

# Full wwPDB X-ray Structure Validation Report (i)

#### Jan 27, 2022 - 06:07 pm GMT

PDB ID	:	7PR0
Title	:	Crystal structure of the receptor binding domain of SARS-CoV-2 Spike glyco-
		protein in complex with FD-5D Fab
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Deposited on	:	2021-09-20
Resolution	:	2.92  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* A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.26
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.26

## 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY \, DIFFRACTION$ 

The reported resolution of this entry is 2.92 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.



Motria	Whole archive	Similar resolution			
	$(\# { m Entries})$	$(\# { m Entries},  { m resolution}  { m range}({ m \AA}))$			
$R_{free}$	130704	2307 (2.94-2.90)			
Clashscore	141614	2531 (2.94-2.90)			
Ramachandran outliers	138981	2462(2.94-2.90)			
Sidechain outliers	138945	2464 (2.94-2.90)			
RSRZ outliers	127900	2248 (2.94-2.90)			

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 >=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 <=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		
			4%		
1	А	205	82%	15%	•
			3%		
1	D	205	88%	8%	•
			7%		
1	Ε	205	86%	10%	•
			5%		
2	В	221	86%	13%	•
			30%		
2	F	221	87%	11%	•



Mol	Chain	Length	Quality of chain								
2	L	221	3% 90%	10%							
3	С	234	<u>6%</u> 86%	9% 5%							
3	G	234	12% 66% 15% •	18%							
3	Н	234	6% 89%	9% •							

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
4	NAG	А	601	-	-	-	Х



## 2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 14592 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	F	197	Total	С	Ν	0	S	0	0	0
			1567	1003	265	291	8			
1	1 A	100	Total	С	Ν	0	S	0	0	0
	199	1581	1011	269	293	8	0	0	0	
1	1 D	107	Total	С	Ν	0	S	0	0	0
	197	1567	1003	265	291	8	0	U	U	

• Molecule 1 is a protein called Spike protein S1.

There are 33 discrepancies between	n the modelled and reference sequences:
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Chain	Residue	Modelled	Actual	Comment	Reference
E	324	GLU	-	expression tag	UNP P0DTC2
Е	325	THR	-	expression tag	UNP P0DTC2
E	326	GLY	-	expression tag	UNP P0DTC2
E	327	HIS	-	expression tag	UNP P0DTC2
E	328	HIS	-	expression tag	UNP P0DTC2
E	329	HIS	-	expression tag	UNP P0DTC2
Е	330	HIS	-	expression tag	UNP P0DTC2
Е	331	HIS	-	expression tag	UNP P0DTC2
Е	332	HIS	-	expression tag	UNP P0DTC2
Е	527	LYS	-	expression tag	UNP P0DTC2
Е	528	LYS	-	expression tag	UNP P0DTC2
А	324	GLU	-	expression tag	UNP P0DTC2
А	325	THR	-	expression tag	UNP P0DTC2
А	326	GLY	-	expression tag	UNP P0DTC2
А	327	HIS	-	expression tag	UNP P0DTC2
А	328	HIS	-	expression tag	UNP P0DTC2
А	329	HIS	-	expression tag	UNP P0DTC2
А	330	HIS	-	expression tag	UNP P0DTC2
А	331	HIS	-	expression tag	UNP P0DTC2
А	332	HIS	-	expression tag	UNP P0DTC2
А	527	LYS	-	expression tag	UNP P0DTC2
А	528	LYS	-	expression tag	UNP P0DTC2
D	324	GLU	-	expression tag	UNP P0DTC2



Chain	Residue	Modelled	Actual	Comment	Reference	
D	325	THR	-	expression tag	UNP P0DTC2	
D	326	GLY	-	expression tag	UNP P0DTC2	
D	327	HIS	-	expression tag	UNP P0DTC2	
D	328	HIS	-	expression tag	UNP P0DTC2	
D	329	HIS	-	expression tag	UNP P0DTC2	
D	330	HIS	-	expression tag	UNP P0DTC2	
D	331	HIS	-	expression tag	UNP P0DTC2	
D	332	HIS	-	expression tag	UNP P0DTC2	
D	527	LYS	-	expression tag	UNP P0DTC2	
D	528	LYS	-	expression tag	UNP P0DTC2	

• Molecule 2 is a protein called FD-5D Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
0	т	221	Total	С	Ν	0	S	0	0	0
		221	1699	1065	285	342	$\overline{7}$	0		
0	0 D	910	Total	С	Ν	0	S	0	0	0
	219	1684	1057	283	338	6	0	0	0	
0	9 F	917	Total	С	Ν	0	S	0	0	0
2 Г	217	1669	1049	278	336	6	U	0	0	

• Molecule 3 is a protein called FD-5D Fab heavy chain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
2	ц	228	Total	С	Ν	0	$\mathbf{S}$	0	0	0
0	11	220	1676	1056	278	335	7	0	0	0
2	3 C	223	Total	С	Ν	0	S	0	0	0
0			1644	1038	272	327	$\overline{7}$			
9	C	101	Total	С	Ν	0	S	0	0	0
3 G	191	1421	898	234	282	7	0	0	0	

• Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	Е	1	Total C N O 14 8 1 5	0	0
4	А	1	Total C N O 14 8 1 5	0	0
4	D	1	Total         C         N         O           14         8         1         5	0	0



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
5	Е	1	Total 5	0 4	S 1	0	0
Continued on next page							

D W I D E

$\alpha$ $\cdot$ 1	C		
Continued	from	previous	page
	5	1	1 0

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	L	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
5	Н	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0

• Molecule 6 is NITRATE ION (three-letter code: NO3) (formula: NO<sub>3</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	L	1	$\begin{array}{ccc} \text{Total} & \text{N} & \text{O} \\ 4 & 1 & 3 \end{array}$	0	0
6	Н	1	Total N O 4 1 3	0	0
6	С	1	Total N O 4 1 3	0	0

• Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	L	1	Total Cl 1 1	0	0
7	Н	1	Total Cl 1 1	0	0
7	G	1	Total Cl 1 1	0	0

![](_page_6_Picture_11.jpeg)

![](_page_7_Figure_3.jpeg)

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
8	F	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0

![](_page_7_Picture_5.jpeg)

## 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.

![](_page_8_Figure_5.jpeg)

• Molecule 1: Spike protein S1

• Molecule 2: FD-5D Fab light chain

![](_page_8_Picture_8.jpeg)

![](_page_9_Figure_3.jpeg)

![](_page_10_Figure_3.jpeg)

![](_page_10_Picture_4.jpeg)

![](_page_10_Picture_5.jpeg)

## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	231.31Å 146.06Å 78.58Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $103.68^{\circ}$ $90.00^{\circ}$	Depositor
Bosolution (Å)	71.50 - 2.92	Depositor
Resolution (A)	73.03 - 2.92	EDS
% Data completeness	92.5(71.50-2.92)	Depositor
(in resolution range)	92.5(73.03-2.92)	EDS
R <sub>merge</sub>	0.28	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.00 (at 2.91 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.19_4092	Depositor
P. P.	0.214 , $0.251$	Depositor
$n, n_{free}$	0.216 , $0.251$	DCC
$R_{free}$ test set	2528 reflections $(4.96%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	104.8	Xtriage
Anisotropy	0.283	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	(Not available), (Not available)	EDS
L-test for twinning <sup>2</sup>	$ L  > = 0.44, < L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	14592	wwPDB-VP
Average B, all atoms $(Å^2)$	125.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.63% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;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.

![](_page_11_Picture_8.jpeg)

<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

## 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, GOL, NO3, NAG, 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).

Mal	Chain	Bond	lengths	Bond angles	
	Unam	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	А	0.27	0/1628	0.50	0/2216
1	D	0.27	0/1613	0.49	0/2196
1	Е	0.29	0/1613	0.51	0/2196
2	В	0.28	0/1722	0.51	0/2342
2	F	0.27	0/1707	0.50	0/2323
2	L	0.27	0/1737	0.52	0/2362
3	С	0.28	0/1683	0.52	0/2295
3	G	0.28	0/1454	0.51	0/1978
3	Н	0.28	0/1716	0.53	0/2340
All	All	0.28	0/14873	0.51	0/20248

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	А	1581	0	1482	20	0
1	D	1567	0	1472	9	0
1	Е	1567	0	1472	13	0
2	В	1684	0	1642	16	1

![](_page_12_Picture_16.jpeg)

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	1669	0	1626	13	0
2	L	1699	0	1653	13	1
3	С	1644	0	1599	12	0
3	G	1421	0	1367	19	0
3	Н	1676	0	1633	12	0
4	А	14	0	13	0	0
4	D	14	0	13	0	0
4	Ε	14	0	13	0	0
5	Ε	5	0	0	0	0
5	Н	5	0	0	0	0
5	L	5	0	0	0	0
6	С	4	0	0	0	0
6	Н	4	0	0	0	0
6	L	4	0	0	0	0
7	G	1	0	0	0	0
7	Н	1	0	0	0	0
7	L	1	0	0	0	0
8	В	6	0	8	0	0
8	F	6	0	8	0	0
All	All	14592	0	14001	118	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 4.

All (118) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:418:ILE:HA	1:A:422:ASN:HD22	1.58	0.69
3:G:52:SER:HB2	3:G:103:THR:HG21	1.76	0.67
2:L:168:GLU:HB2	2:L:182:LEU:HD11	1.75	0.67
3:C:179:VAL:O	3:C:180:HIS:ND1	2.28	0.66
3:G:93:VAL:HG22	3:G:124:THR:HG22	1.77	0.66
1:E:418:ILE:HA	1:E:422:ASN:HD22	1.60	0.66
2:B:168:GLU:HB2	2:B:182:LEU:HD11	1.78	0.66
3:H:143:SER:H	3:H:146:SER:HB3	1.61	0.65
1:E:403:ARG:NH2	1:E:405:ASP:OD2	2.30	0.65
3:G:57:THR:HG21	3:G:108:SER:HB3	1.81	0.61
3:G:67:ARG:NH2	3:G:90:ASP:OD2	2.34	0.60
3:C:93:VAL:HG22	3:C:124:THR:HG22	1.83	0.60
3:H:30:SER:O	3:H:53:SER:OG	2.20	0.60
3:G:83:MET:HB3	3:G:86:LEU:HD21	1.83	0.59

![](_page_13_Picture_9.jpeg)

		Interatomic	Clash	
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)	
2:B:37:TYR:HD2	2:B:97:LEU:HA	1.66	0.59	
1:E:346:ARG:NH2	3:H:117:ASP:OD1	2.35	0.58	
2:B:66:ARG:NH1	2:B:87:ASP:OD2	2.35	0.57	
2:F:29:LEU:HA	2:F:97:LEU:HD22	1.87	0.56	
3:H:148:SER:OG	3:H:149:GLY:N	2.39	0.56	
2:L:129:ASP:HA	2:L:132:LEU:HB2	1.87	0.56	
1:D:418:ILE:HA	1:D:422:ASN:HD22	1.71	0.55	
3:H:34:MET:HB3	3:H:79:LEU:HD22	1.87	0.55	
3:H:91:THR:HG23	3:H:126:THR:HA	1.88	0.55	
1:A:389:ASP:HA	1:D:521:PRO:HG3	1.90	0.53	
3:C:157:LEU:HD22	3:C:159:LYS:HB2	1.91	0.53	
2:F:120:PRO:HB3	2:F:146:PHE:HB3	1.90	0.53	
2:F:191:ALA:O	2:F:195:LYS:HG2	2.09	0.52	
2:F:156:LYS:HB3	2:F:159:ASN:HA	1.90	0.52	
2:F:168:GLU:HB2	2:F:182:LEU:HD11	1.91	0.52	
1:E:384:PRO:HA	1:E:387:LEU:HG	1.92	0.52	
3:H:157:LEU:HD22	3:H:159:LYS:HB2	1.91	0.52	
3:C:34:MET:HB3	3:C:79:LEU:HD22	1.91	0.52	
1:A:518:LEU:HD12	1:A:520:ALA:HB2	1.92	0.51	
1:D:434:ILE:HB	1:D:511:VAL:HG22	1.93	0.51	
3:G:91:THR:HG23	3:G:126:THR:HA	1.92	0.51	
2:B:88:VAL:HG21	2:B:113:ILE:HD11	1.93	0.51	
2:L:196:HIS:O	2:L:218:ARG:HD2	2.11	0.50	
1:E:445:VAL:HG21	2:L:58:ASN:CG	2.32	0.50	
1:A:376:THR:HB	1:A:435:ALA:HB3	1.93	0.50	
1:A:341:VAL:HG22	1:A:356:LYS:HD2	1.94	0.50	
2:B:3:VAL:HG12	2:B:26:SER:HB3	1.93	0.50	
2:F:64:PRO:HG2	2:F:66:ARG:HH21	1.77	0.50	
3:G:166:VAL:HG12	3:G:216:HIS:HD2	1.76	0.50	
1:A:384:PRO:HA	1:A:387:LEU:HG	1.94	0.49	
1:A:403:ARG:HE	1:A:405:ASP:HB2	1.76	0.49	
3:G:3:GLN:O	3:G:4:LEU:HD12	2.12	0.49	
2:B:88:VAL:HG13	2:B:111:VAL:O	2.12	0.49	
1:A:403:ARG:NH2	1:A:405:ASP:OD2	2.26	0.49	
3:G:216:HIS:CE1	3:G:218:PRO:HG2	2.47	0.49	
1:E:392:PHE:HB2	1:A:519:HIS:HB2	1.95	0.48	
3:G:30:SER:O	3:G:53:SER:OG	2.32	0.48	
3:G:168:VAL:HG23	3:G:214:VAL:HG22	1.96	0.48	
2:L:42:LEU:HD13	2:L:91:TYR:CZ	2.49	0.48	
3:C:30:SER:O	3:C:53:SER:OG	2.32	0.47	
2:F:40:TRP:CD2	2:F:78:LEU:HG	2.49	0.47	

![](_page_14_Picture_6.jpeg)

		Interatomic	Clash	
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)	
2:L:220:GLU:HG2	2:L:221:CYS:H	1.79	0.47	
2:B:59:ARG:NH1	2:B:65:ASP:HA	2.30	0.47	
2:B:149:ARG:HB2	2:B:180:TYR:CE2	2.49	0.47	
2:B:23:CYS:HB2	2:B:40:TRP:CH2	2.50	0.46	
3:G:36:TRP:HD1	3:G:70:ILE:HD12	1.81	0.46	
2:L:194:GLU:HG2	2:L:218:ARG:NH2	2.30	0.46	
3:H:70:ILE:HD11	3:H:79:LEU:HD11	1.96	0.46	
1:D:379:CYS:HA	1:D:432:CYS:HA	1.98	0.46	
3:G:60:TYR:CE1	3:G:70:ILE:HG22	2.51	0.46	
3:C:91:THR:HG23	3:C:126:THR:HA	1.98	0.46	
1:A:396:TYR:HB2	1:A:514:SER:HB2	1.98	0.46	
2:B:191:ALA:O	2:B:195:LYS:HG2	2.16	0.46	
3:G:133:LYS:HD3	3:G:191:LEU:HD21	1.98	0.46	
1:A:440:ASN:OD1	1:A:440:ASN:N	2.49	0.46	
1:E:389:ASP:HA	1:A:521:PRO:HG3	1.96	0.45	
2:L:194:GLU:HG2	2:L:218:ARG:HH21	1.81	0.45	
3:G:51:ILE:HG22	3:G:52:SER:O	2.17	0.45	
1:A:339:GLY:O	1:A:343:ASN:HB2	2.17	0.45	
3:H:83:MET:HB3	3:H:86:LEU:HD21	1.98	0.45	
2:B:127:PRO:HB2	2:B:132:LEU:HG	1.99	0.45	
1:A:346:ARG:NH2	3:C:117:ASP:OD1	2.49	0.45	
3:C:83:MET:HE2	3:C:86:LEU:HD21	1.99	0.45	
1:E:440:ASN:OD1	1:E:440:ASN:N	2.50	0.45	
1:E:518:LEU:HD13	1:A:518:LEU:HD21	1.98	0.45	
2:F:88:VAL:HG21	2:F:113:ILE:HD11	1.99	0.44	
3:G:34:MET:SD	3:G:98:SER:HB2	2.57	0.44	
3:H:83:MET:HE2	3:H:86:LEU:HD21	2.00	0.44	
2:B:42:LEU:HD13	2:B:91:TYR:CZ	2.52	0.44	
1:E:350:VAL:HA	1:E:400:PHE:HB2	1.99	0.44	
1:A:379:CYS:HA	1:A:432:CYS:HA	2.00	0.44	
1:A:385:THR:HG23	1:A:386:LYS:HG3	2.00	0.44	
3:C:67:ARG:NH2	3:C:90:ASP:OD2	2.49	0.44	
2:F:23:CYS:HB2	2:F:40:TRP:CH2	2.53	0.43	
2:F:40:TRP:CE2	2:F:78:LEU:HG	2.53	0.43	
2:B:173:GLN:HG3	2:B:180:TYR:CZ	2.54	0.43	
1:E:396:TYR:HB2	1:E:514:SER:HB2	2.00	0.43	
2:F:127:PRO:HD3	2:F:139:VAL:HG22	2.00	0.43	
1:E:386:LYS:O	1:E:390:LEU:HG	2.19	0.42	
2:L:173:GLN:HG3	2:L:180:TYR:CZ	2.54	0.42	
2:B:144:ASN:ND2	3:C:199:THR:HG21	2.34	0.42	
1:A:338:PHE:CD2	1:A:368:LEU:HD21	2.54	0.42	

![](_page_15_Picture_6.jpeg)

Atom 1	Atom 2	Interatomic	Clash	
Atom-1	Atom-2	$distance (\text{\AA})$	overlap (Å)	
2:B:66:ARG:HD2	2:B:82:ARG:O	2.20	0.42	
1:D:385:THR:HG23	1:D:386:LYS:HG3	2.01	0.42	
3:H:18:LEU:HD23	3:H:86:LEU:HD11	2.02	0.42	
1:A:350:VAL:HA	1:A:400:PHE:HB2	2.01	0.42	
1:D:440:ASN:OD1	1:D:440:ASN:N	2.53	0.42	
2:F:2:ILE:HG23	2:F:27:GLN:HG2	2.01	0.42	
3:G:51:ILE:HG13	3:G:70:ILE:HD13	2.02	0.42	
2:B:40:TRP:CD2	2:B:78:LEU:HG	2.54	0.42	
3:G:12:VAL:HG13	3:G:127:VAL:HG22	2.02	0.42	
2:L:71:GLY:HA3	2:L:76:PHE:HA	2.02	0.41	
1:A:444:LYS:HG3	3:C:114:TYR:CG	2.55	0.41	
1:D:384:PRO:HA	1:D:387:LEU:HG	2.01	0.41	
2:F:30:LEU:HD23	2:F:31:HIS:O	2.21	0.41	
3:H:4:LEU:HD22	3:H:22:CYS:SG	2.60	0.41	
3:C:18:LEU:HD23	3:C:86:LEU:HD11	2.02	0.41	
1:D:350:VAL:HG22	1:D:422:ASN:HB3	2.02	0.41	
2:L:40:TRP:CE2	2:L:78:LEU:HG	2.56	0.41	
2:L:40:TRP:CD2	2:L:78:LEU:HG	2.56	0.40	
3:G:184:ALA:HA	3:G:194:LEU:HB3	2.02	0.40	
1:E:371:SER:C	1:E:373:SER:H	2.25	0.40	
2:L:59:ARG:HD3	2:L:67:PHE:O	2.21	0.40	
1:D:396:TYR:O	1:D:513:LEU:HA	2.22	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)
2:L:117:VAL:O	2:B:156:LYS:NZ[4_444]	2.18	0.02

#### 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.

![](_page_16_Picture_11.jpeg)

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
1	А	197/205~(96%)	189 (96%)	8 (4%)	0	100	100
1	D	195/205~(95%)	187~(96%)	8 (4%)	0	100	100
1	Е	195/205~(95%)	185~(95%)	10 (5%)	0	100	100
2	В	217/221~(98%)	211 (97%)	6 (3%)	0	100	100
2	F	215/221~(97%)	211 (98%)	4 (2%)	0	100	100
2	L	219/221~(99%)	211 (96%)	8 (4%)	0	100	100
3	С	219/234~(94%)	211 (96%)	7(3%)	1 (0%)	29	60
3	G	185/234~(79%)	170 (92%)	14 (8%)	1 (0%)	29	60
3	Н	226/234 (97%)	214 (95%)	11 (5%)	1 (0%)	34	65
All	All	1868/1980~(94%)	1789 (96%)	76 (4%)	3 (0%)	47	77

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	С	160	ASP
3	G	165	PRO
3	Н	160	ASP

#### 5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Perce	$\mathbf{ntiles}$
1	А	171/177~(97%)	170 (99%)	1 (1%)	86	95
1	D	170/177~(96%)	167~(98%)	3~(2%)	59	83
1	Ε	170/177~(96%)	170 (100%)	0	100	100
2	В	193/195~(99%)	191 (99%)	2(1%)	76	91
2	F	192/195~(98%)	190~(99%)	2(1%)	76	91
2	L	195/195~(100%)	194 (100%)	1 (0%)	88	96
3	С	184/194~(95%)	184 (100%)	0	100	100
3	G	158/194~(81%)	154 (98%)	4 (2%)	47	77
3	Η	188/194~(97%)	188 (100%)	0	100	100

![](_page_17_Picture_11.jpeg)

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles		
All	All	1621/1698~(96%)	1608 (99%)	13 (1%)	81 93		

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	L	65	ASP
1	А	382	VAL
2	В	65	ASP
2	В	192	ASP
1	D	333	THR
1	D	382	VAL
1	D	511	VAL
2	F	39	ASP
2	F	65	ASP
3	G	51	ILE
3	G	111	PHE
3	G	133	LYS
3	G	213	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

#### 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 monosaccharides in this entry.

#### 5.6 Ligand geometry (i)

Of 14 ligands modelled in this entry, 3 are monoatomic - leaving 11 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

![](_page_18_Picture_17.jpeg)

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).

Mal	Mol Tuno Chain		Deg Link		Bond lengths		Bond angles			
	туре	Chain	nes		Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	А	601	1	14,14,15	0.53	0	17,19,21	0.88	1 (5%)
8	GOL	F	301	-	$5,\!5,\!5$	0.87	0	$5,\!5,\!5$	0.97	0
5	SO4	E	602	-	4,4,4	0.15	0	6,6,6	0.07	0
8	GOL	В	301	-	$5,\!5,\!5$	0.86	0	$5,\!5,\!5$	0.96	0
6	NO3	L	301	-	1,3,3	0.60	0	0,3,3	-	-
4	NAG	D	601	1	14,14,15	0.34	0	17,19,21	0.55	0
5	SO4	Н	402	-	4,4,4	0.14	0	6,6,6	0.07	0
6	NO3	С	301	-	1,3,3	0.65	0	0,3,3	-	-
6	NO3	Н	401	-	$1,\!3,\!3$	0.59	0	0,3,3	-	-
4	NAG	E	601	1	14,14,15	0.29	0	17,19,21	0.51	0
5	SO4	L	302	-	4,4,4	0.15	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
4	NAG	А	601	1	-	2/6/23/26	0/1/1/1
8	GOL	F	301	-	-	4/4/4/4	-
8	GOL	В	301	-	-	2/4/4/4	-
4	NAG	D	601	1	-	0/6/23/26	0/1/1/1
4	NAG	Е	601	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
4	А	601	NAG	C1-O5-C5	3.21	116.54	112.19

There are no chirality outliers.

All (10) torsion outliers are listed below:

![](_page_19_Picture_12.jpeg)

Mol	Chain	Res	Type	Atoms
8	F	301	GOL	O1-C1-C2-C3
4	А	601	NAG	O5-C5-C6-O6
4	Е	601	NAG	O5-C5-C6-O6
4	А	601	NAG	C4-C5-C6-O6
4	Е	601	NAG	C4-C5-C6-O6
8	В	301	GOL	C1-C2-C3-O3
8	F	301	GOL	C1-C2-C3-O3
8	F	301	GOL	O1-C1-C2-O2
8	F	301	GOL	O2-C2-C3-O3
8	В	301	GOL	O2-C2-C3-O3

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.

![](_page_20_Picture_10.jpeg)

## 6 Fit of model and data (i)

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

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median,  $95^{th}$  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	$\langle RSRZ \rangle$	#RSRZ>2	$\mathbf{OWAB}(\mathrm{\AA}^2)$	Q<0.9
1	А	199/205~(97%)	0.48	9 (4%) 33 30	92, 114, 187, 223	0
1	D	197/205~(96%)	0.48	6 (3%) 50 46	86, 119, 203, 230	0
1	Е	197/205~(96%)	0.48	15 (7%) 13 11	91, 110, 188, 223	0
2	В	219/221~(99%)	0.48	10 (4%) 32 29	92, 118, 160, 209	0
2	F	217/221~(98%)	1.46	66 (30%) 0 0	103, 167, 224, 243	0
2	L	221/221~(100%)	0.47	6 (2%) 54 51	88, 105, 137, 195	0
3	С	223/234~(95%)	0.57	14 (6%) 20 17	88, 122, 156, 171	0
3	G	191/234~(81%)	0.87	27 (14%) 2 2	83, 111, 206, 329	0
3	Н	228/234~(97%)	0.49	14 (6%) 21 18	89, 115, 151, 192	0
All	All	1892/1980~(95%)	0.64	167 (8%) 10 7	83, 117, 194, 329	0

All (167) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	203	VAL	8.5
2	F	151	ALA	8.2
2	F	142	LEU	7.6
3	G	174	ALA	6.9
2	F	183	SER	6.3
2	F	208	LEU	5.9
2	F	123	PHE	5.8
2	F	193	TYR	5.6
2	F	141	CYS	5.5
2	F	140	VAL	5.5
3	G	179	VAL	5.4
2	F	153	VAL	5.4
3	G	197	VAL	5.3
3	G	156	CYS	5.0
2	F	205	HIS	4.9

![](_page_21_Picture_10.jpeg)

Mol	Chain	Res	Type	RSRZ
3	G	196	SER	4.9
2	F	118	ALA	4.6
2	F	155	TRP	4.5
3	G	195	SER	4.5
2	F	216	PHE	4.4
2	F	182	LEU	4.4
2	F	13	VAL	4.2
2	F	212	VAL	4.1
3	С	110	LEU	4.1
2	В	37	TYR	4.1
2	F	113	ILE	4.0
3	G	211	ILE	4.0
2	В	103	TRP	3.9
2	F	206	GLN	3.9
2	F	210	SER	3.9
3	G	119	TRP	3.8
3	G	180	HIS	3.8
3	G	138	PHE	3.7
2	F	150	GLU	3.7
2	F	137	ALA	3.6
3	G	157	LEU	3.6
1	Е	451	TYR	3.6
2	F	29	LEU	3.5
2	F	200	ALA	3.5
3	G	170	TRP	3.5
2	F	122	VAL	3.5
3	G	1	GLU	3.4
2	F	125	PHE	3.4
3	G	29	PHE	3.4
3	С	154	LEU	3.4
3	С	35	ASN	3.4
2	В	55	LEU	3.4
2	В	52	LEU	3.3
2	F	143	LEU	3.3
2	F	152	LYS	3.3
2	F	199	TYR	3.3
1	E	486	PHE	3.2
3	G	221	THR	3.2
3	Н	227	VAL	3.2
2	F	170	VAL	3.2
2	F	138	SER	3.2
1	D	410	ILE	3.2

![](_page_22_Picture_6.jpeg)

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Mol	Chain	Res	Type	RSRZ
3	С	99	PRO	3.1
3	G	137	VAL	3.1
1	А	365	TYR	3.1
2	F	161	LEU	3.0
2	F	156	LYS	3.0
2	F	80	ILE	3.0
3	G	212	CYS	3.0
3	С	37	VAL	3.0
3	Н	36	TRP	2.9
2	F	119	ALA	2.9
3	С	111	PHE	2.9
3	G	172	SER	2.9
3	С	50	TYR	2.9
3	Н	94	TYR	2.8
3	G	37	VAL	2.8
1	Е	402	ILE	2.8
2	F	67	PHE	2.7
2	F	78	LEU	2.7
1	D	450	ASN	2.7
2	F	117	VAL	2.7
3	G	214	VAL	2.6
2	F	215	SER	2.6
2	F	126	PRO	2.6
3	Н	86	LEU	2.6
3	С	140	LEU	2.6
1	D	449	TYR	2.6
2	F	40	TRP	2.6
2	F	207	GLY	2.6
3	С	45	LEU	2.6
1	Е	510	VAL	2.5
2	F	83	VAL	2.5
1	A	455	LEU	2.5
1	Е	356	LYS	2.5
2	F	129	ASP	2.5
3	H	48	VAL	2.5
2	L	67	PHE	2.5
2	F	167	GLN	2.5
3	Н	45	LEU	2.5
1	D	400	PHE	2.5
1	A	452	LEU	2.5
3	G	182	PHE	2.5
2	F	124	ILE	2.5

![](_page_23_Picture_6.jpeg)

Mol	Chain	Res	Type	RSRZ
2	F	116	THR	2.5
3	G	177	SER	2.5
3	С	113	TYR	2.5
2	F	107	GLN	2.4
2	F	37	TYR	2.4
3	С	59	TYR	2.4
1	А	392	PHE	2.4
2	В	21	ILE	2.4
3	G	110	LEU	2.4
2	F	127	PRO	2.4
2	F	121	SER	2.4
2	F	157	VAL	2.4
2	L	97	LEU	2.4
3	Н	157	LEU	2.4
2	F	187	THR	2.4
2	F	36	ASN	2.4
2	F	188	LEU	2.4
2	F	21	ILE	2.4
2	В	105	PHE	2.4
2	L	2	ILE	2.4
1	Е	338	PHE	2.4
3	Н	47	TRP	2.3
1	Е	487	ASN	2.3
1	А	341	VAL	2.3
2	F	189	SER	2.3
1	Е	497	PHE	2.3
2	F	82	ARG	2.3
1	Е	410	ILE	2.3
2	L	52	LEU	2.3
1	А	342	PHE	2.2
2	F	209	SER	2.2
1	Е	461	LEU	2.2
2	F	185	THR	2.2
3	Н	100	GLY	2.2
1	А	335	LEU	2.2
3	Н	110	LEU	2.2
1	А	475	ALA	2.2
1	D	495	TYR	2.2
3	С	34	MET	2.2
2	F	214	LYS	2.2
3	Н	18	LEU	2.2
2	В	67	PHE	2.2

![](_page_24_Picture_6.jpeg)

Mol	Chain	$\operatorname{Res}$	Type	RSRZ
3	G	191	LEU	2.2
2	F	204	THR	2.2
1	Е	387	LEU	2.1
1	Е	513	LEU	2.1
2	F	55	LEU	2.1
2	F	159	ASN	2.1
3	G	176	THR	2.1
1	Е	429	PHE	2.1
1	A	492	LEU	2.1
2	В	41	TYR	2.1
2	F	147	TYR	2.1
2	В	42	LEU	2.1
3	Н	214	VAL	2.1
3	G	166	VAL	2.1
1	D	382	VAL	2.1
2	F	201	CYS	2.1
1	Е	374	PHE	2.1
3	С	36	TRP	2.1
3	С	68	PHE	2.1
2	L	41	TYR	2.1
1	Е	377	PHE	2.1
2	В	53	ILE	2.0
3	Н	145	LYS	2.0
3	Н	192	TYR	2.0
3	G	4	LEU	2.0
2	L	220	GLU	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,  $95^{th}$  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.

![](_page_25_Picture_11.jpeg)

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	Q<0.9
5	SO4	Е	602	5/5	0.54	0.28	160,177,201,328	0
5	SO4	Н	402	5/5	0.63	0.18	187,188,202,288	0
7	CL	Н	403	1/1	0.64	0.17	119,119,119,119	0
4	NAG	А	601	14/15	0.67	0.64	195,202,217,218	0
4	NAG	D	601	14/15	0.75	0.28	126,165,180,190	0
4	NAG	Е	601	14/15	0.81	0.25	141,171,186,190	0
8	GOL	В	301	6/6	0.81	0.57	116,117,121,122	0
5	SO4	L	302	5/5	0.83	0.23	158,173,192,194	0
8	GOL	F	301	6/6	0.86	0.45	129,137,138,141	0
6	NO3	Н	401	4/4	0.87	0.17	123,128,131,139	0
6	NO3	С	301	4/4	0.93	0.13	131,134,135,138	0
6	NO3	L	301	4/4	0.94	0.19	118,121,121,123	0
7	CL	G	301	1/1	0.94	0.08	117,117,117,117	0
7	CL	L	303	1/1	0.95	0.08	116,116,116,116	0

## 6.5 Other polymers (i)

There are no such residues in this entry.

![](_page_26_Picture_6.jpeg)