



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 2, 2025 – 12:14 am GMT

PDB ID : 8RVD  
Title : Unbound murine diabetogenic 4.1 TCR  
Authors : Lopez-Sagaseta, J.; Erausquin, E.  
Deposited on : 2024-02-01  
Resolution : 3.00 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](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 : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.003 (Gargrove)  
Density-Fitness : 1.0.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.40

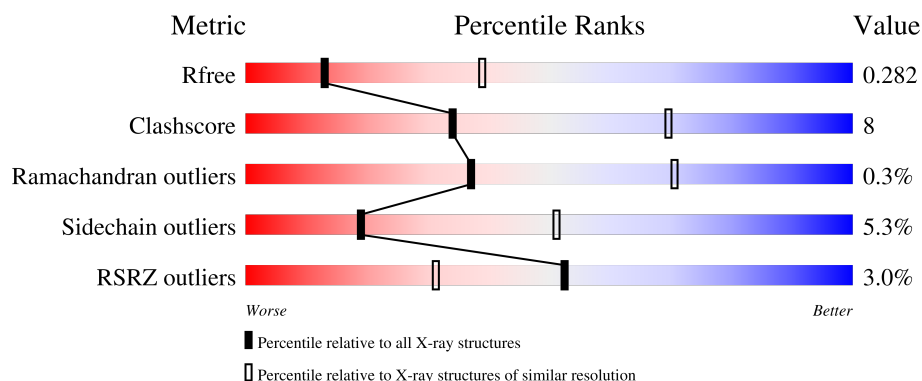
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	2511 (3.00-3.00)
Clashscore	180529	2866 (3.00-3.00)
Ramachandran outliers	177936	2778 (3.00-3.00)
Sidechain outliers	177891	2781 (3.00-3.00)
RSRZ outliers	164620	2523 (3.00-3.00)

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	242	<div> <div>3%</div> <div>83%</div> <div>12%</div> <div>..</div> </div>
1	C	242	<div> <div>%</div> <div>82%</div> <div>14%</div> <div>..</div> </div>
1	E	242	<div> <div>2%</div> <div>81%</div> <div>16%</div> <div>.</div> </div>
1	F	242	<div> <div>%</div> <div>83%</div> <div>15%</div> <div>.</div> </div>
1	I	242	<div> <div>2%</div> <div>83%</div> <div>13%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	K	242	
1	M	242	
1	O	242	
2	B	207	
2	D	207	
2	G	207	
2	H	207	
2	J	207	
2	L	207	
2	N	207	
2	P	207	

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
3	PO4	A	301	-	-	X	-
3	PO4	B	301	-	-	X	-
3	PO4	E	301	-	-	X	-
3	PO4	M	301	-	-	X	-
3	PO4	O	302	-	-	X	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 25719 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 4.1 TCR beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	241	Total	C	N	O	S	0	0	0
			1791	1134	327	323	7			
1	A	238	Total	C	N	O	S	0	0	0
			1729	1088	314	320	7			
1	C	240	Total	C	N	O	S	0	0	0
			1851	1173	329	342	7			
1	F	242	Total	C	N	O	S	0	0	0
			1853	1175	326	344	8			
1	I	241	Total	C	N	O	S	0	0	0
			1838	1164	325	342	7			
1	K	240	Total	C	N	O	S	0	0	0
			1816	1153	315	341	7			
1	M	239	Total	C	N	O	S	0	0	0
			1810	1148	317	338	7			
1	O	239	Total	C	N	O	S	0	0	0
			1831	1160	320	344	7			

- Molecule 2 is a protein called 4.1 TCR alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	195	Total	C	N	O	S	0	0	0
			1388	872	236	272	8			
2	B	198	Total	C	N	O	S	0	0	0
			1348	847	226	266	9			
2	D	172	Total	C	N	O	S	0	0	0
			1290	815	217	250	8			
2	G	195	Total	C	N	O	S	0	0	0
			1477	927	248	293	9			
2	J	192	Total	C	N	O	S	0	0	0
			1440	909	245	278	8			
2	L	189	Total	C	N	O	S	0	0	0
			1400	884	238	269	9			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	N	189	Total	C	N	O	S	0	0	0
			1371	871	222	270	8			
2	P	197	Total	C	N	O	S	0	0	0
			1442	912	241	281	8			

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	E	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	I	1	Total	O	P	0	0
			5	4	1		
3	J	1	Total	O	P	0	0
			5	4	1		
3	M	1	Total	O	P	0	0
			5	4	1		
3	O	1	Total	O	P	0	0
			5	4	1		
3	O	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).

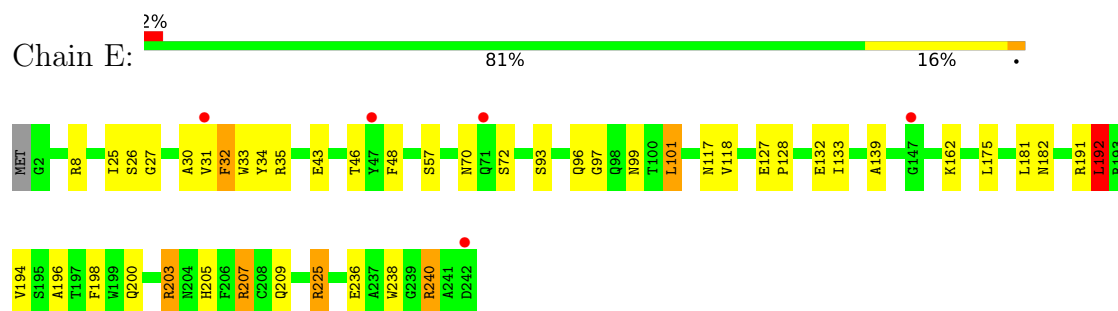


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	O	1	Total	C	O	0	0
			4	2	2		

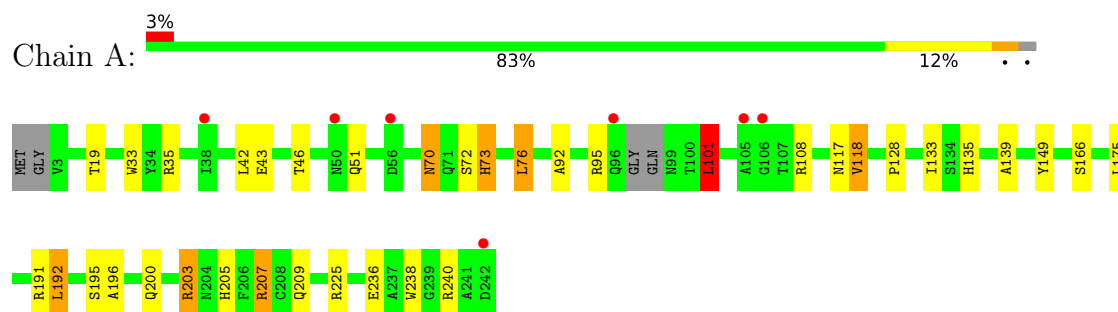
### 3 Residue-property plots [i](#)

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.

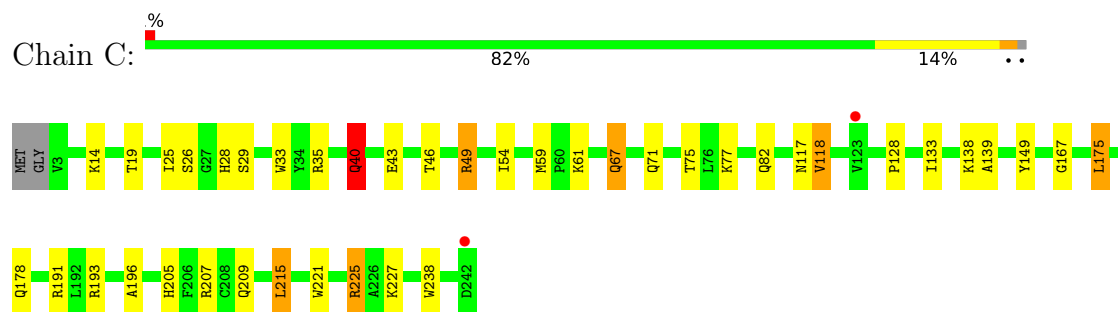
- Molecule 1: 4.1 TCR beta chain



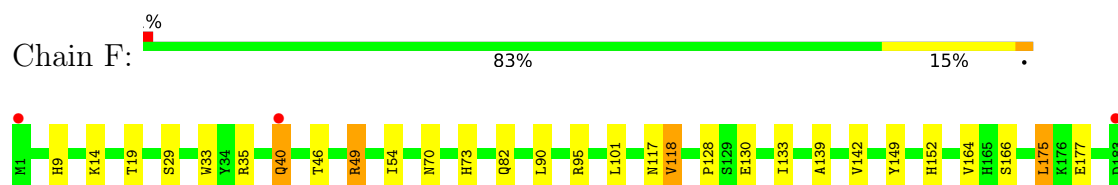
- Molecule 1: 4.1 TCR beta chain



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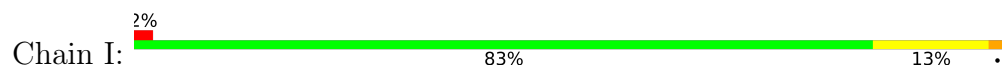


- Molecule 1: 4.1 TCR beta chain

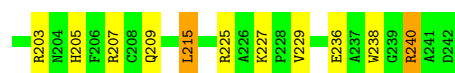
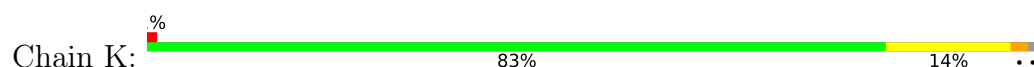




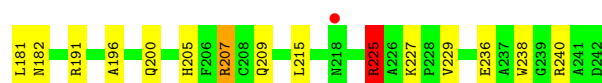
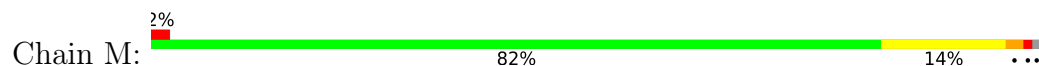
- Molecule 1: 4.1 TCR beta chain



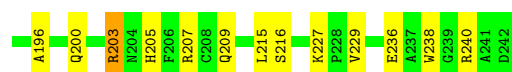
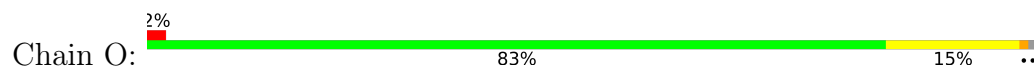
- Molecule 1: 4.1 TCR beta chain



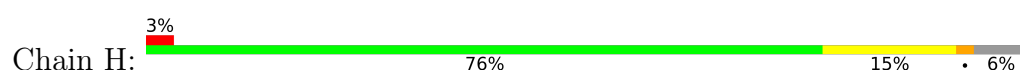
- Molecule 1: 4.1 TCR beta chain



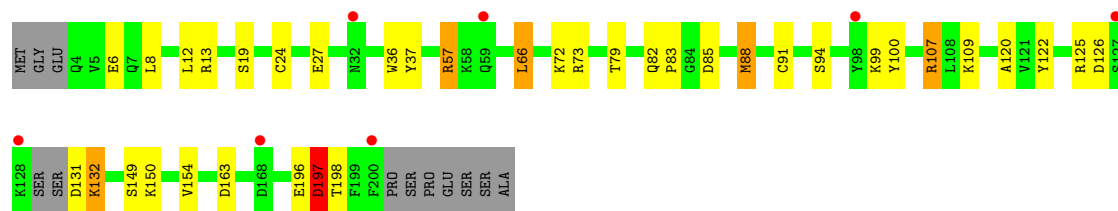
- Molecule 1: 4.1 TCR beta chain



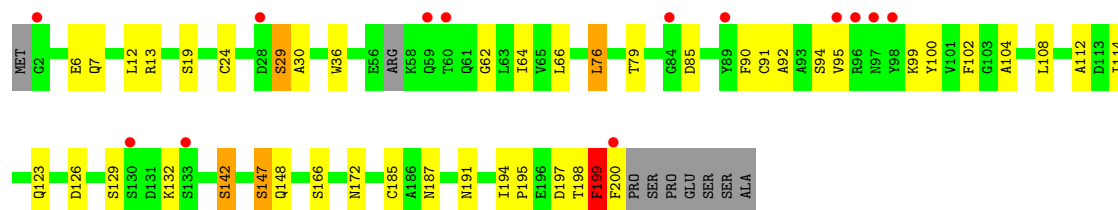
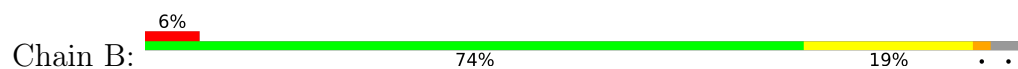
- Molecule 2: 4.1 TCR alpha chain



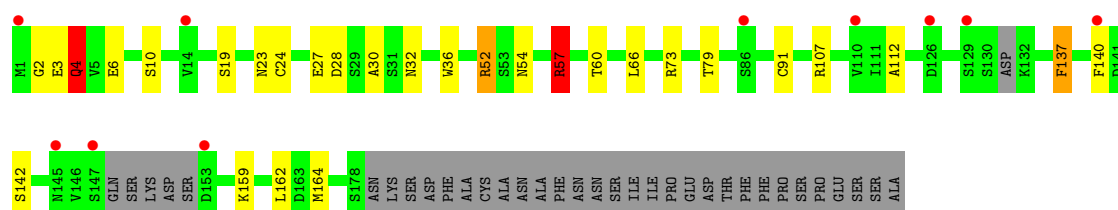




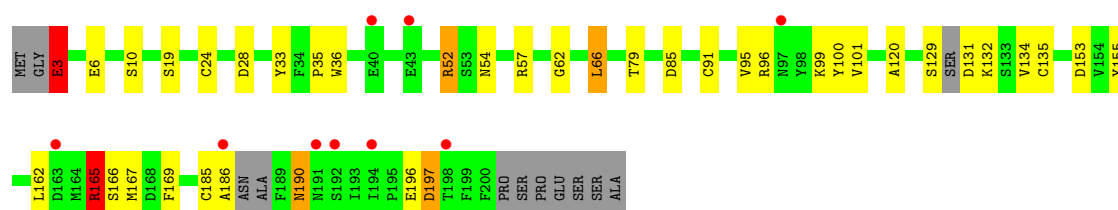
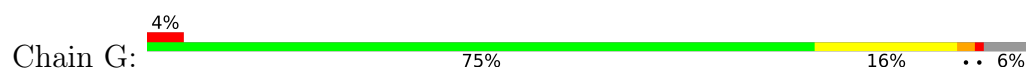
• Molecule 2: 4.1 TCR alpha chain



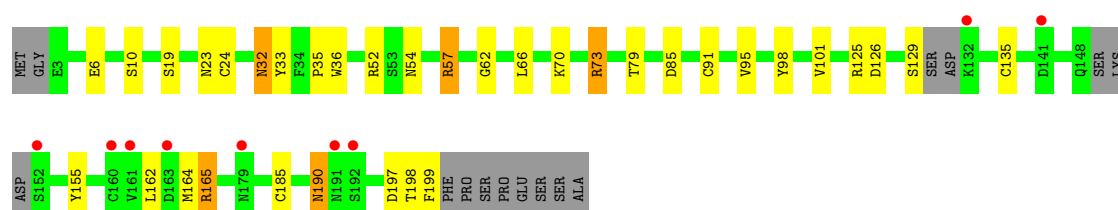
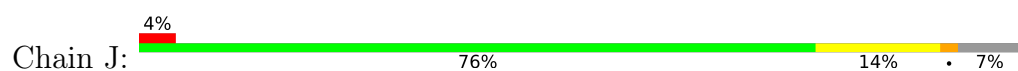
• Molecule 2: 4.1 TCR alpha chain



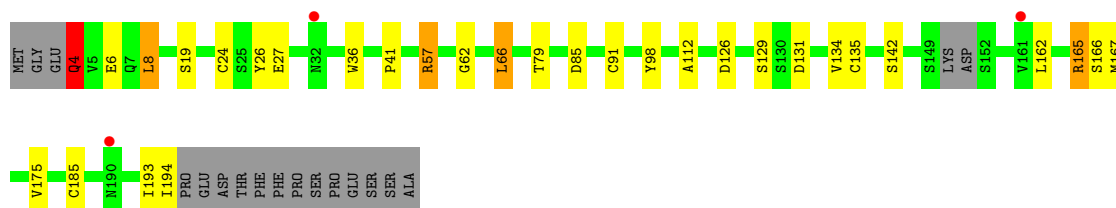
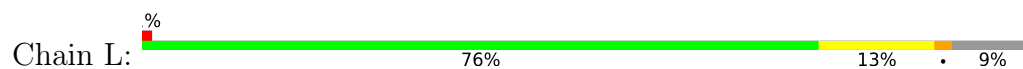
• Molecule 2: 4.1 TCR alpha chain



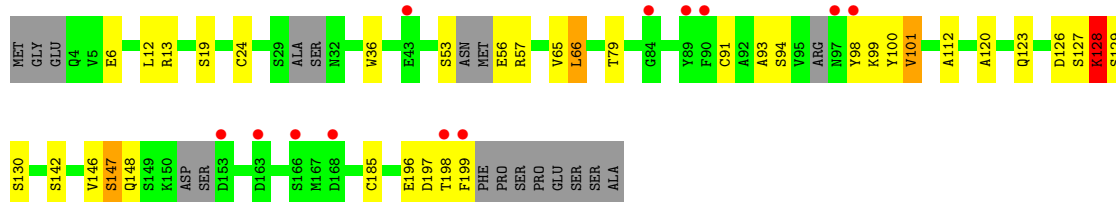
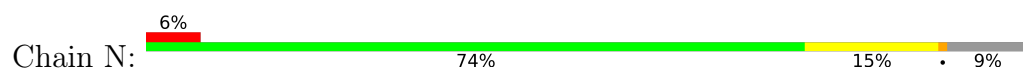
• Molecule 2: 4.1 TCR alpha chain



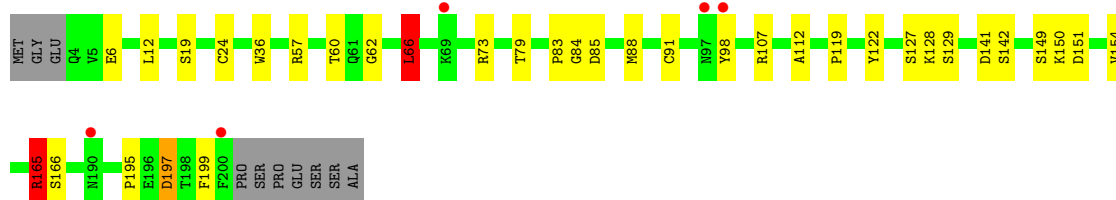
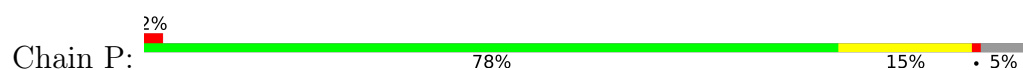
## • Molecule 2: 4.1 TCR alpha chain



## • Molecule 2: 4.1 TCR alpha chain



## • Molecule 2: 4.1 TCR alpha chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	129.99Å 151.13Å 135.55Å 90.00° 92.80° 90.00°	Depositor
Resolution (Å)	135.39 – 3.00 135.39 – 3.15	Depositor EDS
% Data completeness (in resolution range)	86.3 (135.39-3.00) 99.8 (135.39-3.15)	Depositor EDS
$R_{merge}$	0.18	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.70 (at 3.13Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, $R_{free}$	0.216 , 0.266 0.230 , 0.282	Depositor DCC
$R_{free}$ test set	4351 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	68.5	Xtriage
Anisotropy	0.521	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 59.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.009 for l,k,-h 0.076 for h,-k,-l 0.020 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	25719	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 36.79 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.7331e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, EDO

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	0.43	0/1777	0.92	5/2434 (0.2%)
1	C	0.47	0/1903	1.01	6/2599 (0.2%)
1	E	0.46	0/1843	0.96	5/2521 (0.2%)
1	F	0.47	0/1906	0.97	5/2605 (0.2%)
1	I	0.44	0/1890	0.98	7/2586 (0.3%)
1	K	0.47	0/1868	0.98	5/2558 (0.2%)
1	M	0.45	0/1860	1.01	7/2545 (0.3%)
1	O	0.44	0/1883	0.95	3/2576 (0.1%)
2	B	0.47	1/1376 (0.1%)	0.99	3/1888 (0.2%)
2	D	0.47	0/1314	1.06	6/1786 (0.3%)
2	G	0.47	0/1504	1.08	8/2041 (0.4%)
2	H	0.52	0/1415	1.10	8/1932 (0.4%)
2	J	0.49	0/1467	1.03	6/1994 (0.3%)
2	L	0.50	0/1427	1.06	6/1939 (0.3%)
2	N	0.48	1/1396 (0.1%)	1.00	6/1902 (0.3%)
2	P	0.49	0/1471	1.04	6/2005 (0.3%)
All	All	0.47	2/26300 (0.0%)	1.01	92/35911 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	C	0	1
1	E	0	1
1	F	0	1
2	B	0	1
2	D	0	2
2	G	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	H	0	2
2	J	0	2
2	L	0	1
2	N	0	1
2	P	0	4
All	All	0	20

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	147	SER	CA-CB	-5.57	1.44	1.52
2	N	53	SER	C-O	5.05	1.32	1.23

The worst 5 of 92 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	225	ARG	NE-CZ-NH1	12.91	126.75	120.30
1	C	175	LEU	CB-CG-CD2	-12.23	90.21	111.00
1	M	225	ARG	CD-NE-CZ	10.50	138.31	123.60
1	M	181	LEU	CB-CG-CD2	-9.93	94.12	111.00
2	J	165	ARG	NE-CZ-NH2	-9.18	115.71	120.30

There are no chirality outliers.

5 of 20 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	108	ARG	Sidechain
1	A	207	ARG	Sidechain
1	E	207	ARG	Sidechain
2	H	163	ASP	Mainchain
2	H	73	ARG	Sidechain

## 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.

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1729	0	1479	23	0
1	C	1851	0	1730	25	0
1	E	1791	0	1594	33	0
1	F	1853	0	1719	32	0
1	I	1838	0	1689	29	0
1	K	1816	0	1656	30	0
1	M	1810	0	1647	27	0
1	O	1831	0	1679	31	0
2	B	1348	0	1073	26	0
2	D	1290	0	1187	22	0
2	G	1477	0	1352	33	1
2	H	1388	0	1179	22	0
2	J	1440	0	1310	34	0
2	L	1400	0	1271	22	1
2	N	1371	0	1210	18	0
2	P	1442	0	1313	26	0
3	A	5	0	0	2	0
3	B	5	0	0	2	0
3	E	5	0	0	2	0
3	I	5	0	0	0	0
3	J	5	0	0	0	0
3	M	5	0	0	2	0
3	O	10	0	0	2	0
4	O	4	0	6	2	0
All	All	25719	0	23094	364	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 8.

The worst 5 of 364 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)
2:G:165:ARG:HH11	1:O:164:VAL:HB	1.10	1.09
1:M:166:SER:HB2	3:M:301:PO4:O3	1.51	1.08
1:O:11:VAL:O	4:O:303:EDO:H22	1.55	1.06
2:H:57:ARG:HG2	2:H:66:LEU:CD1	1.92	0.99
1:M:207:ARG:NH2	1:M:209:GLN:OE1	1.95	0.98

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:6:GLU:OE1	2:L:19:SER:OG[2_655]	2.12	0.08

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	234/242 (97%)	225 (96%)	9 (4%)	0	100	100
1	C	238/242 (98%)	230 (97%)	8 (3%)	0	100	100
1	E	239/242 (99%)	225 (94%)	12 (5%)	2 (1%)	16	51
1	F	240/242 (99%)	229 (95%)	11 (5%)	0	100	100
1	I	239/242 (99%)	231 (97%)	8 (3%)	0	100	100
1	K	238/242 (98%)	231 (97%)	6 (2%)	1 (0%)	30	66
1	M	235/242 (97%)	226 (96%)	9 (4%)	0	100	100
1	O	235/242 (97%)	225 (96%)	10 (4%)	0	100	100
2	B	194/207 (94%)	175 (90%)	15 (8%)	4 (2%)	5	28
2	D	166/207 (80%)	159 (96%)	7 (4%)	0	100	100
2	G	189/207 (91%)	177 (94%)	12 (6%)	0	100	100
2	H	191/207 (92%)	175 (92%)	16 (8%)	0	100	100
2	J	186/207 (90%)	170 (91%)	16 (9%)	0	100	100
2	L	185/207 (89%)	170 (92%)	14 (8%)	1 (0%)	25	61
2	N	179/207 (86%)	167 (93%)	12 (7%)	0	100	100
2	P	195/207 (94%)	178 (91%)	15 (8%)	2 (1%)	13	46
All	All	3383/3592 (94%)	3193 (94%)	180 (5%)	10 (0%)	37	70

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	26	SER
2	B	29	SER
2	B	195	PRO
1	K	29	SER
2	P	197	ASP

### 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	154/210 (73%)	140 (91%)	14 (9%)	7	30
1	C	190/210 (90%)	176 (93%)	14 (7%)	11	38
1	E	167/210 (80%)	158 (95%)	9 (5%)	18	50
1	F	189/210 (90%)	182 (96%)	7 (4%)	29	63
1	I	185/210 (88%)	179 (97%)	6 (3%)	34	67
1	K	182/210 (87%)	173 (95%)	9 (5%)	21	54
1	M	180/210 (86%)	167 (93%)	13 (7%)	12	39
1	O	187/210 (89%)	180 (96%)	7 (4%)	29	63
2	B	111/185 (60%)	102 (92%)	9 (8%)	9	34
2	D	131/185 (71%)	125 (95%)	6 (5%)	23	56
2	G	153/185 (83%)	145 (95%)	8 (5%)	19	52
2	H	125/185 (68%)	117 (94%)	8 (6%)	14	44
2	J	143/185 (77%)	137 (96%)	6 (4%)	25	59
2	L	138/185 (75%)	133 (96%)	5 (4%)	30	64
2	N	134/185 (72%)	127 (95%)	7 (5%)	19	52
2	P	145/185 (78%)	141 (97%)	4 (3%)	38	70
All	All	2514/3160 (80%)	2382 (95%)	132 (5%)	19	51

5 of 132 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	N	66	LEU

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
2	N	129	SER
2	P	129	SER
1	C	117	ASN
1	C	77	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 40 such sidechains are listed below:

Mol	Chain	Res	Type
2	L	82	GLN
2	N	123	GLN
1	M	40	GLN
1	M	73	HIS
1	O	205	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

9 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	PO4	E	301	-	4,4,4	0.70	0	6,6,6	0.47	0
3	PO4	O	302	-	4,4,4	0.77	0	6,6,6	0.38	0
4	EDO	O	303	-	3,3,3	0.38	0	2,2,2	1.01	0
3	PO4	J	301	-	4,4,4	1.04	0	6,6,6	0.36	0
3	PO4	O	301	-	4,4,4	1.05	0	6,6,6	0.81	0
3	PO4	M	301	-	4,4,4	0.99	0	6,6,6	0.72	0
3	PO4	B	301	-	4,4,4	0.86	0	6,6,6	0.46	0
3	PO4	I	301	-	4,4,4	1.01	0	6,6,6	0.78	0
3	PO4	A	301	-	4,4,4	1.52	1 (25%)	6,6,6	0.41	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	EDO	O	303	-	-	0/1/1/1	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	301	PO4	P-O1	2.74	1.57	1.50

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	301	PO4	2	0
3	O	302	PO4	2	0
4	O	303	EDO	2	0
3	M	301	PO4	2	0
3	B	301	PO4	2	0
3	A	301	PO4	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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	238/242 (98%)	0.15	7 (2%) 54 32	45, 75, 115, 153	0
1	C	240/242 (99%)	-0.20	2 (0%) 82 66	34, 60, 93, 127	0
1	E	241/242 (99%)	0.08	5 (2%) 63 41	34, 62, 101, 122	0
1	F	242/242 (100%)	-0.05	3 (1%) 76 56	37, 63, 103, 138	0
1	I	241/242 (99%)	-0.01	5 (2%) 63 41	35, 63, 104, 136	0
1	K	240/242 (99%)	-0.09	2 (0%) 82 66	38, 62, 94, 118	0
1	M	239/242 (98%)	0.24	6 (2%) 58 36	39, 76, 127, 178	0
1	O	239/242 (98%)	0.12	5 (2%) 63 41	36, 68, 107, 151	0
2	B	198/207 (95%)	0.55	13 (6%) 26 14	43, 78, 114, 164	0
2	D	172/207 (83%)	0.20	10 (5%) 30 17	29, 65, 116, 128	0
2	G	195/207 (94%)	0.19	9 (4%) 38 22	37, 61, 110, 139	0
2	H	195/207 (94%)	0.20	7 (3%) 46 27	35, 60, 95, 115	0
2	J	192/207 (92%)	0.10	9 (4%) 37 21	32, 62, 107, 137	0
2	L	189/207 (91%)	0.12	3 (1%) 70 49	31, 62, 114, 151	0
2	N	189/207 (91%)	0.56	12 (6%) 27 15	48, 79, 115, 158	0
2	P	197/207 (95%)	0.16	5 (2%) 58 36	39, 64, 105, 142	0
All	All	3447/3592 (95%)	0.13	103 (2%) 52 31	29, 66, 110, 178	0

The worst 5 of 103 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	38	ILE	5.7
2	J	161	VAL	4.3
1	A	105	ALA	4.2
2	P	97	ASN	3.9
1	I	183	ASP	3.9

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	PO4	O	302	5/5	0.64	0.11	117,143,162,167	0
4	EDO	O	303	4/4	0.67	0.21	79,80,87,88	0
3	PO4	J	301	5/5	0.75	0.11	95,102,131,136	0
3	PO4	B	301	5/5	0.80	0.16	103,105,115,116	0
3	PO4	E	301	5/5	0.82	0.13	112,120,131,154	0
3	PO4	I	301	5/5	0.89	0.10	56,56,66,71	0
3	PO4	M	301	5/5	0.91	0.08	55,59,66,75	0
3	PO4	A	301	5/5	0.92	0.10	46,60,73,77	0
3	PO4	O	301	5/5	0.95	0.07	43,50,61,76	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.