



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 9, 2022 – 04:07 PM EST

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 wwPDB X-ray Structure Validation Summary 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 ⓘ symbol.

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 : 2.26
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) : 2.26

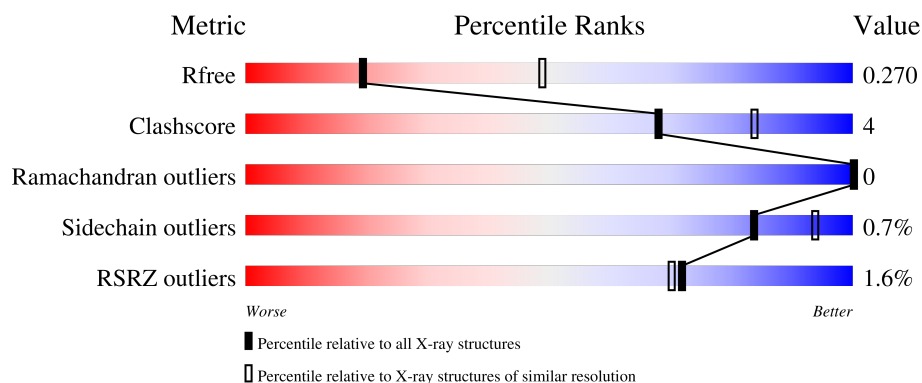
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


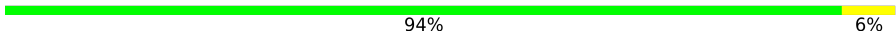
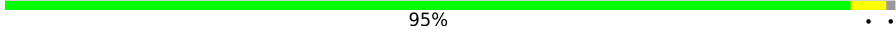


The reported resolution of this entry is 2.85 Å.

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 ≥ 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% 5%
2	C	230	 89% 8% 3%
3	E	601	 88% 10% 2%

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Mol	Chain	Length	Quality of chain
3	F	601	
4	G	215	
4	N	215	
5	H	223	
5	M	223	
6	I	216	
6	S	216	

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
1	A	213	Total	C	N	O	S	0	0	0
			1592	995	271	322	4			
1	D	214	Total	C	N	O	S	0	1	0
			1614	1005	275	330	4			

- Molecule 2 is a protein called S309 heavy chain.

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

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

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

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
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
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
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: C₂H₆O₂).



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

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

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

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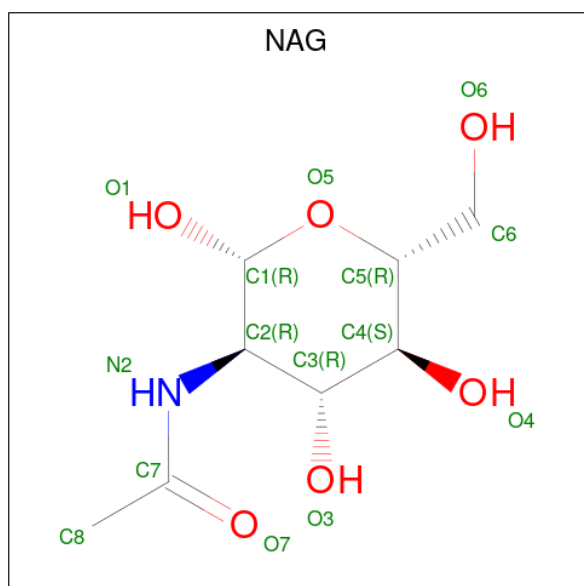
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	2	Total	Cl	0	0
			2	2		
8	C	4	Total	Cl	0	0
			4	4		
8	D	1	Total	Cl	0	0
			1	1		
8	E	4	Total	Cl	0	0
			4	4		
8	F	1	Total	Cl	0	0
			1	1		
8	I	1	Total	Cl	0	0
			1	1		
8	N	1	Total	Cl	0	0
			1	1		
8	S	3	Total	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: C₈H₁₅NO₆).



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	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	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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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	N	9	Total	O	0	0
			9	9		
11	S	20	Total	O	0	0
			20	20		

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: 



- Molecule 1: S309 light chain

Chain D: 




- Molecule 2: S309 heavy chain

Chain B: 




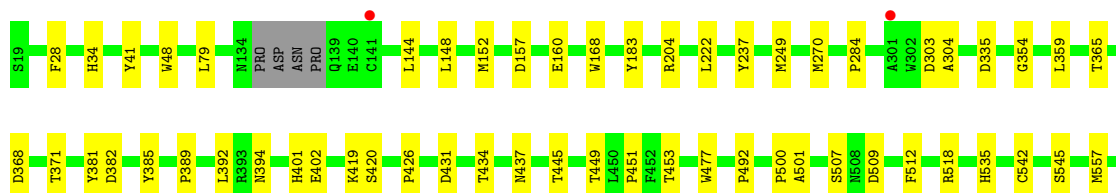
- Molecule 2: S309 heavy chain

Chain C: 



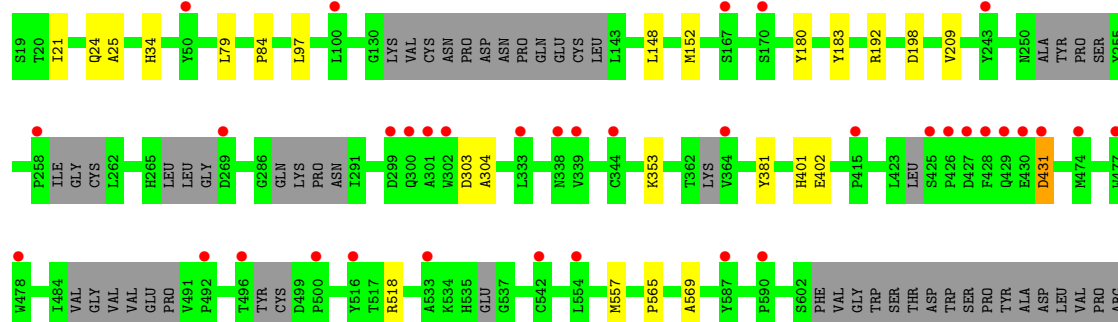
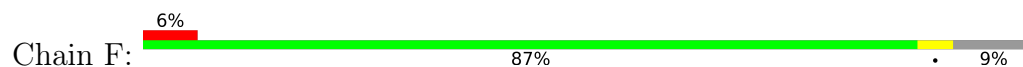
- Molecule 3: Angiotensin-converting enzyme 2

Chain E: 

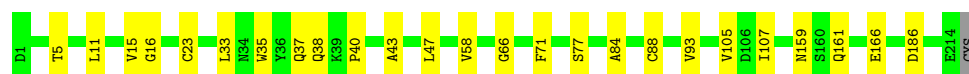
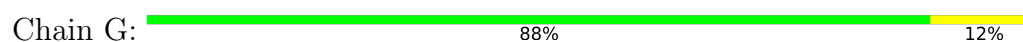




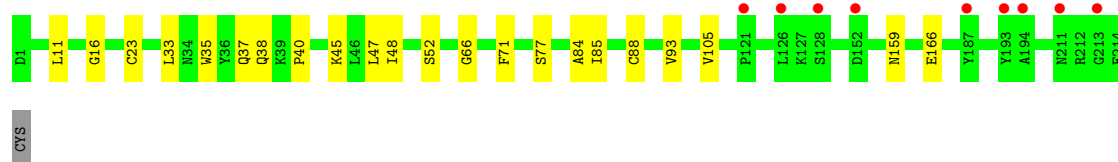
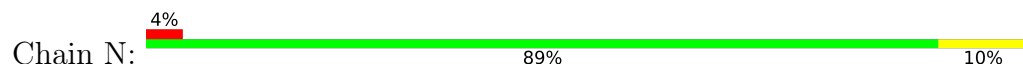
• Molecule 3: Angiotensin-converting enzyme 2



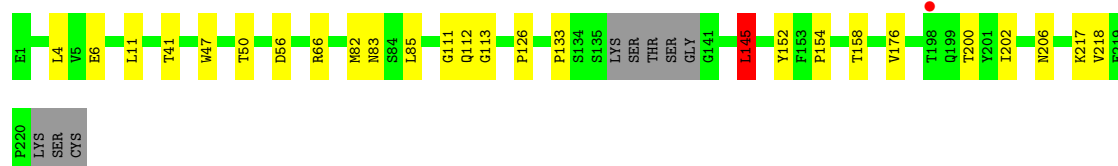
• Molecule 4: S304 Fab light chain



• Molecule 4: S304 Fab light chain



• Molecule 5: S304 Fab heavy chain

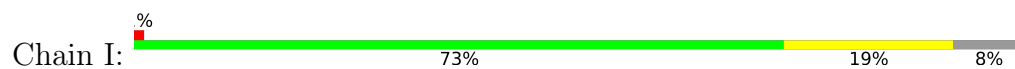


• Molecule 5: S304 Fab heavy chain

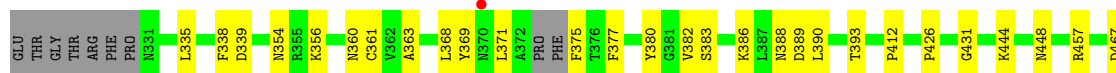




• Molecule 6: Spike protein S1



• 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, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	1.19 (at 2.86Å)	Xtriage
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 ²)	53.5	Xtriage
Anisotropy	0.409	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 44.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	24894	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage'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.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, EDO, CL, NAG

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.

The worst 5 of 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

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 ⓘ

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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	H	145	LEU
4	G	186	ASP
3	E	381	TYR
3	F	431	ASP
1	D	207	LYS

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	$\# Z > 2$
7	EDO	A	301	-	3,3,3	0.48	0	2,2,2	0.18	0
7	EDO	M	301	-	3,3,3	0.48	0	2,2,2	0.26	0
7	EDO	G	302	-	3,3,3	0.44	0	2,2,2	0.41	0
10	NAG	F	703	3	14,14,15	0.21	0	17,19,21	0.56	0
7	EDO	S	602	-	3,3,3	0.49	0	2,2,2	0.20	0
7	EDO	N	303	-	3,3,3	0.44	0	2,2,2	0.42	0
10	NAG	E	709	3	14,14,15	0.30	0	17,19,21	0.57	0
10	NAG	E	710	3	14,14,15	0.28	0	17,19,21	0.43	0
7	EDO	N	301	-	3,3,3	0.47	0	2,2,2	0.17	0
10	NAG	S	605	6	14,14,15	0.17	0	17,19,21	0.44	0
10	NAG	F	701	3	14,14,15	0.25	0	17,19,21	0.51	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
7	EDO	G	301	-	3,3,3	0.42	0	2,2,2	0.42	0
10	NAG	E	703	3	14,14,15	0.30	0	17,19,21	0.49	0
7	EDO	B	1003	-	3,3,3	0.49	0	2,2,2	0.20	0
7	EDO	M	302	-	3,3,3	0.48	0	2,2,2	0.32	0
10	NAG	E	708	3	14,14,15	0.29	0	17,19,21	0.56	0
10	NAG	F	704	3	14,14,15	0.32	0	17,19,21	0.49	0
7	EDO	S	601	-	3,3,3	0.46	0	2,2,2	0.34	0
10	NAG	I	601	6	14,14,15	0.41	0	17,19,21	0.83	1 (5%)
7	EDO	N	304	-	3,3,3	0.44	0	2,2,2	0.38	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
7	EDO	A	301	-	-	0/1/1/1	-
7	EDO	M	301	-	-	1/1/1/1	-
7	EDO	G	302	-	-	0/1/1/1	-
10	NAG	F	703	3	-	0/6/23/26	0/1/1/1
7	EDO	S	602	-	-	0/1/1/1	-
7	EDO	N	303	-	-	0/1/1/1	-
10	NAG	E	709	3	-	0/6/23/26	0/1/1/1
10	NAG	E	710	3	-	2/6/23/26	0/1/1/1
7	EDO	N	301	-	-	0/1/1/1	-
10	NAG	S	605	6	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	NAG	F	701	3	-	1/6/23/26	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
7	EDO	G	301	-	-	0/1/1/1	-
10	NAG	E	703	3	-	0/6/23/26	0/1/1/1
7	EDO	B	1003	-	-	0/1/1/1	-
7	EDO	M	302	-	-	0/1/1/1	-
10	NAG	E	708	3	-	2/6/23/26	0/1/1/1
10	NAG	F	704	3	-	0/6/23/26	0/1/1/1
7	EDO	S	601	-	-	1/1/1/1	-
10	NAG	I	601	6	-	1/6/23/26	0/1/1/1
7	EDO	N	304	-	-	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.

5 of 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
10	E	708	NAG	C4-C5-C6-O6

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	G	302	EDO	1	0
10	E	710	NAG	2	0
7	G	301	EDO	2	0
10	I	601	NAG	2	0
7	N	304	EDO	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 [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, 95th 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 ²)	Q<0.9
1	A	213/214 (99%)	-0.21	0 100 100	36, 52, 69, 87	0
1	D	214/214 (100%)	-0.20	0 100 100	33, 50, 67, 91	0
2	B	228/230 (99%)	-0.13	1 (0%) 92 92	39, 60, 80, 106	0
2	C	224/230 (97%)	-0.19	0 100 100	32, 48, 65, 85	0
3	E	591/601 (98%)	-0.02	2 (0%) 94 94	42, 62, 84, 109	0
3	F	547/601 (91%)	0.22	36 (6%) 18 14	52, 98, 140, 156	0
4	G	214/215 (99%)	-0.21	0 100 100	28, 48, 76, 94	0
4	N	214/215 (99%)	0.08	9 (4%) 36 31	29, 54, 111, 123	0
5	H	215/223 (96%)	-0.19	1 (0%) 91 90	29, 53, 73, 89	0
5	M	214/223 (95%)	-0.06	0 100 100	35, 69, 92, 108	0
6	I	198/216 (91%)	0.02	3 (1%) 73 72	33, 52, 86, 108	0
6	S	197/216 (91%)	-0.02	1 (0%) 91 90	35, 53, 85, 111	0
All	All	3269/3398 (96%)	-0.04	53 (1%) 72 70	28, 59, 115, 156	0

The worst 5 of 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

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, 95th 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(\AA^2)	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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
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.