



# Full wwPDB X-ray Structure Validation Report

Oct 9, 2023 – 07:00 AM EDT


PDB ID : 7TN0  
Title : SARS-CoV-2 Omicron RBD in complex with human ACE2 and S304 Fab and S309 Fab  
Authors : McCallum, M.; Czudnochowski, N.; Nix, J.C.; Croll, T.I.; SSGCID; Dillen, J.R.; Snell, G.; Veesler, D.; Seattle Structural Genomics Center for Infectious Disease (SSGCID)  
Deposited on : 2022-01-20  
Resolution : 2.85 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 : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (Phenix) : 1.13  
EDS : 2.35.1  
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) : 2.35.1

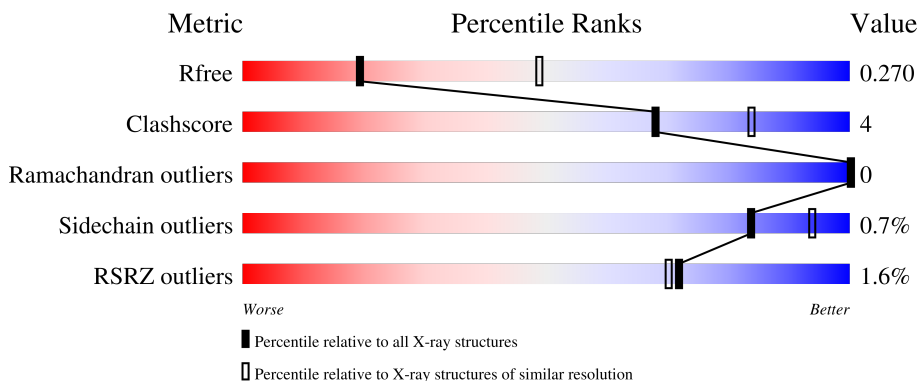
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

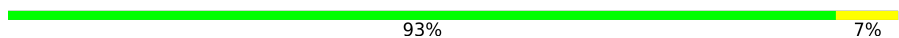
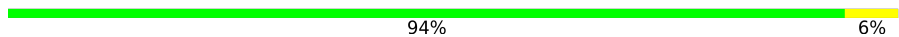
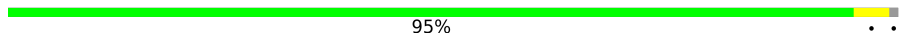

The reported resolution of this entry is 2.85 Å.

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	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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	214	 93% 7%
1	D	214	 94% 6%
2	B	230	 95% . .
2	C	230	 89% 8% .

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Mol	Chain	Length	Quality of chain
3	E	601	 88% 10%
3	F	601	 6% 87% 9%
4	G	215	 88% 12%
4	N	215	 4% 89% 10%
5	H	223	 85% 11%
5	M	223	 87% 9%
6	I	216	 1% 73% 19% 8%
6	S	216	 74% 18% 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
7	EDO	S	601	-	-	-	X
8	CL	B	1002	-	-	-	X

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 24894 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 S309 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	213	Total 1592	C 995	N 271	O 322	S 4	0	0	0
1	D	214	Total 1614	C 1005	N 275	O 330	S 4	0	1	0

- Molecule 2 is a protein called S309 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	228	Total 1684	C 1062	N 287	O 328	S 7	0	0	0
2	C	224	Total 1671	C 1054	N 282	O 328	S 7	0	0	0

- Molecule 3 is a protein called Angiotensin-converting enzyme 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	E	591	Total 4747	C 3042	N 790	O 886	S 29	0	0	0
3	F	547	Total 3745	C 2351	N 668	O 707	S 19	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	616	LEU	-	expression tag	UNP Q9BYF1
E	617	VAL	-	expression tag	UNP Q9BYF1
E	618	PRO	-	expression tag	UNP Q9BYF1
E	619	ARG	-	expression tag	UNP Q9BYF1
F	616	LEU	-	expression tag	UNP Q9BYF1
F	617	VAL	-	expression tag	UNP Q9BYF1
F	618	PRO	-	expression tag	UNP Q9BYF1
F	619	ARG	-	expression tag	UNP Q9BYF1

- Molecule 4 is a protein called S304 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	G	214	Total	C	N	O	S	0	0	0
			1607	1009	269	324	5			
4	N	214	Total	C	N	O	S	0	0	0
			1562	982	262	313	5			

- Molecule 5 is a protein called S304 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	H	215	Total	C	N	O	S	0	0	0
			1591	1009	262	314	6			
5	M	214	Total	C	N	O	S	0	0	0
			1543	979	254	304	6			

- Molecule 6 is a protein called Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	I	198	Total	C	N	O	S	0	1	0
			1565	1008	264	285	8			
6	S	197	Total	C	N	O	S	0	1	0
			1565	1007	268	282	8			

There are 52 discrepancies between the modelled and reference sequences:

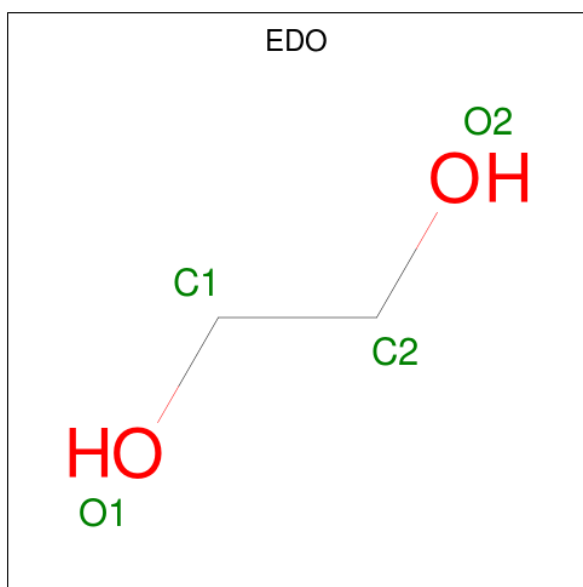
Chain	Residue	Modelled	Actual	Comment	Reference
I	325	THR	SER	variant	UNP P0DTC2
I	326	GLY	ILE	variant	UNP P0DTC2
I	327	THR	VAL	variant	UNP P0DTC2
I	339	ASP	GLY	variant	UNP P0DTC2
I	371	LEU	SER	variant	UNP P0DTC2
I	373	PRO	SER	variant	UNP P0DTC2
I	375	PHE	SER	variant	UNP P0DTC2
I	417	ASN	LYS	variant	UNP P0DTC2
I	440	LYS	ASN	variant	UNP P0DTC2
I	446	SER	GLY	variant	UNP P0DTC2
I	477	ASN	SER	variant	UNP P0DTC2
I	478	LYS	THR	variant	UNP P0DTC2
I	484	ALA	GLU	variant	UNP P0DTC2
I	493	ARG	GLN	variant	UNP P0DTC2
I	496	SER	GLY	variant	UNP P0DTC2
I	498	ARG	GLN	variant	UNP P0DTC2
I	501	TYR	ASN	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
I	505	HIS	TYR	variant	UNP P0DTC2
I	532	HIS	-	expression tag	UNP P0DTC2
I	533	HIS	-	expression tag	UNP P0DTC2
I	534	HIS	-	expression tag	UNP P0DTC2
I	535	HIS	-	expression tag	UNP P0DTC2
I	536	HIS	-	expression tag	UNP P0DTC2
I	537	HIS	-	expression tag	UNP P0DTC2
I	538	HIS	-	expression tag	UNP P0DTC2
I	539	HIS	-	expression tag	UNP P0DTC2
S	325	THR	SER	variant	UNP P0DTC2
S	326	GLY	ILE	variant	UNP P0DTC2
S	327	THR	VAL	variant	UNP P0DTC2
S	339	ASP	GLY	variant	UNP P0DTC2
S	371	LEU	SER	variant	UNP P0DTC2
S	373	PRO	SER	variant	UNP P0DTC2
S	375	PHE	SER	variant	UNP P0DTC2
S	417	ASN	LYS	variant	UNP P0DTC2
S	440	LYS	ASN	variant	UNP P0DTC2
S	446	SER	GLY	variant	UNP P0DTC2
S	477	ASN	SER	variant	UNP P0DTC2
S	478	LYS	THR	variant	UNP P0DTC2
S	484	ALA	GLU	variant	UNP P0DTC2
S	493	ARG	GLN	variant	UNP P0DTC2
S	496	SER	GLY	variant	UNP P0DTC2
S	498	ARG	GLN	variant	UNP P0DTC2
S	501	TYR	ASN	variant	UNP P0DTC2
S	505	HIS	TYR	variant	UNP P0DTC2
S	532	HIS	-	expression tag	UNP P0DTC2
S	533	HIS	-	expression tag	UNP P0DTC2
S	534	HIS	-	expression tag	UNP P0DTC2
S	535	HIS	-	expression tag	UNP P0DTC2
S	536	HIS	-	expression tag	UNP P0DTC2
S	537	HIS	-	expression tag	UNP P0DTC2
S	538	HIS	-	expression tag	UNP P0DTC2
S	539	HIS	-	expression tag	UNP P0DTC2

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 4 2 2	0	0
7	B	1	Total C O 4 2 2	0	0
7	G	1	Total C O 4 2 2	0	0
7	G	1	Total C O 4 2 2	0	0
7	M	1	Total C O 4 2 2	0	0
7	M	1	Total C O 4 2 2	0	0
7	N	1	Total C O 4 2 2	0	0
7	N	1	Total C O 4 2 2	0	0
7	N	1	Total C O 4 2 2	0	0
7	S	1	Total C O 4 2 2	0	0
7	S	1	Total C O 4 2 2	0	0

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	4	Total Cl 4 4	0	0

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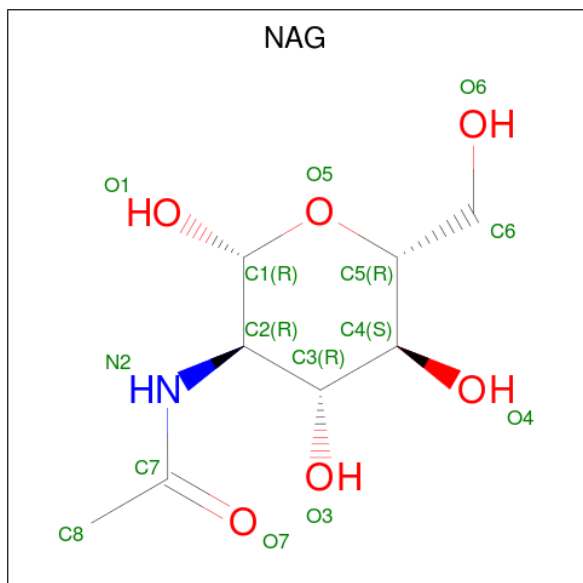
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	2	Total	Cl	0	0
			2	2		
8	C	4	Total	Cl	0	0
			4	4		
8	D	1	Total	Cl	0	0
			1	1		
8	E	4	Total	Cl	0	0
			4	4		
8	F	1	Total	Cl	0	0
			1	1		
8	I	1	Total	Cl	0	0
			1	1		
8	N	1	Total	Cl	0	0
			1	1		
8	S	3	Total	Cl	0	0
			3	3		

- Molecule 9 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	E	1	Total	Zn	0	0
			1	1		
9	F	1	Total	Zn	0	0
			1	1		

- Molecule 10 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	E	1	Total	C	N	O	0	0
			14	8	1	5		
10	E	1	Total	C	N	O	0	0
			14	8	1	5		
10	E	1	Total	C	N	O	0	0
			14	8	1	5		
10	E	1	Total	C	N	O	0	0
			14	8	1	5		
10	F	1	Total	C	N	O	0	0
			14	8	1	5		
10	F	1	Total	C	N	O	0	0
			14	8	1	5		
10	F	1	Total	C	N	O	0	0
			14	8	1	5		
10	I	1	Total	C	N	O	0	0
			14	8	1	5		
10	S	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	15	Total	O	0	0
			15	15		
11	B	13	Total	O	0	0
			13	13		
11	C	31	Total	O	0	0
			31	31		
11	D	27	Total	O	0	0
			27	27		
11	E	32	Total	O	0	0
			32	32		
11	G	12	Total	O	0	0
			12	12		
11	H	9	Total	O	0	0
			9	9		
11	I	10	Total	O	0	0
			10	10		
11	M	9	Total	O	0	0
			9	9		

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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>	<b>ZeroOcc</b>	<b>AltConf</b>
11	N	9	Total O 9 9	0	0
11	S	20	Total O 20 20	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: S309 light chain

Chain A:  93% 7%



- Molecule 1: S309 light chain

Chain D:  94% 6%



- Molecule 2: S309 heavy chain

Chain B:  95%




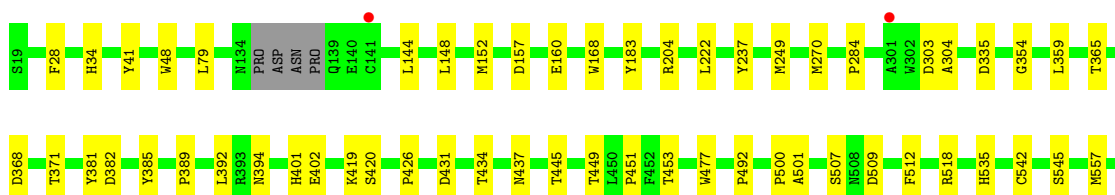
- Molecule 2: S309 heavy chain

Chain C:  89% 8%



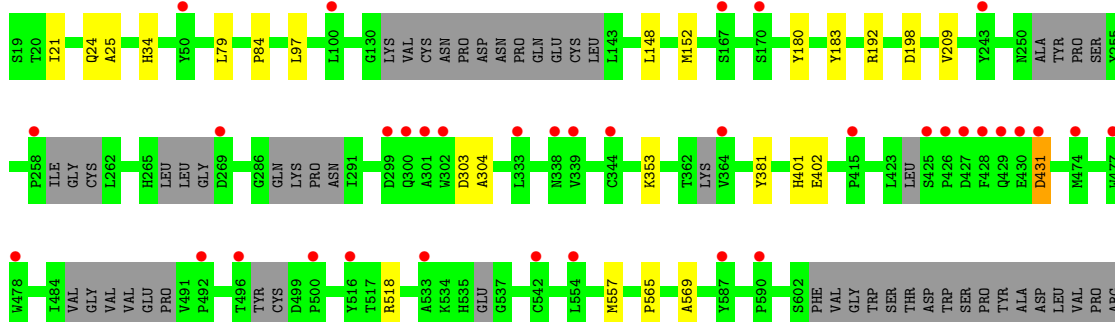
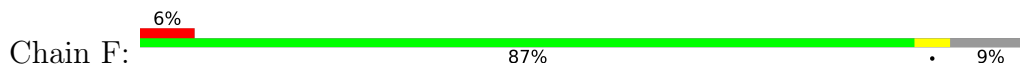
- Molecule 3: Angiotensin-converting enzyme 2

Chain E:  88% 10%





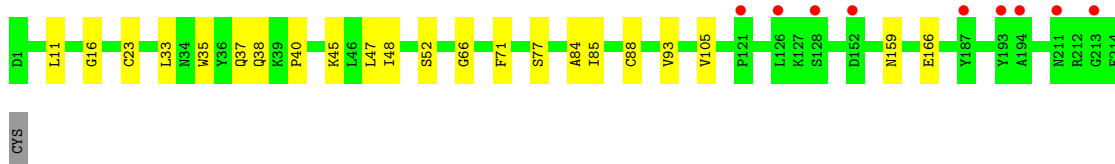
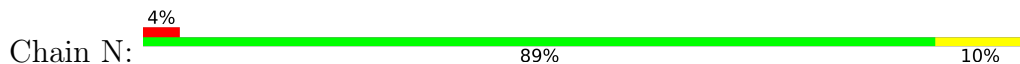
- Molecule 3: Angiotensin-converting enzyme 2



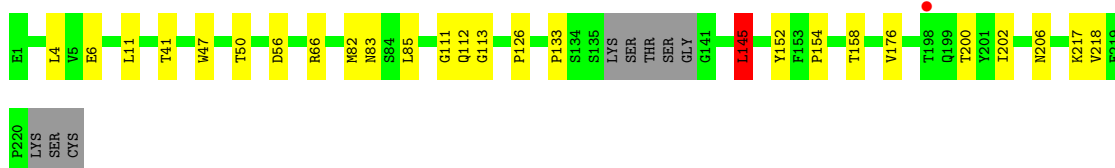
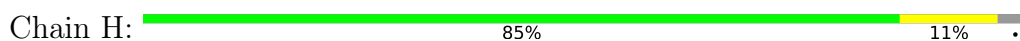
- Molecule 4: S304 Fab light chain



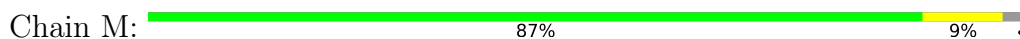
- Molecule 4: S304 Fab light chain



- Molecule 5: S304 Fab heavy chain

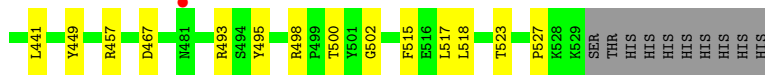
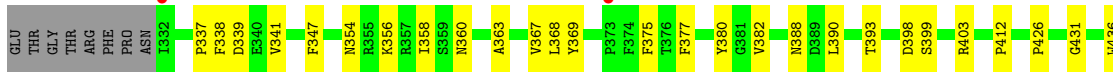
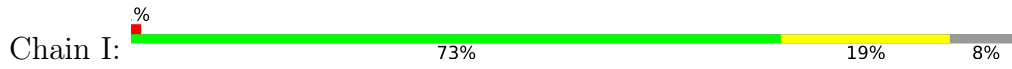


- Molecule 5: S304 Fab heavy chain

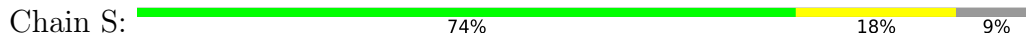




• Molecule 6: Spike protein S1



• Molecule 6: Spike protein S1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	78.28Å 183.65Å 194.55Å 90.00° 95.98° 90.00°	Depositor
Resolution (Å)	48.91 – 2.85 48.91 – 2.85	Depositor EDS
% Data completeness (in resolution range)	95.2 (48.91-2.85) 95.2 (48.91-2.85)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.19 (at 2.86Å)	Xtrriage
Refinement program	PHENIX 1.20_4459, PHENIX 1.20_4459	Depositor
R, $R_{free}$	0.230 , 0.268 0.231 , 0.270	Depositor DCC
$R_{free}$ test set	6055 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	53.5	Xtrriage
Anisotropy	0.409	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 44.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	24894	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	63.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.99% 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: ZN, NAG, EDO, 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	0.26	0/1625	0.51	0/2214
1	D	0.26	0/1650	0.52	0/2246
2	B	0.26	0/1727	0.50	0/2359
2	C	0.27	0/1713	0.53	0/2337
3	E	0.25	0/4880	0.44	0/6637
3	F	0.24	0/3831	0.41	0/5249
4	G	0.28	0/1643	0.58	0/2239
4	N	0.29	0/1598	0.58	0/2188
5	H	0.26	0/1632	0.52	1/2229 (0.0%)
5	M	0.32	1/1584 (0.1%)	0.50	0/2171
6	I	0.31	0/1614	0.62	0/2203
6	S	0.30	0/1612	0.62	0/2193
All	All	0.27	1/25109 (0.0%)	0.51	1/34265 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	1	GLU	CD-OE2	7.10	1.33	1.25

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	145	LEU	CA-CB-CG	5.68	128.38	115.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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	1592	0	1506	8	0
1	D	1614	0	1537	7	0
2	B	1684	0	1584	5	0
2	C	1671	0	1602	11	0
3	E	4747	0	4474	38	0
3	F	3745	0	2841	15	0
4	G	1607	0	1532	18	0
4	N	1562	0	1428	14	0
5	H	1591	0	1502	16	1
5	M	1543	0	1369	11	1
6	I	1565	0	1463	28	0
6	S	1565	0	1470	27	0
7	A	4	0	6	0	0
7	B	4	0	6	0	0
7	G	8	0	12	3	0
7	M	8	0	12	0	0
7	N	12	0	18	1	0
7	S	8	0	12	0	0
8	A	4	0	0	0	0
8	B	2	0	0	0	0
8	C	4	0	0	0	0
8	D	1	0	0	0	0
8	E	4	0	0	0	0
8	F	1	0	0	0	0
8	I	1	0	0	0	0
8	N	1	0	0	0	0
8	S	3	0	0	0	0
9	E	1	0	0	0	0
9	F	1	0	0	0	0
10	E	70	0	65	2	0
10	F	56	0	52	0	0
10	I	14	0	13	2	0
10	S	14	0	13	0	0
11	A	15	0	0	1	0
11	B	13	0	0	1	0
11	C	31	0	0	2	0
11	D	27	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	E	32	0	0	2	0
11	G	12	0	0	0	0
11	H	9	0	0	1	0
11	I	10	0	0	0	0
11	M	9	0	0	1	0
11	N	9	0	0	1	0
11	S	20	0	0	1	0
All	All	24894	0	22517	180	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 (180) 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)
6:S:371:LEU:HB3	6:S:375:PHE:HD2	1.42	0.84
2:B:32:TYR:O	11:B:1101:HOH:O	1.98	0.81
5:H:41:THR:OG1	11:H:301:HOH:O	2.01	0.78
6:S:354:ASN:OD1	6:S:356:LYS:NZ	2.17	0.77
5:M:101:SER:OG	11:M:401:HOH:O	2.05	0.74
6:S:393:THR:HG23	6:S:517:LEU:HD12	1.75	0.69
4:G:11:LEU:HD22	4:G:105:VAL:HG13	1.75	0.68
4:N:33:LEU:HD21	4:N:88:CYS:HB2	1.77	0.67
2:C:226:GLU:OE2	11:C:401:HOH:O	2.13	0.66
4:N:52:SER:O	11:N:401:HOH:O	2.14	0.65
2:B:91:THR:HG23	2:B:124:THR:HA	1.80	0.64
1:A:38:GLN:HB2	1:A:48:LEU:HD11	1.80	0.64
1:D:112:ALA:O	11:D:401:HOH:O	2.14	0.64
6:S:371:LEU:HB3	6:S:375:PHE:CD2	2.29	0.63
6:S:388:ASN:HB3	6:S:527:PRO:HD2	1.79	0.63
4:G:15:VAL:HG22	4:G:107:ILE:HD11	1.81	0.62
6:I:393:THR:HG23	6:I:517:LEU:HD12	1.83	0.61
6:I:388:ASN:HB3	6:I:527:PRO:HD2	1.81	0.61
5:H:202:ILE:HG12	5:H:217:LYS:HA	1.84	0.60
5:H:6:GLU:HG3	5:H:113:GLY:H	1.67	0.60
6:I:449:TYR:OH	6:I:498:ARG:NH2	2.36	0.59
2:C:91:THR:HG23	2:C:124:THR:HA	1.85	0.58
5:M:47:TRP:HE1	5:M:50:THR:HG1	1.50	0.58
6:S:360:ASN:H	6:S:523:THR:HB	1.67	0.58
3:E:445:THR:O	3:E:449:THR:OG1	2.21	0.58
3:F:21:ILE:HD11	3:F:84:PRO:HD2	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:38:GLN:O	4:N:84:ALA:HB1	2.04	0.58
1:D:108:ARG:NH2	11:D:404:HOH:O	2.36	0.57
3:F:402:GLU:HB2	3:F:518:ARG:HG3	1.87	0.57
3:E:501:ALA:O	3:E:507:SER:OG	2.21	0.56
2:C:28:PRO:HB3	6:S:335:LEU:HD13	1.87	0.56
4:N:37:GLN:HB2	4:N:47:LEU:HD11	1.87	0.56
4:G:40:PRO:HB3	4:G:166:GLU:HG3	1.87	0.56
4:G:38:GLN:O	4:G:84:ALA:HB1	2.06	0.55
3:E:535:HIS:CD2	3:E:542:CYS:HB2	2.41	0.55
2:C:35:SER:OG	2:C:99:ASP:OD2	2.22	0.55
3:E:41:TYR:OH	6:I:500:THR:OG1	2.20	0.55
4:G:33:LEU:HD21	4:G:88:CYS:HB2	1.88	0.55
3:E:389:PRO:HD2	3:E:392:LEU:HD12	1.88	0.55
5:H:126:PRO:HB3	5:H:152:TYR:HB3	1.89	0.55
4:G:37:GLN:HB2	4:G:47:LEU:HD11	1.89	0.54
1:D:38:GLN:HB2	1:D:48:LEU:HD11	1.89	0.54
2:B:100:TYR:OH	6:I:339:ASP:HB2	2.07	0.54
6:I:382:VAL:HG21	6:I:390:LEU:CD1	2.38	0.53
5:H:158:THR:HB	5:H:206:ASN:HB3	1.89	0.53
4:G:40:PRO:HG3	7:G:302:EDO:H11	1.91	0.53
5:H:6:GLU:HG3	5:H:113:GLY:N	2.23	0.53
3:F:34:HIS:CE1	6:S:493:ARG:HB3	2.45	0.52
4:G:5:THR:HG22	7:G:301:EDO:H22	1.92	0.52
5:H:4:LEU:O	5:H:112:GLN:NE2	2.42	0.52
6:S:444:LYS:HG2	6:S:448:ASN:HB2	1.91	0.52
6:S:457:ARG:NH1	6:S:467:ASP:OD2	2.42	0.52
6:I:382:VAL:HG21	6:I:390:LEU:HD11	1.92	0.52
5:H:56:ASP:HB3	6:I:369:TYR:CG	2.44	0.52
1:A:190:LYS:HE3	1:A:210:ASN:HB3	1.91	0.52
4:N:40:PRO:HB3	4:N:166:GLU:HG3	1.92	0.51
3:F:79:LEU:HD12	6:S:486:PHE:HD1	1.75	0.51
3:E:402:GLU:HB2	3:E:518:ARG:HG3	1.91	0.51
3:E:144:LEU:HB2	3:E:168:TRP:CZ3	2.46	0.51
3:F:24:GLN:HG2	6:S:475:ALA:O	2.11	0.50
3:E:592:PHE:CZ	3:E:596:LYS:HE3	2.47	0.50
4:G:16:GLY:HA2	4:G:77:SER:OG	2.11	0.50
3:E:270:MET:N	11:E:802:HOH:O	2.24	0.50
6:I:393:THR:HG23	6:I:517:LEU:HA	1.93	0.49
3:F:353:LYS:HD3	6:S:501:TYR:CZ	2.47	0.49
5:H:133:PRO:HD3	5:H:145:LEU:HD12	1.93	0.49
6:S:431:GLY:HA2	6:S:515:PHE:CD2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:ASN:ND2	2:B:197:THR:HG21	2.27	0.49
6:I:338:PHE:O	6:I:341:VAL:HG22	2.12	0.49
1:A:50:TYR:CZ	10:I:601:NAG:H62	2.48	0.49
2:C:50:TRP:CD2	2:C:102:ARG:HD2	2.47	0.49
3:E:365:THR:HG23	3:E:368:ASP:H	1.77	0.48
3:F:180:TYR:HA	3:F:183:TYR:HB3	1.95	0.48
3:E:557:MET:HG2	3:E:569:ALA:HB1	1.95	0.48
3:E:249:MET:HB2	3:E:249:MET:HE2	1.59	0.48
5:H:11:LEU:HB2	5:H:154:PRO:HG3	1.95	0.48
4:G:161:GLN:HB3	5:H:176:VAL:HG11	1.96	0.48
4:N:16:GLY:HA2	4:N:77:SER:OG	2.13	0.48
1:A:32:THR:HG22	6:I:441:LEU:HD22	1.94	0.48
2:C:50:TRP:CH2	2:C:52:SER:HB2	2.49	0.48
5:M:219:GLU:HG2	5:M:220:PRO:HD2	1.96	0.48
4:N:11:LEU:HD22	4:N:105:VAL:HG13	1.96	0.48
6:I:354:ASN:OD1	6:I:356:LYS:HE2	2.14	0.47
6:I:393:THR:HG21	6:I:518:LEU:H	1.78	0.47
5:M:126:PRO:HB3	5:M:152:TYR:HB3	1.95	0.47
4:N:85:ILE:HG13	7:N:304:EDO:H21	1.96	0.47
4:G:15:VAL:CG2	4:G:107:ILE:HD11	2.45	0.47
6:I:338:PHE:HE2	6:I:363:ALA:HB1	1.79	0.47
6:I:368:LEU:HD22	6:I:377:PHE:CE1	2.49	0.47
3:E:431:ASP:HB3	3:E:434:THR:HB	1.97	0.47
2:C:89:ASP:HB3	11:C:421:HOH:O	2.14	0.47
3:E:48:TRP:CZ3	3:E:359:LEU:HB2	2.50	0.47
3:F:25:ALA:HB1	3:F:97:LEU:HD11	1.95	0.47
3:E:34:HIS:NE2	6:I:493:ARG:HB3	2.30	0.46
2:C:6:GLN:H	2:C:119:GLN:HE22	1.64	0.46
3:F:148:LEU:O	3:F:152:MET:HG2	2.15	0.46
1:D:21:LEU:HD23	1:D:102:THR:HB	1.96	0.46
6:S:382:VAL:HG21	6:S:390:LEU:CD1	2.46	0.46
6:S:338:PHE:HE2	6:S:363:ALA:HB1	1.79	0.46
6:S:493:ARG:NH2	11:S:702:HOH:O	2.35	0.46
3:E:477:TRP:CD2	3:E:500:PRO:HG3	2.51	0.46
3:E:394:ASN:HB3	3:E:562:LYS:HE3	1.98	0.46
5:M:56:ASP:HB3	6:S:369:TYR:CG	2.51	0.46
4:G:47:LEU:HA	4:G:58:VAL:HG21	1.98	0.46
5:H:47:TRP:HE1	5:H:50:THR:HG1	1.64	0.46
2:C:11:VAL:O	2:C:12:LYS:HD2	2.15	0.46
6:S:368:LEU:HB3	6:S:377:PHE:CZ	2.51	0.46
4:N:159:ASN:OD1	4:N:159:ASN:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:43:ALA:HB2	5:H:111:GLY:O	2.17	0.45
1:A:98:PHE:O	11:A:401:HOH:O	2.21	0.45
4:G:93:VAL:HG22	6:I:380:TYR:CD2	2.51	0.45
5:M:11:LEU:HB2	5:M:154:PRO:HG3	1.98	0.45
3:E:419:LYS:HE3	3:E:426:PRO:HA	1.99	0.45
3:E:382:ASP:HA	3:E:385:TYR:CZ	2.52	0.45
6:I:367:VAL:HB	10:I:601:NAG:H83	1.99	0.44
6:S:382:VAL:HG22	6:S:383:SER:N	2.32	0.44
3:E:157:ASP:HB3	3:E:160:GLU:HB3	1.99	0.44
4:G:5:THR:O	7:G:301:EDO:H11	2.18	0.44
6:I:347:PHE:CE2	6:I:399:SER:HB2	2.53	0.44
6:S:368:LEU:HD22	6:S:377:PHE:CE1	2.51	0.44
3:E:303:ASP:OD1	3:E:304:ALA:N	2.50	0.44
3:E:371:THR:OG1	11:E:801:HOH:O	2.21	0.44
3:E:335:ASP:N	3:E:335:ASP:OD1	2.50	0.44
3:E:354:GLY:HA3	6:I:502:GLY:HA3	2.00	0.44
3:E:382:ASP:OD1	3:E:385:TYR:OH	2.21	0.44
3:F:192:ARG:HH21	3:F:198:ASP:HB3	1.83	0.44
1:A:21:LEU:HD23	1:A:102:THR:HB	1.98	0.44
4:G:159:ASN:OD1	4:G:159:ASN:N	2.51	0.44
1:A:49:ILE:HD13	1:A:55:ARG:HA	2.00	0.43
3:E:492:PRO:HD3	3:E:613:TYR:CG	2.52	0.43
5:M:66:ARG:NH2	5:M:89:ASP:OD2	2.33	0.43
4:G:23:CYS:HB2	4:G:35:TRP:CH2	2.53	0.43
3:E:183:TYR:OH	3:E:509:ASP:OD1	2.20	0.43
3:E:420:SER:HB2	10:E:710:NAG:O3	2.18	0.43
3:E:453:THR:HG23	3:E:512:PHE:CD2	2.54	0.43
6:I:354:ASN:O	6:I:398:ASP:HA	2.19	0.43
3:F:303:ASP:OD1	3:F:304:ALA:N	2.50	0.42
4:N:66:GLY:HA3	4:N:71:PHE:HA	2.01	0.42
2:C:210:CYS:O	2:C:222:ASP:HA	2.19	0.42
3:F:431:ASP:OD1	3:F:431:ASP:N	2.51	0.42
5:H:82:MET:HB3	5:H:85:LEU:HD21	2.01	0.42
3:F:79:LEU:HD12	6:S:486:PHE:CD1	2.52	0.42
6:I:375:PHE:CD2	6:I:436:TRP:HB3	2.54	0.42
2:B:51:ILE:HD13	2:B:72:THR:HG23	2.02	0.42
3:E:284:PRO:HB3	3:E:594:TRP:CH2	2.53	0.42
5:M:56:ASP:OD1	5:M:56:ASP:N	2.43	0.42
4:N:37:GLN:O	4:N:45:LYS:N	2.41	0.42
3:E:237:TYR:CE1	3:E:451:PRO:HG2	2.54	0.42
5:M:7:SER:N	5:M:21:SER:O	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:284:PRO:HG2	3:E:437:ASN:OD1	2.20	0.42
3:E:545:SER:HB2	10:E:710:NAG:H82	2.01	0.42
6:I:403:ARG:HG3	6:I:495:TYR:CD1	2.55	0.42
6:I:412:PRO:HB3	6:I:426:PRO:O	2.20	0.41
3:E:359:LEU:HD23	3:E:359:LEU:C	2.40	0.41
6:I:457:ARG:NH1	6:I:467:ASP:OD2	2.53	0.41
3:E:204:ARG:HG2	3:E:222:LEU:HD23	2.03	0.41
4:G:66:GLY:HA3	4:G:71:PHE:HA	2.01	0.41
3:F:557:MET:HG2	3:F:569:ALA:HB1	2.01	0.41
6:S:361:CYS:O	6:S:524:VAL:HA	2.21	0.41
2:C:36:TRP:CE2	2:C:81:MET:HB2	2.56	0.41
1:D:83:ASP:O	1:D:87:TYR:OH	2.31	0.41
3:E:28:PHE:HE1	3:E:79:LEU:HD23	1.86	0.41
5:M:155:GLU:OE1	5:M:156:PRO:HA	2.21	0.41
6:S:412:PRO:HB3	6:S:426:PRO:O	2.21	0.41
3:E:477:TRP:CE3	3:E:500:PRO:HG3	2.55	0.41
3:F:209:VAL:HG11	3:F:565:PRO:HB3	2.03	0.41
5:M:34:MET:HB3	5:M:78:LEU:HD22	2.02	0.41
5:H:145:LEU:HG	5:H:218:VAL:HG11	2.02	0.41
6:I:431:GLY:HA2	6:I:515:PHE:CD2	2.56	0.41
3:E:148:LEU:O	3:E:152:MET:HG2	2.21	0.40
4:N:23:CYS:HB2	4:N:35:TRP:CH2	2.55	0.40
4:N:35:TRP:HB2	4:N:48:ILE:HB	2.03	0.40
5:H:66:ARG:HB3	5:H:83:ASN:O	2.21	0.40
6:I:360:ASN:H	6:I:523:THR:HB	1.85	0.40
6:S:386:LYS:HE2	6:S:386:LYS:HB3	1.94	0.40
1:D:29:VAL:HG13	1:D:93:ASP:HB2	2.02	0.40
6:S:389:ASP:OD1	6:S:528:LYS:HD2	2.22	0.40
1:D:49:ILE:HD13	1:D:55:ARG:HA	2.02	0.40
6:I:337:PRO:HD2	6:I:358:ILE:HG23	2.03	0.40
4:N:93:VAL:HG22	6:S:380:TYR:CD2	2.57	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)
5:H:200:THR:OG1	5:M:200:THR:OG1[1_655]	2.07	0.13

## 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	211/214 (99%)	207 (98%)	4 (2%)	0	100	100
1	D	213/214 (100%)	209 (98%)	4 (2%)	0	100	100
2	B	226/230 (98%)	221 (98%)	5 (2%)	0	100	100
2	C	220/230 (96%)	213 (97%)	7 (3%)	0	100	100
3	E	587/601 (98%)	578 (98%)	9 (2%)	0	100	100
3	F	525/601 (87%)	516 (98%)	9 (2%)	0	100	100
4	G	212/215 (99%)	206 (97%)	6 (3%)	0	100	100
4	N	212/215 (99%)	206 (97%)	6 (3%)	0	100	100
5	H	211/223 (95%)	208 (99%)	3 (1%)	0	100	100
5	M	210/223 (94%)	206 (98%)	4 (2%)	0	100	100
6	I	197/216 (91%)	187 (95%)	10 (5%)	0	100	100
6	S	194/216 (90%)	184 (95%)	10 (5%)	0	100	100
All	All	3218/3398 (95%)	3141 (98%)	77 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	171/185 (92%)	169 (99%)	2 (1%)	71	89
1	D	177/185 (96%)	176 (99%)	1 (1%)	86	95

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	175/192 (91%)	173 (99%)	2 (1%)	73	90
2	C	181/192 (94%)	178 (98%)	3 (2%)	60	83
3	E	501/531 (94%)	499 (100%)	2 (0%)	91	96
3	F	269/531 (51%)	266 (99%)	3 (1%)	73	90
4	G	177/188 (94%)	176 (99%)	1 (1%)	86	95
4	N	161/188 (86%)	161 (100%)	0	100	100
5	H	170/186 (91%)	169 (99%)	1 (1%)	86	95
5	M	150/186 (81%)	150 (100%)	0	100	100
6	I	165/190 (87%)	165 (100%)	0	100	100
6	S	163/190 (86%)	162 (99%)	1 (1%)	86	95
All	All	2460/2944 (84%)	2444 (99%)	16 (1%)	84	94

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	LEU
1	A	90	GLN
2	B	81	MET
2	B	130	THR
2	C	25	SER
2	C	205	THR
2	C	210	CYS
1	D	207	LYS
3	E	381	TYR
3	E	401	HIS
3	F	381	TYR
3	F	401	HIS
3	F	431	ASP
4	G	186	ASP
5	H	145	LEU
6	S	339	ASP

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 45 ligands modelled in this entry, 23 are monoatomic - leaving 22 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	$\# Z  > 2$
10	NAG	E	710	3	14,14,15	0.28	0	17,19,21	0.43	0
10	NAG	I	601	6	14,14,15	0.41	0	17,19,21	0.83	1 (5%)
7	EDO	B	1003	-	3,3,3	0.49	0	2,2,2	0.20	0
10	NAG	E	703	3	14,14,15	0.30	0	17,19,21	0.49	0
10	NAG	E	709	3	14,14,15	0.30	0	17,19,21	0.57	0
7	EDO	S	601	-	3,3,3	0.46	0	2,2,2	0.34	0
7	EDO	N	301	-	3,3,3	0.47	0	2,2,2	0.17	0
10	NAG	F	701	3	14,14,15	0.25	0	17,19,21	0.51	0
7	EDO	M	302	-	3,3,3	0.48	0	2,2,2	0.32	0
10	NAG	F	704	3	14,14,15	0.32	0	17,19,21	0.49	0
7	EDO	M	301	-	3,3,3	0.48	0	2,2,2	0.26	0
10	NAG	F	703	3	14,14,15	0.21	0	17,19,21	0.56	0
7	EDO	N	304	-	3,3,3	0.44	0	2,2,2	0.38	0
7	EDO	G	302	-	3,3,3	0.44	0	2,2,2	0.41	0
7	EDO	S	602	-	3,3,3	0.49	0	2,2,2	0.20	0
7	EDO	G	301	-	3,3,3	0.42	0	2,2,2	0.42	0
7	EDO	A	301	-	3,3,3	0.48	0	2,2,2	0.18	0
7	EDO	N	303	-	3,3,3	0.44	0	2,2,2	0.42	0
10	NAG	S	605	6	14,14,15	0.17	0	17,19,21	0.44	0
10	NAG	E	708	3	14,14,15	0.29	0	17,19,21	0.56	0
10	NAG	E	706	3	14,14,15	0.23	0	17,19,21	0.50	0
10	NAG	F	705	3	14,14,15	0.27	0	17,19,21	0.45	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
10	NAG	E	710	3	-	2/6/23/26	0/1/1/1
10	NAG	I	601	6	-	1/6/23/26	0/1/1/1
7	EDO	B	1003	-	-	0/1/1/1	-
10	NAG	E	703	3	-	0/6/23/26	0/1/1/1
10	NAG	E	709	3	-	0/6/23/26	0/1/1/1
7	EDO	S	601	-	-	1/1/1/1	-
7	EDO	N	301	-	-	0/1/1/1	-
10	NAG	F	701	3	-	1/6/23/26	0/1/1/1
7	EDO	M	302	-	-	0/1/1/1	-
10	NAG	F	704	3	-	0/6/23/26	0/1/1/1
7	EDO	M	301	-	-	1/1/1/1	-
10	NAG	F	703	3	-	0/6/23/26	0/1/1/1
7	EDO	N	304	-	-	0/1/1/1	-
7	EDO	G	302	-	-	0/1/1/1	-
7	EDO	S	602	-	-	0/1/1/1	-
7	EDO	G	301	-	-	0/1/1/1	-
7	EDO	A	301	-	-	0/1/1/1	-
7	EDO	N	303	-	-	0/1/1/1	-
10	NAG	S	605	6	-	3/6/23/26	0/1/1/1
10	NAG	E	708	3	-	2/6/23/26	0/1/1/1
10	NAG	E	706	3	-	0/6/23/26	0/1/1/1
10	NAG	F	705	3	-	0/6/23/26	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(°)	Ideal(°)
10	I	601	NAG	C1-O5-C5	3.06	116.34	112.19

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	E	710	NAG	O5-C5-C6-O6
10	E	710	NAG	C4-C5-C6-O6
10	S	605	NAG	O5-C5-C6-O6
10	F	701	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
10	E	708	NAG	C4-C5-C6-O6
10	S	605	NAG	C1-C2-N2-C7
10	E	708	NAG	O5-C5-C6-O6
10	S	605	NAG	C4-C5-C6-O6
10	I	601	NAG	C4-C5-C6-O6
7	M	301	EDO	O1-C1-C2-O2
7	S	601	EDO	O1-C1-C2-O2

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	E	710	NAG	2	0
10	I	601	NAG	2	0
7	N	304	EDO	1	0
7	G	302	EDO	1	0
7	G	301	EDO	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data 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<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	213/214 (99%)	-0.21	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	36, 52, 69, 87	0
1	D	214/214 (100%)	-0.20	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	33, 50, 67, 91	0
2	B	228/230 (99%)	-0.13	1 (0%) <span style="border: 1px solid blue; padding: 2px;">92</span> <span style="border: 1px solid blue; padding: 2px;">92</span>	39, 60, 80, 106	0
2	C	224/230 (97%)	-0.19	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	32, 48, 65, 85	0
3	E	591/601 (98%)	-0.02	2 (0%) <span style="border: 1px solid blue; padding: 2px;">94</span> <span style="border: 1px solid blue; padding: 2px;">94</span>	42, 62, 84, 109	0
3	F	547/601 (91%)	0.22	36 (6%) <span style="border: 1px solid red; padding: 2px;">18</span> <span style="border: 1px solid red; padding: 2px;">14</span>	52, 98, 140, 156	0
4	G	214/215 (99%)	-0.21	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	28, 48, 76, 94	0
4	N	214/215 (99%)	0.08	9 (4%) <span style="border: 1px solid red; padding: 2px;">36</span> <span style="border: 1px solid red; padding: 2px;">31</span>	29, 54, 111, 123	0
5	H	215/223 (96%)	-0.19	1 (0%) <span style="border: 1px solid blue; padding: 2px;">91</span> <span style="border: 1px solid blue; padding: 2px;">90</span>	29, 53, 73, 89	0
5	M	214/223 (95%)	-0.06	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	35, 69, 92, 108	0
6	I	198/216 (91%)	0.02	3 (1%) <span style="border: 1px solid blue; padding: 2px;">73</span> <span style="border: 1px solid blue; padding: 2px;">72</span>	33, 52, 86, 108	0
6	S	197/216 (91%)	-0.02	1 (0%) <span style="border: 1px solid blue; padding: 2px;">91</span> <span style="border: 1px solid blue; padding: 2px;">90</span>	35, 53, 85, 111	0
All	All	3269/3398 (96%)	-0.04	53 (1%) <span style="border: 1px solid blue; padding: 2px;">72</span> <span style="border: 1px solid blue; padding: 2px;">70</span>	28, 59, 115, 156	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	427	ASP	5.1
3	F	415	PRO	3.6
3	F	258	PRO	3.6
3	F	429	GLN	3.5
3	F	430	GLU	3.4
4	N	187	TYR	3.2
3	F	542	CYS	3.1
3	F	425	SER	3.1
3	F	590	PRO	3.1
3	F	492	PRO	3.0
3	F	243	TYR	3.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	F	269	ASP	3.0
3	F	301	ALA	2.9
3	F	587	TYR	2.9
3	F	364	VAL	2.9
3	F	302	TRP	2.8
3	F	170	SER	2.8
3	F	533	ALA	2.8
4	N	121	PRO	2.7
3	F	300	GLN	2.6
2	B	146	SER	2.6
3	F	500	PRO	2.5
3	F	339	VAL	2.5
3	E	141	CYS	2.5
4	N	126	LEU	2.5
6	I	373	PRO	2.4
3	F	477	TRP	2.4
3	F	344	CYS	2.4
3	E	301	ALA	2.4
6	S	370	ASN	2.4
4	N	193	TYR	2.3
4	N	152	ASP	2.3
3	F	333	LEU	2.3
3	F	478	TRP	2.3
6	I	481	ASN	2.3
3	F	431	ASP	2.2
3	F	496	THR	2.2
3	F	426	PRO	2.2
3	F	474	MET	2.2
4	N	213	GLY	2.2
3	F	100	LEU	2.2
3	F	50	TYR	2.2
3	F	428	PHE	2.2
4	N	194	ALA	2.2
3	F	167	SER	2.2
4	N	211	ASN	2.1
3	F	554	LEU	2.1
3	F	516	TYR	2.1
3	F	299	ASP	2.1
4	N	128	SER	2.0
3	F	338	ASN	2.0
6	I	332	ILE	2.0
5	H	198	THR	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(Å <sup>2</sup> )	Q<0.9
8	CL	C	304	1/1	0.68	0.30	104,104,104,104	0
8	CL	B	1001	1/1	0.70	0.18	77,77,77,77	0
8	CL	B	1002	1/1	0.73	0.56	80,80,80,80	0
7	EDO	N	301	4/4	0.75	0.37	53,67,74,77	0
10	NAG	F	701	14/15	0.75	0.29	112,122,135,138	0
10	NAG	E	710	14/15	0.77	0.37	81,100,109,110	0
7	EDO	S	601	4/4	0.79	0.49	80,82,83,87	0
7	EDO	B	1003	4/4	0.80	0.26	57,64,79,82	0
8	CL	A	302	1/1	0.81	0.54	84,84,84,84	0
10	NAG	E	706	14/15	0.81	0.23	85,102,112,114	0
7	EDO	M	302	4/4	0.82	0.46	51,59,64,78	0
8	CL	C	301	1/1	0.83	0.22	83,83,83,83	0
8	CL	A	304	1/1	0.84	0.18	70,70,70,70	0
7	EDO	A	301	4/4	0.85	0.21	60,61,64,71	0
10	NAG	F	705	14/15	0.85	0.42	106,116,125,127	0
10	NAG	I	601	14/15	0.85	0.25	75,86,104,106	0
8	CL	S	603	1/1	0.87	0.12	54,54,54,54	0
10	NAG	F	704	14/15	0.87	0.32	97,114,120,125	0
10	NAG	E	708	14/15	0.88	0.20	77,89,98,103	0
8	CL	S	604	1/1	0.88	0.11	74,74,74,74	0
7	EDO	M	301	4/4	0.88	0.26	44,49,53,55	0
10	NAG	E	709	14/15	0.89	0.20	53,68,76,88	0
8	CL	A	305	1/1	0.89	0.37	76,76,76,76	0
10	NAG	E	703	14/15	0.89	0.19	71,89,95,106	0
10	NAG	S	605	14/15	0.89	0.25	71,79,102,105	0
8	CL	E	707	1/1	0.90	0.18	78,78,78,78	0
10	NAG	F	703	14/15	0.90	0.17	61,72,84,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
8	CL	C	303	1/1	0.90	0.11	83,83,83,83	0
9	ZN	E	702	1/1	0.91	0.11	94,94,94,94	0
8	CL	E	701	1/1	0.91	0.37	71,71,71,71	0
9	ZN	F	702	1/1	0.92	0.04	117,117,117,117	0
8	CL	S	606	1/1	0.92	0.14	68,68,68,68	0
8	CL	D	301	1/1	0.93	0.12	63,63,63,63	0
8	CL	F	706	1/1	0.93	0.14	84,84,84,84	0
7	EDO	S	602	4/4	0.93	0.27	46,48,59,62	0
8	CL	E	705	1/1	0.94	0.19	70,70,70,70	0
8	CL	I	602	1/1	0.94	0.17	62,62,62,62	0
7	EDO	N	303	4/4	0.95	0.33	42,45,51,53	0
7	EDO	G	302	4/4	0.95	0.27	35,47,52,54	0
7	EDO	G	301	4/4	0.95	0.43	56,61,62,64	0
7	EDO	N	304	4/4	0.96	0.37	56,57,58,64	0
8	CL	C	302	1/1	0.96	0.12	59,59,59,59	0
8	CL	E	704	1/1	0.97	0.07	57,57,57,57	0
8	CL	N	302	1/1	0.97	0.13	67,67,67,67	0
8	CL	A	303	1/1	0.98	0.11	60,60,60,60	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.