UNP Q8CJ91

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Chain	Residue	Modelled	Actual	Comment	Reference
C	187	ASP	-	expression tag	UNP Q8CJ91
C	188	ASP	-	expression tag	UNP Q8CJ91
C	189	ASP	-	expression tag	UNP Q8CJ91
C	190	LYS	-	expression tag	UNP Q8CJ91

- Molecule 2 is a protein called CD209 ANTIGEN-LIKE PROTEIN B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	D	133	1084	690	184	201	9	0	0	0

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	168	MET	-	expression tag	UNP Q8CJ91
D	169	SER	-	expression tag	UNP Q8CJ91
D	170	ALA	-	expression tag	UNP Q8CJ91
D	171	LEU	-	expression tag	UNP Q8CJ91
D	172	LEU	-	expression tag	UNP Q8CJ91
D	173	ILE	-	expression tag	UNP Q8CJ91
D	174	LEU	-	expression tag	UNP Q8CJ91
D	175	ALA	-	expression tag	UNP Q8CJ91
D	176	LEU	-	expression tag	UNP Q8CJ91
D	177	VAL	-	expression tag	UNP Q8CJ91
D	178	GLY	-	expression tag	UNP Q8CJ91
D	179	ALA	-	expression tag	UNP Q8CJ91
D	180	ALA	-	expression tag	UNP Q8CJ91
D	181	VAL	-	expression tag	UNP Q8CJ91
D	182	ALA	-	expression tag	UNP Q8CJ91
D	183	ASP	-	expression tag	UNP Q8CJ91
D	184	TYR	-	expression tag	UNP Q8CJ91
D	185	LYS	-	expression tag	UNP Q8CJ91
D	186	ASP	-	expression tag	UNP Q8CJ91
D	187	ASP	-	expression tag	UNP Q8CJ91
D	188	ASP	-	expression tag	UNP Q8CJ91
D	189	ASP	-	expression tag	UNP Q8CJ91

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



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	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		

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Ca	0	0
			1	1		
4	A	1	Total	Ca	0	0
			1	1		
4	D	1	Total	Ca	0	0
			1	1		
4	C	1	Total	Ca	0	0
			1	1		

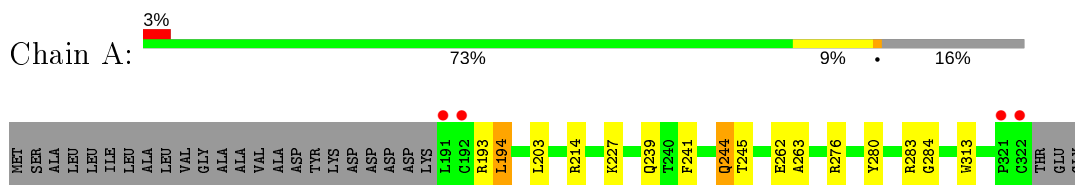
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	138	Total	O	0	0
			138	138		
5	B	66	Total	O	0	0
			66	66		
5	C	129	Total	O	0	0
			129	129		
5	D	73	Total	O	0	0
			73	73		

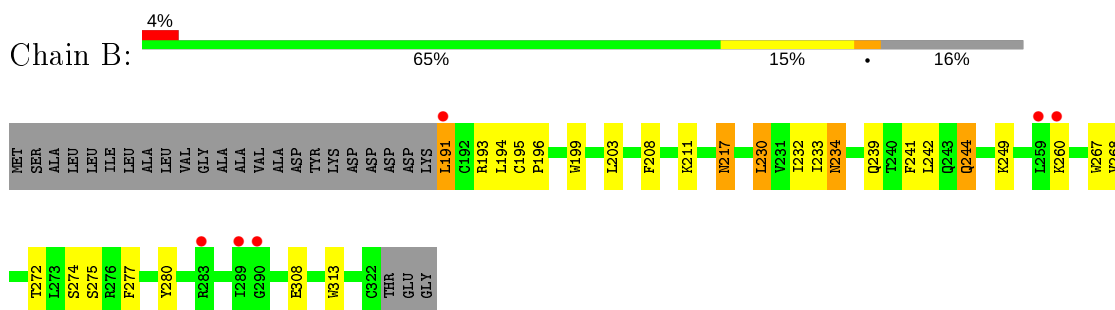
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

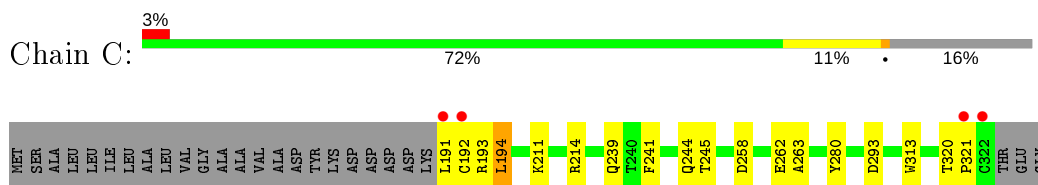
- Molecule 1: CD209 ANTIGEN-LIKE PROTEIN B



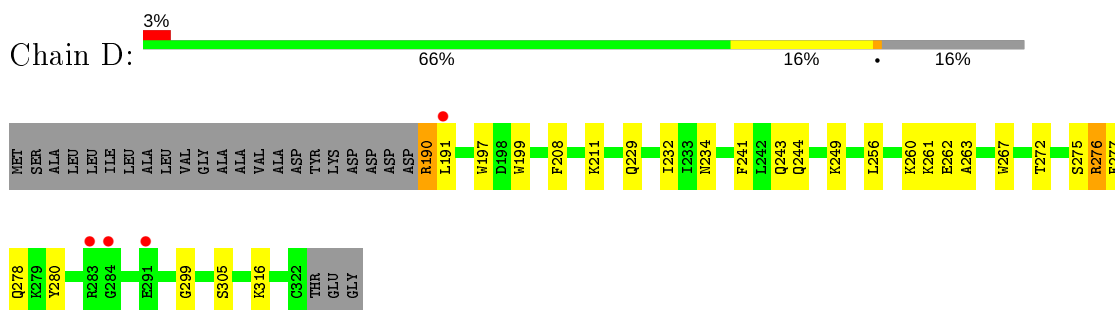
- Molecule 1: CD209 ANTIGEN-LIKE PROTEIN B



- Molecule 1: CD209 ANTIGEN-LIKE PROTEIN B



- Molecule 2: CD209 ANTIGEN-LIKE PROTEIN B





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	146.72Å 92.77Å 77.06Å 90.00° 121.66° 90.00°	Depositor
Resolution (Å)	27.63 – 1.87 74.47 – 1.87	Depositor EDS
% Data completeness (in resolution range)	72.2 (27.63-1.87) 72.2 (74.47-1.87)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.26 (at 1.87Å)	Xtrriage
Refinement program	PHENIX (PHENIX.REFINE: 1.6_289)	Depositor
R, $R_{free}$	0.204 , 0.244 0.199 , 0.237	Depositor DCC
$R_{free}$ test set	3719 reflections (7.09%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.9	Xtrriage
Anisotropy	0.537	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 37.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.477 for -h-2*1,-k,l	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4819	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 35.65 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.6439e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: CA, 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	0.42	0/1114	0.57	0/1507
1	B	0.39	0/1103	0.52	0/1493
1	C	0.41	0/1114	0.55	0/1507
2	D	0.38	0/1114	0.51	0/1507
All	All	0.40	0/4445	0.54	0/6014

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	1081	0	1030	21	0
1	B	1073	0	1017	26	0
1	C	1081	0	1030	13	0
2	D	1084	0	1030	23	0
3	A	30	0	0	1	0
3	B	15	0	0	0	0
3	C	30	0	0	0	0
3	D	15	0	0	1	0
4	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	138	0	0	2	0
5	B	66	0	0	5	0
5	C	129	0	0	0	0
5	D	73	0	0	2	0
All	All	4819	0	4107	73	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 9.

All (73) 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:A:244:GLN:HE22	1:B:203:LEU:H	1.18	0.91
1:C:214:ARG:HG3	1:C:313:TRP:CZ3	2.18	0.79
1:A:214:ARG:HE	1:A:313:TRP:HH2	1.35	0.72
1:A:244:GLN:NE2	1:B:203:LEU:H	1.88	0.71
1:C:244:GLN:NE2	1:C:245:THR:OG1	2.24	0.69
1:A:203:LEU:H	1:B:244:GLN:HE22	1.41	0.68
1:B:277:PHE:CD1	1:B:280:TYR:HE2	2.11	0.68
1:A:214:ARG:HG3	1:A:313:TRP:CZ3	2.29	0.67
1:A:241:PHE:O	1:A:244:GLN:HG3	1.97	0.64
1:A:203:LEU:H	1:B:244:GLN:NE2	1.97	0.61
2:D:229:GLN:HE21	2:D:232:ILE:HD12	1.63	0.61
1:A:214:ARG:NE	1:A:313:TRP:CH2	2.63	0.61
2:D:211:LYS:HD2	2:D:211:LYS:N	2.16	0.61
2:D:277:PHE:CD1	2:D:280:TYR:HE2	2.20	0.60
1:A:283[B]:ARG:HD2	1:A:284:GLY:N	2.17	0.60
1:B:191:LEU:N	5:B:2001:HOH:O	2.36	0.59
1:C:214:ARG:NE	1:C:313:TRP:CH2	2.72	0.58
1:A:194:LEU:HD22	1:B:249:LYS:HE2	1.86	0.58
1:A:214:ARG:NH2	5:A:2026:HOH:O	2.36	0.58
1:C:241:PHE:O	1:C:244:GLN:HG3	2.04	0.57
1:B:232:ILE:HG23	1:B:267:TRP:CD2	2.41	0.56
1:B:268:VAL:HG21	5:B:2031:HOH:O	2.04	0.56
1:B:260:LYS:O	1:B:260:LYS:HG2	2.06	0.55
2:D:190:ARG:N	2:D:190:ARG:HD3	2.21	0.55
1:A:227:LYS:HD2	2:D:197:TRP:CD1	2.42	0.54
1:B:274:SER:HB3	1:B:277:PHE:CD2	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:276:ARG:HD3	2:D:276:ARG:H	1.76	0.51
1:B:217:ASN:H	1:B:217:ASN:ND2	2.09	0.51
1:B:241:PHE:O	1:B:244:GLN:HG3	2.11	0.50
2:D:241:PHE:O	2:D:244:GLN:HG3	2.13	0.49
1:A:276:ARG:NH2	3:A:505:SO4:O3	2.46	0.49
2:D:277:PHE:HD1	2:D:280:TYR:HE2	1.62	0.47
1:A:214:ARG:HH12	1:C:214:ARG:CZ	2.27	0.47
1:B:277:PHE:CD1	1:B:280:TYR:CE2	3.00	0.47
1:C:262:GLU:O	1:C:263:ALA:HB3	2.15	0.47
1:C:194:LEU:HD22	2:D:249:LYS:HE2	1.97	0.47
2:D:199:TRP:CD2	2:D:208:PHE:HB2	2.49	0.46
1:B:217:ASN:ND2	5:B:2023:HOH:O	2.46	0.46
2:D:243:GLN:NE2	2:D:299:GLY:O	2.48	0.46
1:B:211:LYS:HD2	1:B:211:LYS:N	2.31	0.45
1:C:191:LEU:HD23	1:C:192:CYS:N	2.32	0.45
2:D:316:LYS:HD3	5:D:2033:HOH:O	2.16	0.45
1:A:244:GLN:OE1	1:A:245:THR:OG1	2.22	0.45
1:B:193:ARG:HG2	1:B:195:CYS:O	2.16	0.45
2:D:190:ARG:HG2	2:D:191:LEU:N	2.32	0.45
2:D:275:SER:O	2:D:278:GLN:HG3	2.17	0.44
1:B:196:PRO:HB2	1:B:199:TRP:CD1	2.52	0.44
2:D:199:TRP:CE2	2:D:208:PHE:HB2	2.53	0.44
1:B:199:TRP:CD2	1:B:208:PHE:HB2	2.52	0.44
1:C:320:THR:HA	1:C:321:PRO:HD3	1.73	0.44
1:B:234:ASN:ND2	5:B:2032:HOH:O	2.51	0.44
1:C:258:ASP:OD1	1:C:293:ASP:OD1	2.36	0.44
1:A:214:ARG:NH1	1:C:214:ARG:CZ	2.82	0.43
1:B:230:LEU:HD21	1:B:313:TRP:HB2	2.01	0.43
1:B:230:LEU:HA	1:B:230:LEU:HD23	1.93	0.43
1:B:233:ILE:CD1	1:B:242:LEU:HD12	2.49	0.43
1:A:239:GLN:HG2	1:A:280:TYR:CE1	2.54	0.42
1:A:227:LYS:HG2	1:A:227:LYS:O	2.20	0.42
1:C:211:LYS:HB3	2:D:191:LEU:HG	2.02	0.42
1:C:239:GLN:HG2	1:C:280:TYR:CE1	2.55	0.42
1:A:283[B]:ARG:HD2	1:A:284:GLY:H	1.85	0.42
1:A:214:ARG:CZ	5:A:2026:HOH:O	2.67	0.41
2:D:232:ILE:HG23	2:D:267:TRP:CD2	2.55	0.41
1:B:244:GLN:HB3	5:B:2038:HOH:O	2.19	0.41
1:A:262:GLU:O	1:A:263:ALA:HB3	2.21	0.41
1:B:199:TRP:CE2	1:B:208:PHE:HB2	2.56	0.41
1:B:239:GLN:HG2	1:B:280:TYR:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:256:LEU:HB2	2:D:267:TRP:CZ3	2.56	0.41
2:D:229:GLN:HG3	5:D:2033:HOH:O	2.20	0.41
2:D:211:LYS:H	2:D:211:LYS:HD2	1.86	0.40
2:D:262:GLU:O	2:D:263:ALA:HB3	2.22	0.40
2:D:260:LYS:HG2	2:D:260:LYS:O	2.21	0.40
2:D:305:SER:OG	3:D:501:SO4:O1	2.39	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	131/158 (83%)	128 (98%)	3 (2%)	0	100	100
1	B	130/158 (82%)	123 (95%)	7 (5%)	0	100	100
1	C	131/158 (83%)	129 (98%)	2 (2%)	0	100	100
2	D	131/158 (83%)	125 (95%)	5 (4%)	1 (1%)	19	9
All	All	523/632 (83%)	505 (97%)	17 (3%)	1 (0%)	47	37

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	261	LYS

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	118/136 (87%)	115 (98%)	3 (2%)	47	37
1	B	117/136 (86%)	108 (92%)	9 (8%)	13	4
1	C	118/136 (87%)	116 (98%)	2 (2%)	60	54
2	D	118/136 (87%)	114 (97%)	4 (3%)	37	25
All	All	471/544 (87%)	453 (96%)	18 (4%)	33	21

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	193	ARG
1	A	194	LEU
1	A	244	GLN
1	B	191	LEU
1	B	194	LEU
1	B	217	ASN
1	B	230	LEU
1	B	234	ASN
1	B	244	GLN
1	B	272	THR
1	B	275	SER
1	B	308	GLU
1	C	193	ARG
1	C	194	LEU
2	D	190	ARG
2	D	234	ASN
2	D	272	THR
2	D	276	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	234	ASN
1	B	217	ASN
1	B	244	GLN
1	B	278	GLN
1	C	244	GLN
2	D	229	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 22 ligands modelled in this entry, 4 are monoatomic - leaving 18 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	$\# Z  > 2$
3	SO4	A	501	-	4,4,4	0.21	0	6,6,6	0.16	0
3	SO4	B	501	-	4,4,4	0.12	0	6,6,6	0.17	0
3	SO4	C	505	-	4,4,4	0.29	0	6,6,6	0.07	0
3	SO4	C	502	-	4,4,4	0.17	0	6,6,6	0.20	0
3	SO4	A	505	-	4,4,4	0.28	0	6,6,6	0.07	0
3	SO4	A	504	-	4,4,4	0.13	0	6,6,6	0.28	0
3	SO4	C	504	-	4,4,4	0.17	0	6,6,6	0.40	0
3	SO4	A	503	-	4,4,4	0.11	0	6,6,6	0.20	0
3	SO4	C	503	-	4,4,4	0.21	0	6,6,6	0.20	0
3	SO4	D	503	-	4,4,4	0.12	0	6,6,6	0.12	0
3	SO4	C	506	-	4,4,4	0.14	0	6,6,6	0.37	0
3	SO4	D	504	-	4,4,4	0.15	0	6,6,6	0.18	0
3	SO4	A	502	-	4,4,4	0.20	0	6,6,6	0.19	0
3	SO4	B	504	-	4,4,4	0.20	0	6,6,6	0.15	0
3	SO4	B	503	-	4,4,4	0.13	0	6,6,6	0.28	0
3	SO4	A	506	-	4,4,4	0.16	0	6,6,6	0.18	0
3	SO4	C	501	-	4,4,4	0.10	0	6,6,6	0.19	0
3	SO4	D	501	-	4,4,4	0.11	0	6,6,6	0.21	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	A	505	SO4	1	0
3	D	501	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	132/158 (83%)	-0.12	4 (3%) 50 51	18, 28, 44, 74	0
1	B	132/158 (83%)	0.10	6 (4%) 33 34	23, 39, 57, 65	0
1	C	132/158 (83%)	-0.14	4 (3%) 50 51	19, 28, 44, 75	0
2	D	133/158 (84%)	0.11	4 (3%) 50 51	23, 39, 59, 65	0
All	All	529/632 (83%)	-0.01	18 (3%) 45 46	18, 32, 55, 75	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	192	CYS	9.0
1	C	321	PRO	7.2
1	C	322	CYS	7.2
1	A	321	PRO	6.9
1	C	192	CYS	6.7
1	A	322	CYS	5.6
1	A	191	LEU	5.3
2	D	283	ARG	3.8
1	B	259	LEU	3.3
1	B	283	ARG	3.3
1	C	191	LEU	2.8
2	D	191	LEU	2.7
1	B	289	ILE	2.5
2	D	291	GLU	2.4
1	B	191	LEU	2.4
1	B	290	GLY	2.2
1	B	260	LYS	2.1
2	D	284	GLY	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. 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	SO4	C	505	5/5	0.71	0.32	37,37,45,58	0
3	SO4	C	502	5/5	0.83	0.36	45,61,70,72	0
3	SO4	B	504	5/5	0.84	0.29	58,61,74,84	0
3	SO4	D	504	5/5	0.88	0.24	60,60,79,84	0
3	SO4	A	505	5/5	0.91	0.29	32,54,65,73	0
3	SO4	B	503	5/5	0.92	0.12	46,54,64,66	0
3	SO4	C	503	5/5	0.92	0.13	43,44,59,62	0
3	SO4	A	502	5/5	0.92	0.29	40,59,62,66	0
3	SO4	C	501	5/5	0.93	0.20	46,49,56,62	0
3	SO4	A	503	5/5	0.93	0.10	45,46,54,58	0
3	SO4	B	501	5/5	0.94	0.33	55,67,70,72	0
3	SO4	D	501	5/5	0.94	0.22	60,61,68,70	0
4	CA	B	1323	1/1	0.95	0.12	51,51,51,51	0
3	SO4	A	504	5/5	0.96	0.12	48,52,62,62	0
3	SO4	D	503	5/5	0.96	0.09	45,54,63,68	0
4	CA	D	1323	1/1	0.96	0.09	52,52,52,52	0
3	SO4	A	501	5/5	0.96	0.18	44,50,54,57	0
3	SO4	C	504	5/5	0.97	0.17	48,48,58,60	0
3	SO4	A	506	5/5	0.98	0.10	35,36,45,50	0
3	SO4	C	506	5/5	0.98	0.10	33,38,40,49	0
4	CA	C	1323	1/1	0.98	0.04	36,36,36,36	0
4	CA	A	1323	1/1	0.99	0.03	37,37,37,37	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.