



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:57 PM UTC

PDB ID : 4R4N / pdb_00004r4n
Title : Crystal structure of the anti-hiv-1 antibody 2.2c in complex with hiv-1 93ug037 gp120
Authors : Acharya, P.; Louder, R.; Kwong, P.D.
Deposited on : 2014-08-19
Resolution : 3.56 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

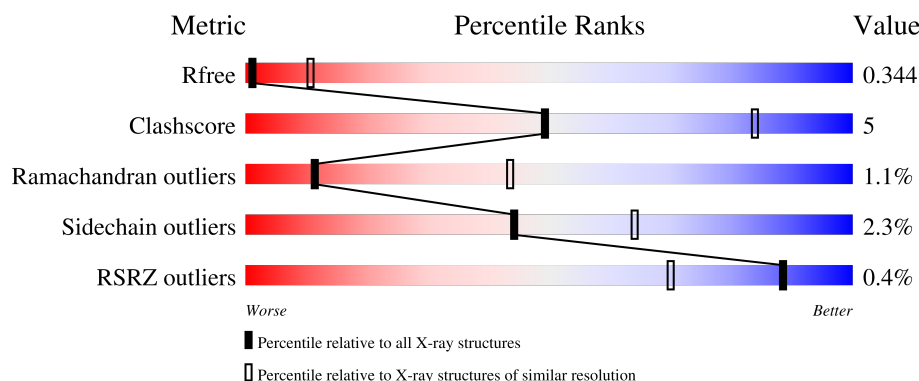
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.56 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.



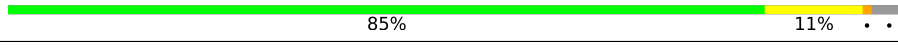
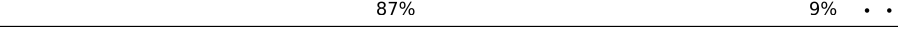
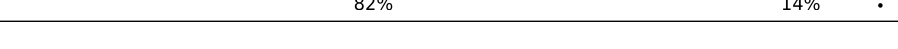
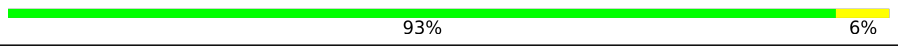
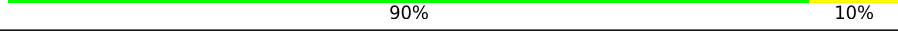
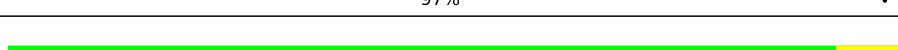
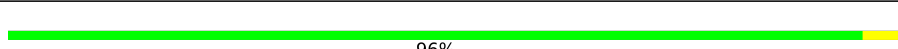
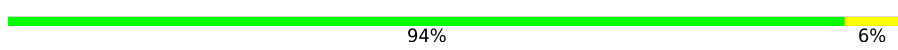
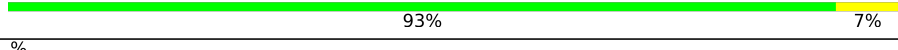
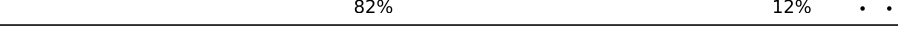
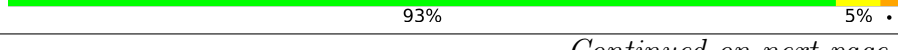
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1410 (3.62-3.50)
Clashscore	190562	1480 (3.62-3.50)
Ramachandran outliers	187476	1440 (3.62-3.50)
Sidechain outliers	187428	1441 (3.62-3.50)
RSRZ outliers	180081	1409 (3.62-3.50)

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	352	% 86% 8% 5%
1	B	352	86% 10%
1	E	352	% 86% 7% 7%
1	I	352	88% 8%
1	M	352	% 87% 9%

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Mol	Chain	Length	Quality of chain
1	P	352	%  87% 8% . .
1	S	352	 85% 11% . .
1	V	352	 87% 9% . .
2	a	28	 82% 14% .
2	b	28	 64% 32% .
2	e	28	 79% 18% .
2	i	28	 82% 14% .
2	m	28	 68% 29% .
2	p	28	 82% 14% .
2	s	28	 82% 14% .
2	v	28	 79% 18% .
3	D	210	 85% 15%
3	G	210	 93% 6%
3	K	210	 90% 10%
3	L	210	 97% .
3	O	210	 93% 7%
3	R	210	 96% .
3	U	210	 94% 6%
3	X	210	 93% 7%
4	C	220	%  82% 12% . .
4	F	220	 86% 11% .
4	H	220	 95% . .
4	J	220	 82% 15% .
4	N	220	 84% 12% .
4	Q	220	93% 5% .

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Mol	Chain	Length	Quality of chain
4	T	220	% 87% 10% •
4	W	220	93% 5% •

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
2	U2X	b	23	-	-	X	-
5	NAG	B	502	-	-	X	-
5	NAG	S	502	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 94738 atoms, of which 45586 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 HIV-1 gp120.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	333	Total	C	H	N	O	S	0	0	0
			5094	1611	2506	458	498	21			
1	B	342	Total	C	H	N	O	S	0	0	0
			5189	1655	2532	469	512	21			
1	I	341	Total	C	H	N	O	S	0	0	0
			5172	1641	2532	466	512	21			
1	E	329	Total	C	H	N	O	S	0	0	0
			5042	1595	2481	453	492	21			
1	M	339	Total	C	H	N	O	S	0	0	0
			5169	1633	2544	463	508	21			
1	P	338	Total	C	H	N	O	S	0	0	0
			5157	1631	2537	462	506	21			
1	S	339	Total	C	H	N	O	S	0	0	0
			5168	1634	2542	463	508	21			
1	V	338	Total	C	H	N	O	S	0	0	0
			5160	1631	2539	463	506	21			

- Molecule 2 is a protein called M48U1 peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	a	28	Total	C	N	O	S	0	0	1
			209	133	38	32	6			
2	b	28	Total	C	N	O	S	0	0	1
			209	133	38	32	6			
2	e	28	Total	C	N	O	S	0	0	1
			209	133	38	32	6			
2	i	28	Total	C	N	O	S	0	0	1
			209	133	38	32	6			
2	m	28	Total	C	N	O	S	0	0	1
			209	133	38	32	6			
2	p	28	Total	C	N	O	S	0	0	1
			209	133	38	32	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	s	28	Total	C	N	O	S	0	0	1
			209	133	38	32	6			
2	v	28	Total	C	N	O	S	0	0	1
			209	133	38	32	6			

- Molecule 3 is a protein called Antibody 2.2c LIGHT CHAIN.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	L	210	Total 3197	C 1012	H 1585	N 272	O 323	S 5	0	0	0
3	D	210	Total 3196	C 1012	H 1584	N 272	O 323	S 5	0	0	0
3	G	210	Total 3194	C 1012	H 1582	N 272	O 323	S 5	0	0	0
3	K	210	Total 3195	C 1012	H 1583	N 272	O 323	S 5	0	0	0
3	O	210	Total 3198	C 1012	H 1586	N 272	O 323	S 5	0	0	0
3	R	210	Total 3195	C 1012	H 1583	N 272	O 323	S 5	0	0	0
3	U	210	Total 3193	C 1012	H 1581	N 272	O 323	S 5	0	0	0
3	X	210	Total 3198	C 1012	H 1586	N 272	O 323	S 5	0	0	0

- Molecule 4 is a protein called Antibody 2.2c heavy CHAIN.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	H	220	Total 3322	C 1066	H 1648	N 283	O 320	S 5	0	0	0
4	C	220	Total 3245	C 1066	H 1571	N 283	O 320	S 5	0	0	0
4	F	220	Total 3186	C 1064	H 1515	N 283	O 319	S 5	0	0	0
4	J	220	Total 3186	C 1064	H 1515	N 283	O 319	S 5	0	0	0
4	N	220	Total 3322	C 1064	H 1651	N 283	O 319	S 5	0	0	0
4	Q	220	Total 3322	C 1064	H 1651	N 283	O 319	S 5	0	0	0
4	T	220	Total 3179	C 1066	H 1505	N 283	O 320	S 5	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
4	W	220	Total	C	H	N	O	S	0	0	0
			3321	1066	1647	283	320	5			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	I	1	Total	C	N	O	0	0
			14	8	1	5		
5	I	1	Total	C	N	O	0	0
			14	8	1	5		
5	I	1	Total	C	N	O	0	0
			14	8	1	5		

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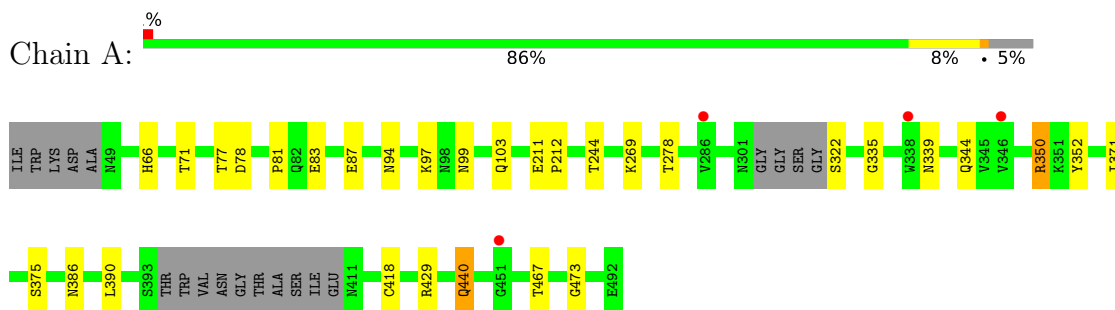
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	E	1	Total	C	N	O	0	0
			14	8	1	5		
5	E	1	Total	C	N	O	0	0
			14	8	1	5		
5	M	1	Total	C	N	O	0	0
			14	8	1	5		
5	P	1	Total	C	N	O	0	0
			14	8	1	5		
5	P	1	Total	C	N	O	0	0
			14	8	1	5		
5	S	1	Total	C	N	O	0	0
			14	8	1	5		
5	S	1	Total	C	N	O	0	0
			14	8	1	5		
5	S	1	Total	C	N	O	0	0
			14	8	1	5		
5	V	1	Total	C	N	O	0	0
			14	8	1	5		

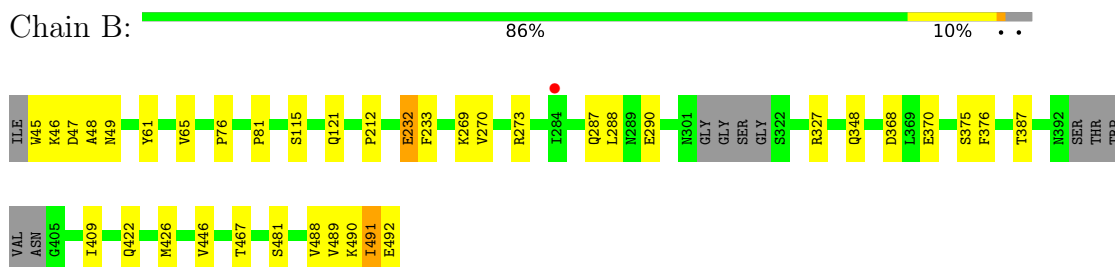
3 Residue-property plots [i](#)

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.

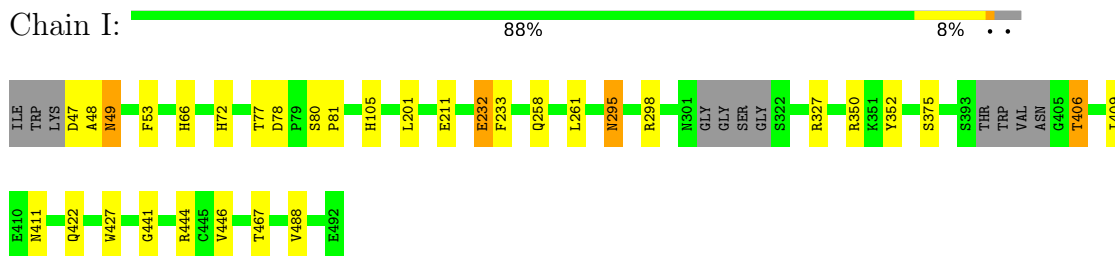
- Molecule 1: HIV-1 gp120



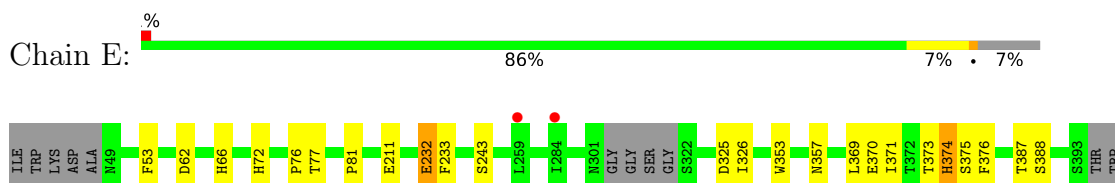
- Molecule 1: HIV-1 gp120

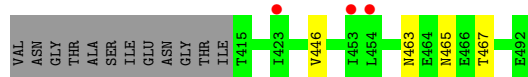


- Molecule 1: HIV-1 gp120

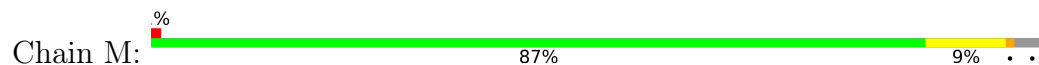


- Molecule 1: HIV-1 gp120

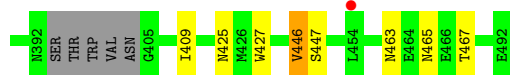
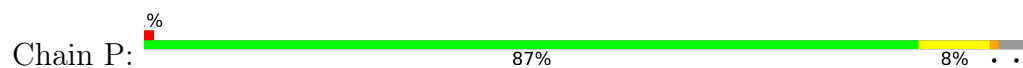




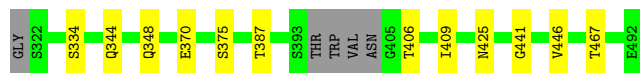
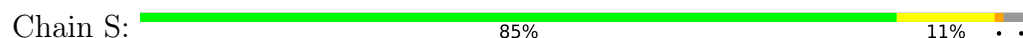
• Molecule 1: HIV-1 gp120



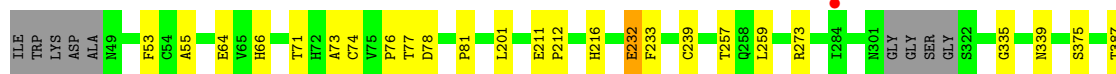
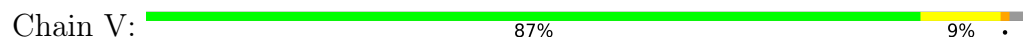
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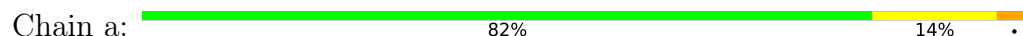
• Molecule 1: HIV-1 gp120



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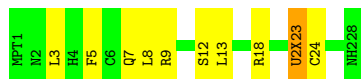


• Molecule 2: M48U1 peptide

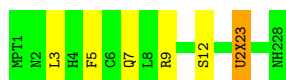
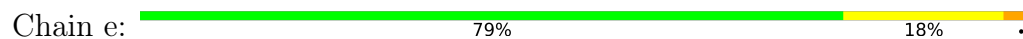




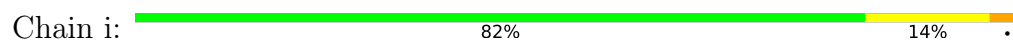
• Molecule 2: M48U1 peptide



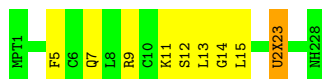
• Molecule 2: M48U1 peptide



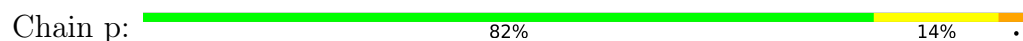
• Molecule 2: M48U1 peptide



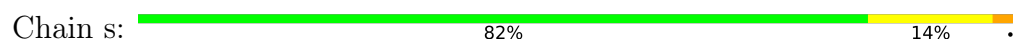
• Molecule 2: M48U1 peptide



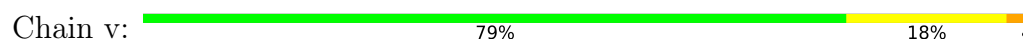
• Molecule 2: M48U1 peptide

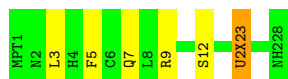


• Molecule 2: M48U1 peptide



• Molecule 2: M48U1 peptide





- Molecule 3: Antibody 2.2c LIGHT CHAIN

Chain L: 97%



- Molecule 3: Antibody 2.2c LIGHT CHAIN

Chain D: 85%



- Molecule 3: Antibody 2.2c LIGHT CHAIN

Chain G: 93%



- Molecule 3: Antibody 2.2c LIGHT CHAIN

Chain K: 90%



- Molecule 3: Antibody 2.2c LIGHT CHAIN

Chain O: 93%



- Molecule 3: Antibody 2.2c LIGHT CHAIN

Chain R: 96%



- Molecule 3: Antibody 2.2c LIGHT CHAIN

Chain U: 94%



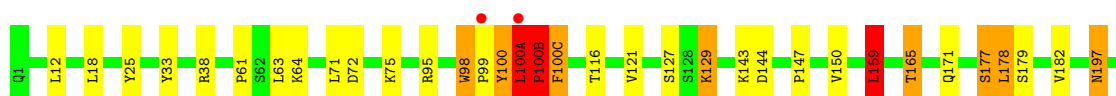
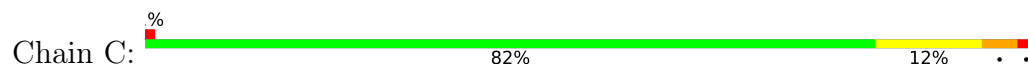
• Molecule 3: Antibody 2.2c LIGHT CHAIN



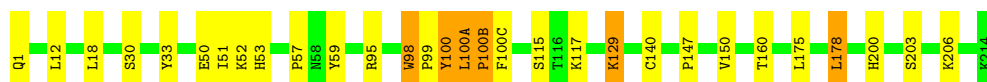
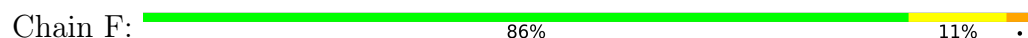
• Molecule 4: Antibody 2.2c heavy CHAIN



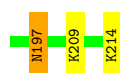
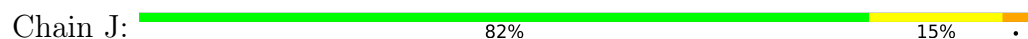
• Molecule 4: Antibody 2.2c heavy CHAIN



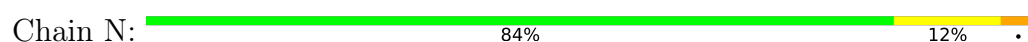
• Molecule 4: Antibody 2.2c heavy CHAIN



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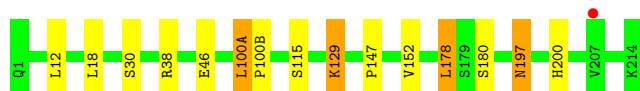
• Molecule 4: Antibody 2.2c heavy CHAIN





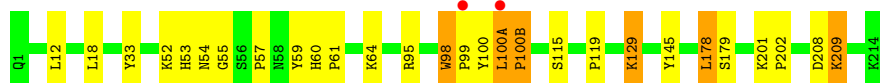
• Molecule 4: Antibody 2.2c heavy CHAIN

Chain Q: 93% 5% •



• Molecule 4: Antibody 2.2c heavy CHAIN

Chain T: 87% 10% •



• Molecule 4: Antibody 2.2c heavy CHAIN

Chain W: 93% 5% •



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	112.97Å 144.18Å 158.35Å 110.58° 92.30° 99.19°	Depositor
Resolution (Å)	49.15 – 3.56 49.15 – 3.56	Depositor EDS
% Data completeness (in resolution range)	62.7 (49.15-3.56) 62.7 (49.15-3.56)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.79 (at 2.86Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.296 , 0.328 0.316 , 0.344	Depositor DCC
R_{free} test set	3686 reflections (1.70%)	wwPDB-VP
Wilson B-factor (Å ²)	99.3	Xtriage
Anisotropy	0.410	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 204.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	94738	wwPDB-VP
Average B, all atoms (Å ²)	217.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.15% 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: OAS, U2X, NAG, MPT, NH2, DPR

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	0.31	0/2639	0.62	0/3583
1	B	0.32	0/2710	0.61	0/3680
1	E	0.31	0/2612	0.60	0/3546
1	I	0.31	0/2691	0.62	0/3654
1	M	0.31	0/2675	0.62	0/3630
1	P	0.31	0/2671	0.61	0/3626
1	S	0.33	0/2677	0.64	0/3634
1	V	0.31	0/2672	0.62	0/3628
2	a	0.44	0/176	0.78	0/231
2	b	0.44	0/176	0.78	0/231
2	e	0.44	0/176	0.78	0/231
2	i	0.44	0/176	0.78	0/231
2	m	0.44	0/176	0.77	0/231
2	p	0.44	0/176	0.78	0/231
2	s	0.44	0/176	0.78	0/231
2	v	0.44	0/176	0.78	0/231
3	D	0.44	0/1646	0.96	2/2231 (0.1%)
3	G	0.32	0/1646	0.72	0/2231
3	K	0.41	0/1646	0.84	0/2231
3	L	0.30	0/1646	0.68	0/2231
3	O	0.30	0/1646	0.66	0/2231
3	R	0.31	0/1646	0.70	0/2231
3	U	0.33	0/1646	0.68	0/2231
3	X	0.31	0/1646	0.66	0/2231
4	C	0.46	0/1713	0.99	7/2341 (0.3%)
4	F	0.32	0/1713	0.71	0/2341
4	H	0.31	0/1713	0.67	0/2341
4	J	0.38	0/1713	0.82	4/2341 (0.2%)
4	N	0.35	0/1713	0.84	6/2341 (0.3%)
4	Q	0.31	0/1713	0.70	0/2341
4	T	0.35	0/1713	0.75	0/2341
4	W	0.34	0/1713	0.82	2/2341 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.34	0/49627	0.71	21/67405 (0.0%)

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
3	K	0	1
4	C	0	1
All	All	0	2

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	118	PHE	CA-C-N	-7.37	112.79	120.38
3	D	118	PHE	C-N-CA	-7.37	112.79	120.38
4	W	207	VAL	N-CA-C	7.17	118.39	107.77
4	J	39	GLN	CA-C-N	-7.16	113.00	120.38
4	J	39	GLN	C-N-CA	-7.16	113.00	120.38
4	C	209	LYS	N-CA-C	6.80	119.92	108.02
4	N	90	TYR	N-CA-C	6.47	120.19	109.46
4	C	209	LYS	CB-CA-C	-6.25	100.68	110.74
4	C	159	LEU	N-CA-C	-6.19	98.64	108.73
4	N	106	GLY	CA-C-N	6.15	130.29	121.50
4	N	106	GLY	C-N-CA	6.15	130.29	121.50
4	W	209	LYS	N-CA-C	6.13	118.39	108.41
4	C	165	THR	N-CA-C	5.76	118.04	108.20
4	C	71	LEU	N-CA-C	5.75	118.33	109.07
4	C	203	SER	N-CA-C	-5.74	104.50	112.30
4	N	93	ALA	N-CA-C	5.62	117.62	109.07
4	C	208	ASP	N-CA-C	5.29	117.52	108.90
4	N	209	LYS	N-CA-C	5.18	116.85	108.41
4	N	207	VAL	N-CA-C	5.17	115.41	107.77
4	J	209	LYS	N-CA-C	5.14	117.17	108.02
4	J	4	LEU	N-CA-C	5.09	117.03	108.73

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	C	159	LEU	Mainchain
3	K	165	GLU	Sidechain

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2588	2506	2508	25	0
1	B	2657	2532	2574	45	0
1	E	2561	2481	2482	20	0
1	I	2640	2532	2554	29	0
1	M	2625	2544	2543	19	0
1	P	2620	2537	2541	24	0
1	S	2626	2542	2545	39	0
1	V	2621	2539	2543	25	0
2	a	209	0	211	7	0
2	b	209	0	211	36	0
2	e	209	0	210	7	6
2	i	209	0	211	6	0
2	m	209	0	211	16	0
2	p	209	0	211	10	0
2	s	209	0	211	10	2
2	v	209	0	211	26	0
3	D	1612	1584	1583	17	1
3	G	1612	1582	1583	20	2
3	K	1612	1583	1583	30	0
3	L	1612	1585	1583	7	0
3	O	1612	1586	1583	8	0
3	R	1612	1583	1583	19	0
3	U	1612	1581	1583	9	6
3	X	1612	1586	1583	7	0
4	C	1674	1571	1650	44	0
4	F	1671	1515	1647	45	0
4	H	1674	1648	1650	7	0
4	J	1671	1515	1647	40	0
4	N	1671	1651	1647	19	0
4	Q	1671	1651	1647	8	1
4	T	1674	1505	1650	36	0
4	W	1674	1647	1650	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	56	0	52	8	0
5	B	28	0	26	10	0
5	E	28	0	26	2	0
5	I	56	0	52	7	0
5	M	14	0	13	1	0
5	P	28	0	26	5	0
5	S	42	0	39	13	0
5	V	14	0	13	3	0
All	All	49152	45586	48076	528	9

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 5.

All (528) 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)
3:K:24:ARG:CZ	2:v:7:GLN:HE22	1.23	1.48
3:K:24:ARG:NE	2:v:7:GLN:HE22	1.18	1.41
2:b:3:LEU:HD11	3:R:24:ARG:CZ	1.59	1.31
2:b:3:LEU:HD11	3:R:24:ARG:NH1	1.41	1.30
3:K:24:ARG:CZ	2:v:7:GLN:NE2	2.02	1.20
3:K:24:ARG:NE	2:v:7:GLN:NE2	1.89	1.19
1:B:375:SER:HB3	2:b:23:U2X:H51	1.23	1.18
2:b:7:GLN:HE21	3:R:24:ARG:NH2	1.40	1.17
2:b:18:ARG:HA	3:R:24:ARG:NH1	1.59	1.15
2:b:3:LEU:CD1	3:R:24:ARG:NH1	2.12	1.11
4:T:100(A):LEU:HB3	4:T:100(B):PRO:HA	1.33	1.10
1:I:48:ALA:HA	1:I:49:ASN:HB2	1.28	1.09
1:B:375:SER:CB	2:b:23:U2X:H51	1.82	1.09
2:b:18:ARG:HA	3:R:24:ARG:HH12	1.08	1.08
3:G:61:ARG:HH21	3:G:79:GLN:HG3	1.14	1.08
4:J:100(A):LEU:HB3	4:J:100(B):PRO:HA	1.36	1.07
2:b:7:GLN:NE2	3:R:24:ARG:HH21	1.51	1.07
4:F:98:TRP:HB3	4:F:100:TYR:H	1.20	1.06
1:S:269:LYS:HB3	5:S:502:NAG:H82	1.37	1.04
4:F:100(A):LEU:HB3	4:F:100(B):PRO:HA	1.34	1.04
4:T:98:TRP:HB3	4:T:100:TYR:H	1.19	1.03
3:L:24:ARG:HH12	2:m:7:GLN:NE2	1.57	1.00
2:b:7:GLN:NE2	3:R:24:ARG:NH2	2.08	0.98
4:C:100(A):LEU:HB3	4:C:100(B):PRO:HA	1.41	0.98
3:L:24:ARG:NH1	2:m:7:GLN:HE22	1.61	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:61:ARG:NH2	3:G:79:GLN:CG	2.27	0.97
3:G:61:ARG:NH2	3:G:79:GLN:HG3	1.80	0.97
4:C:98:TRP:H	4:C:99:PRO:HA	1.34	0.92
1:E:370:GLU:OE1	2:e:23:U2X:H71	1.68	0.92
4:F:98:TRP:H	4:F:99:PRO:HA	1.32	0.92
4:C:98:TRP:HB3	4:C:100:TYR:HB2	1.50	0.91
3:K:24:ARG:NH2	2:v:7:GLN:OE1	2.04	0.91
4:T:98:TRP:HB3	4:T:100:TYR:N	1.85	0.90
1:I:48:ALA:HA	1:I:49:ASN:CB	2.03	0.89
4:T:98:TRP:H	4:T:99:PRO:HA	1.38	0.89
1:B:375:SER:CB	2:b:23:U2X:C5	2.49	0.89
1:I:411:ASN:ND2	2:m:13:LEU:O	2.06	0.88
4:T:95:ARG:HH21	4:T:100(A):LEU:HD13	1.37	0.88
3:G:61:ARG:HH21	3:G:79:GLN:CG	1.86	0.88
3:L:24:ARG:HH12	2:m:7:GLN:HE22	0.91	0.87
1:I:48:ALA:CA	1:I:49:ASN:HB2	2.05	0.86
3:K:24:ARG:NH2	2:v:7:GLN:HE22	1.74	0.85
1:B:269:LYS:HD3	5:B:502:NAG:H61	1.61	0.83
2:b:7:GLN:HE21	3:R:24:ARG:HH21	0.85	0.83
4:J:100(A):LEU:HB3	4:J:100(B):PRO:CA	2.10	0.81
1:B:375:SER:HB2	2:b:23:U2X:C5	2.09	0.81
1:S:375:SER:HB3	2:s:23:U2X:H51	1.63	0.80
2:b:3:LEU:CD1	3:R:24:ARG:CZ	2.51	0.79
1:B:269:LYS:CD	5:B:502:NAG:H61	2.12	0.79
2:b:3:LEU:HD11	3:R:24:ARG:NH2	1.98	0.78
3:K:24:ARG:NH2	2:v:7:GLN:NE2	2.31	0.78
4:J:98:TRP:HB3	4:J:100:TYR:N	1.96	0.78
1:S:375:SER:HB2	2:s:23:U2X:H52	1.64	0.78
1:E:370:GLU:OE1	2:e:23:U2X:HE11	1.84	0.77
2:b:3:LEU:HD11	3:R:24:ARG:HH12	1.46	0.77
4:C:98:TRP:HB3	4:C:100:TYR:N	2.00	0.77
4:J:98:TRP:H	4:J:99:PRO:HA	1.48	0.77
4:C:95:ARG:NH2	4:C:100(A):LEU:HD13	2.00	0.76
1:S:375:SER:CB	2:s:23:U2X:H52	2.14	0.76
3:D:91:LEU:CD2	4:C:100(B):PRO:HB3	2.15	0.76
4:J:95:ARG:NH2	4:J:100(A):LEU:HD13	2.00	0.76
4:F:95:ARG:HH21	4:F:100(A):LEU:HD13	1.50	0.76
1:B:269:LYS:CG	5:B:502:NAG:H61	2.15	0.76
4:C:98:TRP:HB3	4:C:100:TYR:H	1.52	0.74
4:C:100(A):LEU:CB	4:C:100(B):PRO:HA	2.16	0.73
1:I:411:ASN:ND2	2:m:15:LEU:HD21	2.04	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:24:ARG:HE	2:v:7:GLN:HE22	1.36	0.73
1:S:375:SER:HB3	2:s:23:U2X:C5	2.18	0.73
3:K:24:ARG:NH2	2:v:7:GLN:CD	2.47	0.73
4:T:95:ARG:NH2	4:T:100(A):LEU:HD13	2.04	0.72
5:I:501:NAG:O7	5:I:501:NAG:O3	2.06	0.71
1:I:411:ASN:HB2	2:m:14:GLY:HA3	1.72	0.71
1:A:212:PRO:HG3	5:A:501:NAG:H2	1.70	0.71
4:F:98:TRP:H	4:F:99:PRO:CA	2.04	0.71
1:P:233:PHE:O	1:P:273:ARG:NH1	2.24	0.70
4:C:98:TRP:CB	4:C:100:TYR:HB2	2.20	0.70
1:S:370:GLU:OE1	2:s:23:U2X:H71	1.90	0.70
4:F:100(A):LEU:HB3	4:F:100(B):PRO:CA	2.16	0.70
1:S:375:SER:CB	2:s:23:U2X:C5	2.69	0.69
1:I:295:ASN:N	1:I:295:ASN:OD1	2.24	0.69
4:T:100(A):LEU:HB3	4:T:100(B):PRO:CA	2.16	0.69
1:V:375:SER:HB3	2:v:23:U2X:H51	1.74	0.69
3:G:61:ARG:NH2	3:G:79:GLN:CD	2.51	0.69
1:S:348:GLN:NE2	5:S:502:NAG:H81	2.08	0.69
4:F:98:TRP:HB3	4:F:100:TYR:N	2.03	0.69
3:G:91:LEU:CD2	4:F:100(B):PRO:HB3	2.22	0.69
1:V:212:PRO:HG3	5:V:501:NAG:H2	1.74	0.69
4:J:98:TRP:HB3	4:J:100:TYR:H	1.56	0.69
2:b:3:LEU:CD1	3:R:24:ARG:HH12	2.04	0.68
1:V:446:VAL:O	5:V:501:NAG:H5	1.93	0.68
3:K:24:ARG:NH1	2:v:3:LEU:CD2	2.56	0.68
3:K:36:TYR:OH	4:J:100(B):PRO:HB2	1.93	0.68
3:K:36:TYR:HH	4:J:100(C):PHE:HD2	1.41	0.68
1:P:370:GLU:OE1	2:p:23:U2X:H71	1.94	0.68
1:E:370:GLU:OE1	2:e:23:U2X:CE1	2.41	0.68
4:T:98:TRP:CB	4:T:100:TYR:H	2.02	0.68
3:K:24:ARG:HE	2:v:7:GLN:NE2	1.90	0.67
3:D:36:TYR:OH	4:C:100(B):PRO:HB2	1.94	0.67
1:B:48:ALA:HA	1:B:490:LYS:HG3	1.77	0.67
4:F:98:TRP:CB	4:F:100:TYR:H	2.02	0.67
4:C:100(A):LEU:HB3	4:C:100(B):PRO:CA	2.23	0.67
1:B:446:VAL:O	5:B:501:NAG:H5	1.95	0.67
1:B:491:ILE:HG22	1:B:492:GLU:HG3	1.75	0.67
3:K:91:LEU:HD22	4:J:100(A):LEU:HB2	1.75	0.67
1:V:233:PHE:O	1:V:273:ARG:NH1	2.28	0.67
4:F:95:ARG:HE	4:F:100(A):LEU:HD22	1.60	0.66
4:C:98:TRP:H	4:C:99:PRO:CA	2.07	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:62:PHE:CE2	3:G:75:ILE:CD1	2.79	0.66
1:B:376:PHE:CA	2:b:23:U2X:H62	2.25	0.66
1:I:446:VAL:O	5:I:501:NAG:H3	1.96	0.66
1:B:375:SER:C	2:b:23:U2X:H52	2.20	0.66
1:B:368:ASP:OD1	2:b:24:CYS:HB3	1.96	0.66
4:N:94:ARG:NH2	4:N:101:ASP:OD1	2.29	0.66
3:D:93:GLY:O	3:D:96:ARG:NH1	2.26	0.66
5:I:501:NAG:H62	5:I:504:NAG:H81	1.77	0.66
3:K:122:ASP:OD2	4:J:214:LYS:NZ	2.29	0.66
4:F:147:PRO:O	4:F:200:HIS:NE2	2.28	0.65
3:D:26:SER:HA	2:p:3:LEU:HD23	1.78	0.65
1:M:232:GLU:CB	1:M:233:PHE:HA	2.27	0.65
4:Q:147:PRO:O	4:Q:200:HIS:NE2	2.30	0.65
1:B:121:GLN:NE2	1:B:426:MET:SD	2.69	0.65
3:G:62:PHE:CE2	3:G:75:ILE:HD11	2.31	0.65
3:G:91:LEU:HD22	4:F:100(B):PRO:HB3	1.78	0.65
4:J:33:TYR:CE1	4:J:52:LYS:HB2	2.33	0.64
4:C:98:TRP:HB3	4:C:100:TYR:CB	2.26	0.64
1:P:269:LYS:HD3	5:P:502:NAG:H61	1.80	0.64
1:S:298:ARG:NH2	1:S:441:GLY:O	2.31	0.64
4:H:30:OAS:HC22	4:H:31:GLY:H	1.62	0.63
4:T:100(A):LEU:CB	4:T:100(B):PRO:HA	2.20	0.63
4:F:117:LYS:HB2	3:U:126:LYS:HZ3	1.63	0.63
1:E:232:GLU:CB	1:E:233:PHE:HA	2.28	0.62
1:S:270:VAL:O	1:S:348:GLN:NE2	2.31	0.62
4:F:100(A):LEU:CB	4:F:100(B):PRO:HA	2.22	0.62
4:J:95:ARG:HH21	4:J:100(A):LEU:HD13	1.62	0.62
1:I:261:LEU:HD13	5:I:501:NAG:H83	1.81	0.62
1:A:269:LYS:HE2	5:A:502:NAG:H4	1.81	0.62
1:A:375:SER:HB2	2:a:23:U2X:H51	1.82	0.62
1:P:232:GLU:CB	1:P:233:PHE:HA	2.30	0.62
1:V:232:GLU:CB	1:V:233:PHE:HA	2.29	0.61
3:G:61:ARG:NH2	3:G:79:GLN:CB	2.63	0.61
1:B:376:PHE:HA	2:b:23:U2X:H62	1.83	0.61
4:J:98:TRP:HB3	4:J:100:TYR:HB2	1.81	0.61
4:T:98:TRP:N	4:T:99:PRO:HA	2.12	0.61
3:O:37:GLN:O	3:O:45:LYS:N	2.33	0.61
1:A:375:SER:HB2	2:a:23:U2X:C5	2.31	0.60
1:M:298:ARG:NH2	1:M:441:GLY:O	2.34	0.60
3:U:91:LEU:HD22	4:T:100(B):PRO:HB3	1.81	0.60
2:b:3:LEU:HD21	3:R:24:ARG:NE	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:24:ARG:HH11	2:v:3:LEU:HD21	1.66	0.60
4:J:100(A):LEU:CB	4:J:100(B):PRO:CA	2.80	0.60
4:F:33:TYR:CE2	4:F:52:LYS:HD3	2.36	0.60
1:S:232:GLU:CB	1:S:233:PHE:HA	2.32	0.60
1:B:287:GLN:NE2	1:B:481:SER:O	2.35	0.60
1:M:66:HIS:ND1	1:M:211:GLU:O	2.35	0.60
1:I:66:HIS:ND1	1:I:211:GLU:O	2.35	0.59
1:I:232:GLU:CB	1:I:233:PHE:HA	2.31	0.59
1:P:344:GLN:OE1	5:P:502:NAG:H62	2.01	0.59
1:I:411:ASN:CG	2:m:15:LEU:HD21	2.27	0.59
4:J:52:LYS:HG3	4:J:54:ASN:H	1.68	0.59
1:M:370:GLU:OE1	2:m:23:U2X:CE1	2.51	0.59
4:J:57:PRO:HB2	4:J:59:TYR:CZ	2.38	0.59
1:S:212:PRO:HG3	5:S:501:NAG:H2	1.84	0.59
3:G:61:ARG:HH22	3:G:79:GLN:HB2	1.67	0.59
1:M:368:ASP:OD2	1:M:425:ASN:ND2	2.36	0.59
1:A:344:GLN:OE1	5:A:502:NAG:H62	2.02	0.58
3:L:24:ARG:NH1	2:m:7:GLN:NE2	2.35	0.58
2:b:3:LEU:HD13	3:R:24:ARG:NH1	2.15	0.58
1:S:375:SER:HB2	2:s:23:U2X:C5	2.33	0.58
1:I:327:ARG:NH2	1:I:422:GLN:OE1	2.37	0.57
1:E:353:TRP:O	1:E:357:ASN:ND2	2.36	0.57
4:F:95:ARG:NH2	4:F:100(A):LEU:HD13	2.19	0.57
1:B:232:GLU:CB	1:B:233:PHE:HA	2.34	0.57
1:S:348:GLN:HE21	5:S:502:NAG:H81	1.70	0.57
1:B:375:SER:HB2	2:b:23:U2X:H52	1.85	0.57
4:T:33:TYR:CE1	4:T:52:LYS:HB2	2.38	0.57
1:V:212:PRO:CG	5:V:501:NAG:H2	2.34	0.57
1:P:269:LYS:HE2	5:P:502:NAG:H4	1.87	0.57
3:K:93:GLY:O	3:K:96:ARG:NH1	2.34	0.57
1:V:66:HIS:ND1	1:V:211:GLU:O	2.38	0.57
1:S:66:HIS:ND1	1:S:211:GLU:O	2.37	0.57
3:D:91:LEU:HD22	4:C:100(B):PRO:HB3	1.86	0.56
4:F:100:TYR:C	4:F:100(A):LEU:HG	2.31	0.56
3:U:91:LEU:HD21	4:T:100(B):PRO:HG3	1.86	0.56
1:I:375:SER:HB3	2:i:23:U2X:H51	1.88	0.56
3:G:61:ARG:NH2	3:G:79:GLN:HB2	2.21	0.56
3:K:24:ARG:NH1	2:v:3:LEU:HD21	2.20	0.56
1:S:290:GLU:OE2	5:S:502:NAG:O6	2.20	0.56
1:A:212:PRO:CG	5:A:501:NAG:H2	2.35	0.56
3:K:24:ARG:NH1	2:v:3:LEU:HD23	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:55:GLY:O	4:J:57:PRO:HD3	2.06	0.56
1:P:446:VAL:O	5:P:501:NAG:H5	2.05	0.56
1:E:446:VAL:O	5:E:501:NAG:H5	2.05	0.56
3:G:126:LYS:HD2	4:T:115:SER:HB2	1.88	0.55
1:M:76:PRO:O	1:M:77:THR:OG1	2.22	0.55
1:E:66:HIS:ND1	1:E:211:GLU:O	2.39	0.55
4:J:197:ASN:OD1	4:J:197:ASN:N	2.38	0.55
4:T:55:GLY:O	4:T:57:PRO:HD3	2.07	0.55
1:I:406:THR:O	2:m:11:LYS:O	2.25	0.55
4:T:98:TRP:HB3	4:T:100:TYR:HB2	1.89	0.55
4:W:197:ASN:N	4:W:197:ASN:OD1	2.41	0.54
1:E:77:THR:O	4:F:33:TYR:OH	2.24	0.54
1:P:447:SER:OG	5:P:501:NAG:N2	2.41	0.54
4:F:95:ARG:NE	4:F:100(A):LEU:HD22	2.21	0.54
4:Q:197:ASN:OD1	4:Q:197:ASN:N	2.39	0.54
1:S:446:VAL:O	5:S:501:NAG:H5	2.08	0.53
4:T:52:LYS:HG3	4:T:53:HIS:N	2.22	0.53
1:A:375:SER:CB	2:a:23:U2X:H51	2.38	0.53
1:M:232:GLU:HB2	1:M:233:PHE:HA	1.90	0.53
4:T:100(A):LEU:CB	4:T:100(B):PRO:CA	2.85	0.53
1:A:66:HIS:ND1	1:A:211:GLU:O	2.41	0.53
1:E:369:LEU:O	1:E:373:THR:OG1	2.23	0.53
4:F:95:ARG:HH21	4:F:100(A):LEU:CD1	2.20	0.53
4:J:98:TRP:N	4:J:99:PRO:HA	2.22	0.53
4:F:57:PRO:HB2	4:F:59:TYR:CE2	2.43	0.53
1:P:375:SER:HB2	2:p:23:U2X:H52	1.91	0.53
1:B:375:SER:C	2:b:23:U2X:C5	2.82	0.53
5:B:502:NAG:O7	5:B:502:NAG:O3	2.23	0.53
4:C:33:TYR:HB2	4:C:95:ARG:HB2	1.91	0.53
1:S:425:ASN:O	2:s:23:U2X:H72	2.08	0.53
1:A:99:ASN:OD1	1:A:103:GLN:NE2	2.42	0.53
4:F:52:LYS:HG3	4:F:53:HIS:N	2.24	0.53
1:I:232:GLU:HB2	1:I:233:PHE:HA	1.91	0.53
4:F:98:TRP:HB3	4:F:100:TYR:HB2	1.91	0.53
4:C:121:VAL:HG12	4:C:209:LYS:HD2	1.92	0.52
3:U:91:LEU:CD2	4:T:100(B):PRO:HG3	2.39	0.52
3:X:164:THR:HG21	4:W:164:HIS:HB3	1.92	0.52
1:E:232:GLU:HB2	1:E:233:PHE:HA	1.90	0.52
4:J:129:LYS:H	4:J:129:LYS:HD3	1.74	0.52
3:G:62:PHE:HE2	3:G:75:ILE:HD11	1.73	0.52
1:A:335:GLY:O	1:A:339:ASN:ND2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:211:GLU:OE2	5:I:501:NAG:H4	2.10	0.52
1:M:55:ALA:N	1:M:216:HIS:O	2.43	0.52
1:V:375:SER:HB2	2:v:23:U2X:H52	1.91	0.52
3:G:61:ARG:NH2	3:G:82:ASP:OD2	2.43	0.52
4:T:33:TYR:CE1	4:T:52:LYS:HD3	2.45	0.52
1:V:335:GLY:O	1:V:339:ASN:ND2	2.42	0.51
1:P:232:GLU:HB2	1:P:233:PHE:HA	1.93	0.51
4:C:95:ARG:HD3	4:C:100(C):PHE:CE1	2.45	0.51
1:V:375:SER:CB	2:v:23:U2X:C5	2.88	0.51
4:W:12:LEU:HD11	4:W:18:LEU:HA	1.93	0.51
3:D:91:LEU:HD21	4:C:100(B):PRO:HB3	1.90	0.51
4:C:95:ARG:HB3	4:C:100(A):LEU:CD2	2.41	0.51
1:V:375:SER:CB	2:v:23:U2X:H51	2.40	0.51
2:v:9:ARG:O	2:v:12:SER:OG	2.27	0.51
2:i:9:ARG:O	2:i:12:SER:OG	2.27	0.51
1:M:232:GLU:HB3	1:M:233:PHE:HA	1.93	0.50
2:s:9:ARG:O	2:s:12:SER:OG	2.27	0.50
4:F:57:PRO:HB2	4:F:59:TYR:CZ	2.47	0.50
4:N:100(A):LEU:N	4:N:100(B):PRO:HD2	2.26	0.50
1:V:232:GLU:HB2	1:V:233:PHE:HA	1.93	0.50
3:K:24:ARG:HH11	2:v:3:LEU:CD2	2.21	0.50
1:P:375:SER:HB3	2:p:23:U2X:H51	1.94	0.50
1:B:212:PRO:HG3	5:B:501:NAG:H2	1.94	0.50
4:J:52:LYS:HG3	4:J:53:HIS:N	2.26	0.50
1:I:427:TRP:HB2	2:i:23:U2X:OH	2.12	0.50
4:Q:100(A):LEU:N	4:Q:100(B):PRO:CD	2.75	0.50
5:I:501:NAG:H62	5:I:504:NAG:C8	2.41	0.50
4:F:95:ARG:HD3	4:F:100(C):PHE:CD1	2.47	0.50
4:C:25:TYR:OH	1:S:86:MET:SD	2.52	0.50
2:p:9:ARG:O	2:p:12:SER:OG	2.27	0.50
4:T:98:TRP:H	4:T:99:PRO:CA	2.16	0.50
4:F:129:LYS:HD3	4:F:129:LYS:H	1.77	0.49
4:J:98:TRP:CB	4:J:100:TYR:HB2	2.42	0.49
3:O:61:ARG:NH2	3:O:81:GLU:OE2	2.43	0.49
1:E:388:SER:OG	5:E:502:NAG:H62	2.13	0.49
1:S:269:LYS:HA	1:S:289:ASN:HD22	1.76	0.49
1:A:269:LYS:HD3	5:A:502:NAG:H61	1.95	0.49
1:B:375:SER:CB	2:b:23:U2X:H52	2.38	0.49
4:C:150:VAL:HG12	4:C:200:HIS:HB2	1.93	0.49
1:A:87:GLU:N	1:A:87:GLU:OE1	2.45	0.49
1:B:376:PHE:N	2:b:23:U2X:H62	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:37:GLN:O	3:X:45:LYS:N	2.46	0.49
3:X:186:TYR:O	3:X:192:TYR:OH	2.30	0.49
4:H:100(A):LEU:N	4:H:100(B):PRO:CD	2.76	0.48
4:F:206:LYS:HB2	4:T:208:ASP:HB2	1.95	0.48
4:C:144:ASP:OD1	4:C:171:GLN:NE2	2.47	0.48
4:F:95:ARG:HH21	4:F:100(A):LEU:HD22	1.78	0.48
2:b:3:LEU:HD21	3:R:24:ARG:CZ	2.44	0.48
1:B:233:PHE:O	1:B:273:ARG:NH1	2.46	0.48
1:S:99:ASN:OD1	1:S:103:GLN:NE2	2.44	0.48
1:I:350:ARG:O	1:I:352:TYR:N	2.46	0.48
4:F:50:GLU:OE1	4:F:95:ARG:NH1	2.47	0.48
4:T:33:TYR:CZ	4:T:52:LYS:HD3	2.49	0.48
4:H:129:LYS:H	4:H:129:LYS:HD3	1.79	0.48
4:C:165:THR:O	4:C:165:THR:HG22	2.13	0.48
4:F:115:SER:HB2	3:U:126:LYS:HD2	1.94	0.48
1:B:46:LYS:HD2	1:B:491:ILE:HD13	1.96	0.47
1:V:76:PRO:O	1:V:77:THR:OG1	2.31	0.47
4:J:33:TYR:CE1	4:J:52:LYS:HD3	2.48	0.47
1:P:66:HIS:ND1	1:P:211:GLU:O	2.47	0.47
1:S:269:LYS:HG2	5:S:502:NAG:HN2	1.79	0.47
1:S:344:GLN:OE1	5:S:502:NAG:O3	2.28	0.47
1:I:375:SER:HB2	2:i:23:U2X:H52	1.96	0.47
2:e:9:ARG:O	2:e:12:SER:OG	2.27	0.47
4:F:100(A):LEU:CB	4:F:100(B):PRO:CA	2.89	0.47
3:O:164:THR:HG21	4:N:164:HIS:HB3	1.96	0.47
4:N:34:TRP:CH2	4:N:94:ARG:HG3	2.49	0.47
1:B:232:GLU:HB2	1:B:233:PHE:HA	1.96	0.47
4:J:50:GLU:OE1	4:J:95:ARG:NH1	2.48	0.47
1:V:232:GLU:HB3	1:V:233:PHE:HA	1.96	0.47
4:W:129:LYS:HD3	4:W:129:LYS:H	1.78	0.47
2:a:9:ARG:O	2:a:12:SER:OG	2.27	0.47
3:D:108:ARG:NH1	3:D:111:ALA:HB2	2.30	0.47
1:M:461:ASN:O	1:M:463:ASN:N	2.47	0.47
1:S:348:GLN:NE2	5:S:502:NAG:C8	2.76	0.47
2:s:5:PHE:O	2:s:9:ARG:HG3	2.15	0.47
4:T:178:LEU:C	4:T:178:LEU:HD23	2.40	0.47
1:B:46:LYS:HD2	1:B:491:ILE:CD1	2.44	0.47
1:E:376:PHE:N	2:e:23:U2X:H62	2.30	0.47
2:e:5:PHE:O	2:e:9:ARG:HG3	2.15	0.47
2:i:5:PHE:O	2:i:9:ARG:HG3	2.15	0.47
1:M:232:GLU:CB	1:M:233:PHE:CA	2.92	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:375:SER:HB3	2:m:23:U2X:H51	1.95	0.47
4:N:29:LEU:HD23	4:N:34:TRP:CZ2	2.50	0.47
1:S:344:GLN:HB3	5:S:502:NAG:O7	2.15	0.47
3:X:82:ASP:O	3:X:86:TYR:OH	2.30	0.47
1:S:232:GLU:CB	1:S:233:PHE:CA	2.93	0.46
2:b:9:ARG:O	2:b:12:SER:OG	2.27	0.46
1:P:232:GLU:HB3	1:P:233:PHE:HA	1.98	0.46
1:S:232:GLU:HB3	1:S:233:PHE:HA	1.97	0.46
4:F:98:TRP:N	4:F:99:PRO:CA	2.75	0.46
1:I:427:TRP:O	2:i:22:THR:HG21	2.15	0.46
4:C:100(A):LEU:CB	4:C:100(B):PRO:CA	2.88	0.46
1:A:350:ARG:O	1:A:352:TYR:N	2.45	0.46
2:a:5:PHE:O	2:a:9:ARG:HG3	2.15	0.46
3:K:37:GLN:O	3:K:45:LYS:N	2.47	0.46
2:m:5:PHE:O	2:m:9:ARG:HG3	2.15	0.46
1:A:278:THR:HG22	5:A:504:NAG:H62	1.98	0.46
2:b:5:PHE:O	2:b:9:ARG:HG3	2.15	0.46
1:M:218:CYS:HB2	4:N:98:TRP:CZ2	2.51	0.46
4:N:34:TRP:CZ3	4:N:94:ARG:HB2	2.50	0.46
3:U:36:TYR:OH	4:T:100(B):PRO:HG2	2.16	0.46
1:V:232:GLU:CB	1:V:233:PHE:CA	2.94	0.46
4:J:38:ARG:HB3	4:J:48:ILE:HD11	1.97	0.46
1:M:446:VAL:O	5:M:501:NAG:H5	2.16	0.46
1:P:427:TRP:CE3	2:p:23:U2X:H21	2.51	0.46
3:K:34:ALA:CB	4:J:100(B):PRO:HG3	2.46	0.46
1:S:232:GLU:HB2	1:S:233:PHE:HA	1.97	0.46
3:U:93:GLY:O	3:U:96:ARG:NH1	2.34	0.46
1:V:375:SER:HB3	2:v:23:U2X:C5	2.43	0.46
4:C:143:LYS:HG3	4:C:177:SER:HB2	1.97	0.46
2:p:5:PHE:O	2:p:9:ARG:HG3	2.15	0.46
1:S:65:VAL:HB	1:S:115:SER:HB3	1.97	0.46
1:E:232:GLU:HB3	1:E:233:PHE:HA	1.97	0.45
3:O:10:PHE:CZ	3:O:105:GLU:HG2	2.51	0.45
1:A:322:SER:N	2:b:13:LEU:HG	2.31	0.45
1:B:269:LYS:CB	5:B:502:NAG:H61	2.46	0.45
4:J:98:TRP:H	4:J:99:PRO:CA	2.24	0.45
1:P:375:SER:CB	2:p:23:U2X:H52	2.46	0.45
1:S:348:GLN:HE21	5:S:502:NAG:C8	2.29	0.45
1:V:375:SER:HB2	2:v:23:U2X:C5	2.46	0.45
2:v:5:PHE:O	2:v:9:ARG:HG3	2.15	0.45
3:K:6:GLN:HE22	3:K:87:TYR:HA	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:375:SER:O	2:b:23:U2X:H52	2.16	0.45
3:L:61:ARG:NH2	3:L:81:GLU:OE2	2.49	0.45
1:A:94:ASN:OD1	1:A:97:LYS:N	2.50	0.45
1:B:269:LYS:HG2	1:B:348:GLN:NE2	2.31	0.45
2:m:9:ARG:O	2:m:12:SER:OG	2.27	0.45
4:T:60:HIS:CG	4:T:61:PRO:HD2	2.52	0.45
1:B:270:VAL:HG22	1:B:288:LEU:HA	1.98	0.45
1:I:411:ASN:ND2	2:m:15:LEU:CD2	2.76	0.45
1:P:112:TRP:CE3	1:P:427:TRP:CZ2	3.05	0.45
4:Q:152:VAL:HG11	4:Q:180:SER:CB	2.47	0.45
4:N:152:VAL:HG11	4:N:180:SER:CB	2.47	0.45
1:A:375:SER:HB2	2:a:23:U2X:H52	1.99	0.44
1:V:257:THR:O	1:V:259:LEU:N	2.49	0.44
4:C:98:TRP:HB3	4:C:100:TYR:CA	2.47	0.44
1:E:232:GLU:CB	1:E:233:PHE:CA	2.94	0.44
3:O:166:GLN:HG3	3:O:173:TYR:CZ	2.52	0.44
1:B:270:VAL:HB	1:B:348:GLN:HE22	1.82	0.44
4:F:175:LEU:HD21	3:U:126:LYS:NZ	2.32	0.44
1:P:425:ASN:O	2:p:23:U2X:HE11	2.17	0.44
4:Q:129:LYS:H	4:Q:129:LYS:HD3	1.82	0.44
3:D:33:LEU:HD22	3:D:71:PHE:CG	2.53	0.44
4:C:200:HIS:CE1	4:C:202:PRO:HB2	2.53	0.44
1:B:327:ARG:NH2	1:B:422:GLN:OE1	2.49	0.44
4:H:178:LEU:C	4:H:178:LEU:HD23	2.43	0.44
4:C:100(B):PRO:HB2	4:C:100(C):PHE:H	1.62	0.44
4:J:178:LEU:C	4:J:178:LEU:HD23	2.42	0.44
4:N:188:SER:O	4:N:192:GLN:N	2.50	0.44
4:W:100(A):LEU:N	4:W:100(B):PRO:HD2	2.31	0.44
1:A:77:THR:HB	1:A:78:ASP:CB	2.47	0.44
1:B:48:ALA:HB1	1:B:488:VAL:HG12	2.00	0.44
4:C:116:THR:CG2	4:C:203:SER:HB3	2.48	0.44
3:G:61:ARG:CZ	3:G:79:GLN:NE2	2.81	0.44
4:F:95:ARG:HD3	4:F:100(C):PHE:CE1	2.53	0.44
1:P:232:GLU:CB	1:P:233:PHE:CA	2.95	0.44
3:K:118:PHE:HB3	4:J:124:LEU:HD22	1.99	0.44
4:T:98:TRP:N	4:T:99:PRO:CA	2.79	0.44
4:C:12:LEU:HD11	4:C:18:LEU:HA	2.00	0.44
1:I:295:ASN:HD22	1:I:444:ARG:NH2	2.15	0.44
1:E:76:PRO:O	1:E:77:THR:OG1	2.24	0.44
4:F:33:TYR:HB2	4:F:95:ARG:HB2	2.00	0.44
1:S:269:LYS:HD3	5:S:502:NAG:C8	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:463:ASN:C	1:V:465:ASN:H	2.26	0.44
4:W:178:LEU:HD23	4:W:178:LEU:C	2.43	0.44
3:D:58:VAL:HA	3:D:59:PRO:HD3	1.90	0.43
1:S:269:LYS:HD3	5:S:502:NAG:H83	1.99	0.43
4:W:100(A):LEU:N	4:W:100(B):PRO:CD	2.81	0.43
3:O:46:LEU:HD22	4:N:100(B):PRO:HB2	2.01	0.43
1:B:61:TYR:HD2	4:C:61:PRO:HA	1.83	0.43
4:C:95:ARG:HB3	4:C:100(A):LEU:HD22	2.01	0.43
4:C:178:LEU:C	4:C:178:LEU:HD23	2.44	0.43
1:I:105:HIS:CE1	1:I:427:TRP:CZ2	3.06	0.43
4:H:100(A):LEU:N	4:H:100(B):PRO:HD2	2.34	0.43
4:F:178:LEU:HD23	4:F:178:LEU:C	2.43	0.43
4:J:68:THR:HB	4:J:81:ASN:HB2	2.00	0.43
1:M:427:TRP:HB3	2:m:23:U2X:OH	2.18	0.43
4:T:129:LYS:H	4:T:129:LYS:HD3	1.82	0.43
1:A:71:THR:HG22	3:L:93:GLY:HA2	2.01	0.43
3:D:209:PHE:HB3	4:C:129:LYS:NZ	2.33	0.43
4:F:12:LEU:HD11	4:F:18:LEU:HA	2.00	0.43
4:J:98:TRP:HB3	4:J:100:TYR:CB	2.49	0.43
4:N:129:LYS:H	4:N:129:LYS:HD3	1.82	0.43
3:U:33:LEU:HD22	3:U:71:PHE:CD1	2.53	0.43
4:F:95:ARG:NH2	4:F:100(A):LEU:HD22	2.33	0.43
1:B:290:GLU:OE2	5:B:502:NAG:H82	2.19	0.43
1:V:375:SER:CB	2:v:23:U2X:H52	2.48	0.43
1:A:386:ASN:HD22	5:A:503:NAG:H83	1.84	0.43
1:B:61:TYR:CG	4:C:64:LYS:HD3	2.53	0.43
4:N:90:TYR:CD1	4:N:90:TYR:N	2.86	0.43
4:N:178:LEU:C	4:N:178:LEU:HD23	2.44	0.43
1:V:77:THR:HB	1:V:78:ASP:HB3	2.01	0.43
1:V:77:THR:HB	1:V:78:ASP:HA	2.01	0.43
1:B:48:ALA:HB2	1:B:489:VAL:HA	2.01	0.42
5:I:504:NAG:O7	5:I:504:NAG:O3	2.29	0.42
4:F:203:SER:O	4:T:209:LYS:NZ	2.51	0.42
1:P:77:THR:HB	1:P:78:ASP:HB3	1.99	0.42
4:T:119:PRO:HB3	4:T:145:TYR:HB3	2.01	0.42
4:T:201:LYS:N	4:T:202:PRO:CD	2.82	0.42
4:C:147:PRO:O	4:C:200:HIS:NE2	2.48	0.42
3:X:4:MET:HE1	3:X:25:ALA:HB2	2.01	0.42
3:G:33:LEU:HD22	3:G:71:PHE:CG	2.54	0.42
4:F:33:TYR:CZ	4:F:52:LYS:HD3	2.54	0.42
3:K:44:PRO:HG3	4:J:45:LEU:HD11	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:269:LYS:HG3	5:B:502:NAG:H61	1.96	0.42
3:D:185:ASP:O	3:D:188:LYS:HG2	2.19	0.42
3:D:191:VAL:HG22	3:D:210:ASN:OD1	2.18	0.42
4:F:51:ILE:HG13	4:F:52:LYS:N	2.33	0.42
4:J:94:ARG:O	4:J:100(C):PHE:HA	2.20	0.42
4:N:95:ARG:HA	4:N:100(C):PHE:HB3	2.01	0.42
4:N:98:TRP:CD1	4:N:99:PRO:HA	2.54	0.42
3:R:7:SER:HA	3:R:8:PRO:C	2.45	0.42
1:V:425:ASN:O	2:v:23:U2X:HE11	2.20	0.42
3:X:124:GLN:O	3:X:127:SER:OG	2.33	0.42
1:B:232:GLU:CB	1:B:233:PHE:CA	2.96	0.42
4:C:75:LYS:HG2	1:S:85:LYS:HD2	2.02	0.42
4:C:197:ASN:OD1	4:C:197:ASN:N	2.53	0.42
1:E:375:SER:C	2:e:23:U2X:C5	2.93	0.42
4:J:97:ASN:O	4:J:98:TRP:HB2	2.18	0.42
1:M:257:THR:O	1:M:259:LEU:N	2.51	0.42
3:O:43:ALA:HB1	4:N:103:TRP:HB2	2.02	0.42
1:P:375:SER:CB	2:p:23:U2X:C5	2.97	0.42
4:Q:12:LEU:HD11	4:Q:18:LEU:HA	2.01	0.42
4:C:98:TRP:N	4:C:99:PRO:CA	2.77	0.42
4:T:57:PRO:HB2	4:T:59:TYR:CE2	2.55	0.42
1:A:278:THR:CG2	5:A:504:NAG:H62	2.50	0.42
3:G:91:LEU:HD21	4:F:100(B):PRO:HG3	2.02	0.42
1:P:112:TRP:CE3	1:P:427:TRP:CH2	3.07	0.42
1:S:61:TYR:CG	4:T:64:LYS:HD3	2.54	0.42
1:I:77:THR:HB	1:I:78:ASP:HB3	2.02	0.42
2:b:18:ARG:CA	3:R:24:ARG:NH1	2.54	0.42
3:D:89:GLN:NE2	4:C:100(C):PHE:HE2	2.18	0.42
1:S:83:GLU:OE2	1:S:227:LYS:NZ	2.52	0.42
4:H:55:GLY:O	4:H:56:SER:OG	2.25	0.42
1:E:373:THR:O	1:E:374:HIS:CB	2.68	0.42
3:K:124:GLN:HG3	4:J:122:PHE:CE2	2.55	0.42
4:T:12:LEU:HD11	4:T:18:LEU:HA	2.02	0.42
4:N:28:SER:OG	4:N:29:LEU:N	2.41	0.41
4:Q:38:ARG:NH2	4:Q:46:GLU:OE1	2.52	0.41
1:B:212:PRO:CG	5:B:501:NAG:H2	2.50	0.41
1:I:48:ALA:CB	1:I:49:ASN:HB2	2.50	0.41
3:K:13:ALA:HB3	3:K:104:LEU:HD11	2.02	0.41
1:B:61:TYR:CD1	1:B:61:TYR:C	2.98	0.41
1:I:298:ARG:NH2	1:I:441:GLY:O	2.52	0.41
4:J:127:SER:HB2	4:J:129:LYS:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:132:SER:N	4:J:135:THR:O	2.53	0.41
1:M:370:GLU:OE1	2:m:23:U2X:HE11	2.20	0.41
3:K:24:ARG:CZ	2:v:7:GLN:CD	2.79	0.41
1:S:55:ALA:N	1:S:216:HIS:O	2.53	0.41
3:X:116:PHE:CE2	4:W:132:SER:HB2	2.56	0.41
4:J:51:ILE:HG13	4:J:52:LYS:N	2.35	0.41
1:A:473:GLY:HA2	2:a:23:U2X:HE21	2.03	0.41
4:F:100(B):PRO:HB2	4:F:100(C):PHE:H	1.53	0.41
1:P:463:ASN:C	1:P:465:ASN:H	2.29	0.41
1:B:45:TRP:O	1:B:47:ASP:N	2.51	0.41
1:I:232:GLU:CB	1:I:233:PHE:CA	2.96	0.41
4:C:201:LYS:N	4:C:202:PRO:CD	2.84	0.41
1:M:201:LEU:HD23	1:M:202:THR:N	2.35	0.41
4:N:103:TRP:CD1	4:N:103:TRP:N	2.88	0.41
4:T:52:LYS:HG3	4:T:54:ASN:H	1.85	0.41
1:V:66:HIS:CE1	1:V:212:PRO:HA	2.55	0.41
1:E:463:ASN:C	1:E:465:ASN:H	2.28	0.41
4:J:119:PRO:HB3	4:J:145:TYR:HB3	2.03	0.41
1:P:350:ARG:O	1:P:352:TYR:N	2.46	0.41
1:A:77:THR:HB	1:A:78:ASP:CA	2.51	0.41
3:L:49:TYR:HB3	4:H:100(B):PRO:HG3	2.03	0.41
3:D:149:LYS:N	3:D:193:ALA:O	2.43	0.41
4:C:72:ASP:OD1	4:C:72:ASP:C	2.64	0.41
1:E:374:HIS:CD2	1:E:375:SER:N	2.89	0.41
3:G:62:PHE:CZ	3:G:75:ILE:HD13	2.56	0.41
3:G:209:PHE:HB3	4:F:129:LYS:NZ	2.35	0.41
1:M:96:TRP:CD2	1:M:275:GLU:HG3	2.56	0.41
3:O:4:MET:HE1	3:O:25:ALA:HB2	2.02	0.41
4:Q:178:LEU:C	4:Q:178:LEU:HD23	2.45	0.41
1:A:440:GLN:HE22	2:b:8:LEU:HD21	1.86	0.41
4:F:150:VAL:HG12	4:F:200:HIS:HB2	2.03	0.41
1:S:76:PRO:O	1:S:77:THR:OG1	2.32	0.41
1:B:370:GLU:OE1	2:b:23:U2X:HE11	2.22	0.40
3:K:108:ARG:HH21	3:K:170:ASP:HB2	1.86	0.40
3:K:185:ASP:O	3:K:188:LYS:HG2	2.21	0.40
3:D:142:ARG:O	3:D:142:ARG:HG2	2.20	0.40
3:D:158:ASN:O	3:D:179:LEU:HD12	2.21	0.40
4:C:127:SER:OG	4:C:129:LYS:CE	2.69	0.40
1:P:55:ALA:N	1:P:216:HIS:O	2.54	0.40
1:V:55:ALA:N	1:V:216:HIS:O	2.53	0.40
1:A:440:GLN:OE1	2:b:8:LEU:HG	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:VAL:HB	1:B:115:SER:HB3	2.04	0.40
4:N:105:GLN:OE1	4:N:105:GLN:N	2.44	0.40
3:R:33:LEU:HD22	3:R:71:PHE:CG	2.57	0.40
1:I:48:ALA:HB3	1:I:488:VAL:HG12	2.03	0.40
4:C:159:LEU:HD21	4:C:182:VAL:HG21	2.03	0.40
1:E:325:ASP:OD1	1:E:326:ILE:N	2.54	0.40
4:J:33:TYR:CZ	4:J:52:LYS:HD3	2.57	0.40
1:B:232:GLU:HB3	1:B:233:PHE:HA	2.04	0.40
3:D:33:LEU:HG	3:D:34:ALA:N	2.37	0.40
1:S:61:TYR:HD2	4:T:61:PRO:HA	1.87	0.40
1:S:77:THR:HB	1:S:78:ASP:CB	2.51	0.40

All (9) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:e:3:LEU:CD1	3:U:24:ARG:CZ[1_545]	1.75	0.45
2:e:3:LEU:CD1	3:U:24:ARG:NH1[1_545]	1.75	0.45
2:e:7:GLN:NE2	3:U:24:ARG:NH2[1_545]	1.84	0.36
2:e:7:GLN:CD	3:U:24:ARG:NH2[1_545]	2.01	0.19
3:G:24:ARG:NH2	2:s:7:GLN:NE2[1_545]	2.05	0.15
2:e:7:GLN:NE2	3:U:24:ARG:HH21[1_545]	1.55	0.05
2:e:3:LEU:CD2	3:U:24:ARG:NE[1_545]	2.16	0.04
3:G:24:ARG:HH22	2:s:7:GLN:NE2[1_545]	1.57	0.03
3:D:126:LYS:HZ2	4:Q:115:SER:O[1_565]	1.59	0.01

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	327/352 (93%)	298 (91%)	26 (8%)	3 (1%)	14 47

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	336/352 (96%)	301 (90%)	29 (9%)	6 (2%)	6	34
1	E	323/352 (92%)	290 (90%)	26 (8%)	7 (2%)	5	30
1	I	335/352 (95%)	285 (85%)	42 (12%)	8 (2%)	4	29
1	M	333/352 (95%)	298 (90%)	28 (8%)	7 (2%)	5	31
1	P	332/352 (94%)	295 (89%)	30 (9%)	7 (2%)	5	31
1	S	333/352 (95%)	293 (88%)	34 (10%)	6 (2%)	6	34
1	V	332/352 (94%)	299 (90%)	29 (9%)	4 (1%)	10	42
2	a	24/28 (86%)	24 (100%)	0	0	100	100
2	b	24/28 (86%)	24 (100%)	0	0	100	100
2	e	24/28 (86%)	24 (100%)	0	0	100	100
2	i	24/28 (86%)	24 (100%)	0	0	100	100
2	m	24/28 (86%)	24 (100%)	0	0	100	100
2	p	24/28 (86%)	24 (100%)	0	0	100	100
2	s	24/28 (86%)	24 (100%)	0	0	100	100
2	v	24/28 (86%)	24 (100%)	0	0	100	100
3	D	208/210 (99%)	194 (93%)	13 (6%)	1 (0%)	24	57
3	G	208/210 (99%)	197 (95%)	11 (5%)	0	100	100
3	K	208/210 (99%)	198 (95%)	10 (5%)	0	100	100
3	L	208/210 (99%)	198 (95%)	10 (5%)	0	100	100
3	O	208/210 (99%)	198 (95%)	10 (5%)	0	100	100
3	R	208/210 (99%)	197 (95%)	11 (5%)	0	100	100
3	U	208/210 (99%)	199 (96%)	9 (4%)	0	100	100
3	X	208/210 (99%)	198 (95%)	10 (5%)	0	100	100
4	C	217/220 (99%)	203 (94%)	11 (5%)	3 (1%)	9	38
4	F	217/220 (99%)	202 (93%)	11 (5%)	4 (2%)	6	34
4	H	217/220 (99%)	204 (94%)	13 (6%)	0	100	100
4	J	217/220 (99%)	202 (93%)	11 (5%)	4 (2%)	6	34
4	N	217/220 (99%)	203 (94%)	11 (5%)	3 (1%)	9	38
4	Q	217/220 (99%)	203 (94%)	13 (6%)	1 (0%)	24	57
4	T	217/220 (99%)	203 (94%)	11 (5%)	3 (1%)	9	38
4	W	217/220 (99%)	198 (91%)	18 (8%)	1 (0%)	24	57

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	6243/6480 (96%)	5748 (92%)	427 (7%)	68 (1%)	11	43

All (68) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	81	PRO
1	B	81	PRO
1	I	81	PRO
4	C	98	TRP
4	C	100(A)	LEU
1	E	81	PRO
1	E	232	GLU
4	F	98	TRP
4	F	100(B)	PRO
4	J	98	TRP
4	J	100(A)	LEU
4	J	100(B)	PRO
1	M	81	PRO
1	M	232	GLU
4	N	53	HIS
4	N	102	PRO
1	P	81	PRO
1	P	232	GLU
1	S	72	HIS
1	S	81	PRO
4	T	98	TRP
4	T	100(B)	PRO
1	V	81	PRO
1	V	232	GLU
1	B	467	THR
1	I	49	ASN
4	C	100(B)	PRO
1	E	72	HIS
1	M	62	ASP
1	P	62	ASP
1	P	72	HIS
1	P	467	THR
1	S	232	GLU
1	S	409	ILE
1	S	467	THR
4	T	100(A)	LEU
1	V	467	THR

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Mol	Chain	Res	Type
4	W	28	SER
1	A	467	THR
1	B	232	GLU
1	I	72	HIS
1	I	258	GLN
1	E	62	ASP
1	E	374	HIS
1	E	467	THR
1	M	462	SER
1	M	467	THR
4	N	130	SER
1	A	350	ARG
1	B	491	ILE
1	I	232	GLU
1	I	406	THR
1	I	409	ILE
1	E	243	SER
4	F	100	TYR
4	F	100(A)	LEU
1	M	406	THR
1	P	350	ARG
1	S	406	THR
1	I	467	THR
4	J	130	SER
1	M	73	ALA
1	V	73	ALA
1	B	76	PRO
1	B	409	ILE
3	D	110	VAL
1	P	409	ILE
4	Q	100(A)	LEU

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	293/306 (96%)	286 (98%)	7 (2%)	43	63
1	B	299/306 (98%)	297 (99%)	2 (1%)	76	78
1	E	290/306 (95%)	287 (99%)	3 (1%)	68	75
1	I	298/306 (97%)	293 (98%)	5 (2%)	53	69
1	M	296/306 (97%)	291 (98%)	5 (2%)	53	69
1	P	295/306 (96%)	289 (98%)	6 (2%)	48	66
1	S	296/306 (97%)	290 (98%)	6 (2%)	48	66
1	V	296/306 (97%)	286 (97%)	10 (3%)	32	57
2	a	20/20 (100%)	19 (95%)	1 (5%)	22	49
2	b	20/20 (100%)	20 (100%)	0	100	100
2	e	20/20 (100%)	20 (100%)	0	100	100
2	i	20/20 (100%)	20 (100%)	0	100	100
2	m	20/20 (100%)	20 (100%)	0	100	100
2	p	20/20 (100%)	20 (100%)	0	100	100
2	s	20/20 (100%)	20 (100%)	0	100	100
2	v	20/20 (100%)	20 (100%)	0	100	100
3	D	183/183 (100%)	176 (96%)	7 (4%)	29	55
3	G	183/183 (100%)	179 (98%)	4 (2%)	45	65
3	K	183/183 (100%)	182 (100%)	1 (0%)	81	80
3	L	183/183 (100%)	181 (99%)	2 (1%)	65	74
3	O	183/183 (100%)	180 (98%)	3 (2%)	55	69
3	R	183/183 (100%)	180 (98%)	3 (2%)	55	69
3	U	183/183 (100%)	178 (97%)	5 (3%)	39	61
3	X	183/183 (100%)	180 (98%)	3 (2%)	55	69
4	C	190/190 (100%)	178 (94%)	12 (6%)	16	43
4	F	190/190 (100%)	185 (97%)	5 (3%)	40	62
4	H	190/190 (100%)	186 (98%)	4 (2%)	47	65
4	J	190/190 (100%)	185 (97%)	5 (3%)	40	62
4	N	190/190 (100%)	176 (93%)	14 (7%)	13	39
4	Q	190/190 (100%)	187 (98%)	3 (2%)	55	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	T	190/190 (100%)	186 (98%)	4 (2%)	47 65
4	W	190/190 (100%)	184 (97%)	6 (3%)	34 58
All	All	5507/5592 (98%)	5381 (98%)	126 (2%)	44 64

All (126) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	83	GLU
1	A	244	THR
1	A	371	ILE
1	A	390	LEU
1	A	418	CYS
1	A	429	ARG
1	A	440	GLN
1	B	49	ASN
1	B	387	THR
2	a	11	LYS
3	L	72	THR
3	L	108	ARG
1	I	47	ASP
1	I	53	PHE
1	I	80	SER
1	I	201	LEU
1	I	295	ASN
4	H	95	ARG
4	H	129	LYS
4	H	178	LEU
4	H	209	LYS
3	D	24	ARG
3	D	37	GLN
3	D	69	THR
3	D	72	THR
3	D	81	GLU
3	D	108	ARG
3	D	134	CYS
4	C	38	ARG
4	C	63	LEU
4	C	100	TYR
4	C	100(A)	LEU
4	C	100(B)	PRO
4	C	100(C)	PHE

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Mol	Chain	Res	Type
4	C	129	LYS
4	C	177	SER
4	C	178	LEU
4	C	179	SER
4	C	197	ASN
4	C	209	LYS
1	E	53	PHE
1	E	371	ILE
1	E	387	THR
3	G	61	ARG
3	G	72	THR
3	G	105	GLU
3	G	108	ARG
4	F	1	GLN
4	F	129	LYS
4	F	140	CYS
4	F	160	THR
4	F	178	LEU
3	K	108	ARG
4	J	101	ASP
4	J	129	LYS
4	J	178	LEU
4	J	186	SER
4	J	197	ASN
1	M	53	PHE
1	M	201	LEU
1	M	368	ASP
1	M	387	THR
1	M	413	THR
3	O	72	THR
3	O	105	GLU
3	O	108	ARG
4	N	13	LYS
4	N	50	GLU
4	N	51	ILE
4	N	52	LYS
4	N	92	CYS
4	N	98	TRP
4	N	100	TYR
4	N	100(A)	LEU
4	N	100(B)	PRO
4	N	100(C)	PHE

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Mol	Chain	Res	Type
4	N	103	TRP
4	N	129	LYS
4	N	178	LEU
4	N	194	TYR
1	P	53	PHE
1	P	80	SER
1	P	201	LEU
1	P	239	CYS
1	P	276	ASN
1	P	446	VAL
3	R	72	THR
3	R	105	GLU
3	R	108	ARG
4	Q	129	LYS
4	Q	178	LEU
4	Q	197	ASN
1	S	80	SER
1	S	201	LEU
1	S	276	ASN
1	S	289	ASN
1	S	334	SER
1	S	387	THR
3	U	7	SER
3	U	72	THR
3	U	81	GLU
3	U	89	GLN
3	U	108	ARG
4	T	129	LYS
4	T	178	LEU
4	T	179	SER
4	T	209	LYS
1	V	53	PHE
1	V	64	GLU
1	V	71	THR
1	V	74	CYS
1	V	201	LEU
1	V	239	CYS
1	V	387	THR
1	V	446	VAL
1	V	464	GLU
1	V	487	LYS
3	X	72	THR

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Mol	Chain	Res	Type
3	X	105	GLU
3	X	108	ARG
4	W	13	LYS
4	W	129	LYS
4	W	178	LEU
4	W	194	TYR
4	W	196	CYS
4	W	197	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	99	ASN
1	B	337	GLN
3	L	37	GLN
3	L	160	GLN
1	I	99	ASN
1	I	229	ASN
1	I	249	HIS
4	H	58	ASN
4	H	81	ASN
2	b	7	GLN
3	D	38	GLN
3	D	79	GLN
3	D	137	ASN
3	D	189	HIS
4	C	39	GLN
4	C	53	HIS
4	C	164	HIS
1	E	229	ASN
1	E	337	GLN
1	E	357	ASN
1	E	374	HIS
3	G	137	ASN
4	F	5	GLN
4	F	58	ASN
4	F	76	ASN
4	F	164	HIS
4	J	76	ASN
4	J	164	HIS
4	J	204	ASN
1	M	337	GLN

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Mol	Chain	Res	Type
1	M	362	ASN
2	m	7	GLN
3	O	189	HIS
1	P	276	ASN
1	P	374	HIS
3	R	137	ASN
3	R	189	HIS
4	Q	164	HIS
4	Q	199	ASN
1	S	249	HIS
1	S	337	GLN
1	S	357	ASN
3	U	89	GLN
3	U	137	ASN
3	U	189	HIS
4	T	164	HIS
1	V	280	ASN
1	V	337	GLN
1	V	362	ASN
1	V	432	GLN
2	v	7	GLN
4	W	39	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

24 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
4	OAS	N	30	4	4,5,9	0.76	0	1,5,11	1.68	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	OAS	Q	30	4	4,5,9	0.82	0	1,5,11	2.56	1 (100%)
2	U2X	b	23	2	19,20,21	2.49	5 (26%)	20,25,27	1.61	5 (25%)
2	U2X	i	23	2	19,20,21	2.49	5 (26%)	20,25,27	1.61	5 (25%)
4	OAS	H	30	4	7,8,9	0.81	0	4,9,11	0.64	0
2	U2X	p	23	2	19,20,21	2.48	5 (26%)	20,25,27	1.61	5 (25%)
4	OAS	T	30	4	7,8,9	0.84	0	4,9,11	0.68	0
4	OAS	C	30	4	7,8,9	0.84	0	4,9,11	0.70	0
4	OAS	J	30	4	4,5,9	0.82	0	1,5,11	1.44	0
2	U2X	e	23	2	19,20,21	2.47	5 (26%)	20,25,27	1.61	5 (25%)
2	U2X	s	23	2	19,20,21	2.48	5 (26%)	20,25,27	1.61	5 (25%)
4	OAS	F	30	4	4,5,9	0.82	0	1,5,11	2.49	1 (100%)
4	OAS	W	30	4	7,8,9	0.84	0	4,9,11	0.68	0
2	U2X	m	23	2	19,20,21	2.48	5 (26%)	20,25,27	1.60	5 (25%)
2	U2X	a	23	2	19,20,21	2.48	5 (26%)	20,25,27	1.61	5 (25%)
2	U2X	v	23	2	19,20,21	2.48	5 (26%)	20,25,27	1.60	5 (25%)

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	OAS	N	30	4	-	0/2/4/9	-
4	OAS	Q	30	4	-	0/2/4/9	-
2	U2X	b	23	2	-	5/10/19/21	0/2/2/2
2	U2X	i	23	2	-	5/10/19/21	0/2/2/2
4	OAS	H	30	4	-	5/5/7/9	-
2	U2X	p	23	2	-	5/10/19/21	0/2/2/2
4	OAS	T	30	4	-	4/5/7/9	-
4	OAS	C	30	4	-	4/5/7/9	-
4	OAS	J	30	4	-	0/2/4/9	-
2	U2X	e	23	2	-	5/10/19/21	0/2/2/2
2	U2X	s	23	2	-	5/10/19/21	0/2/2/2
4	OAS	F	30	4	-	0/2/4/9	-
4	OAS	W	30	4	-	2/5/7/9	-
2	U2X	m	23	2	-	5/10/19/21	0/2/2/2
2	U2X	a	23	2	-	5/10/19/21	0/2/2/2
2	U2X	v	23	2	-	5/10/19/21	0/2/2/2

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	b	23	U2X	CE2-CD2	8.08	1.51	1.38
2	v	23	U2X	CE2-CD2	8.06	1.51	1.38
2	s	23	U2X	CE2-CD2	8.05	1.51	1.38
2	i	23	U2X	CE2-CD2	8.05	1.51	1.38
2	a	23	U2X	CE2-CD2	8.03	1.51	1.38
2	m	23	U2X	CE2-CD2	8.02	1.51	1.38
2	p	23	U2X	CE2-CD2	8.01	1.51	1.38
2	e	23	U2X	CE2-CD2	7.99	1.51	1.38
2	i	23	U2X	CE1-CD1	4.69	1.46	1.38
2	p	23	U2X	CE1-CD1	4.69	1.46	1.38
2	e	23	U2X	CE1-CD1	4.68	1.46	1.38
2	b	23	U2X	CE1-CD1	4.66	1.46	1.38
2	a	23	U2X	CE1-CD1	4.66	1.46	1.38
2	m	23	U2X	CE1-CD1	4.65	1.46	1.38
2	s	23	U2X	CE1-CD1	4.65	1.46	1.38
2	v	23	U2X	CE1-CD1	4.61	1.46	1.38
2	m	23	U2X	CE1-CZ	2.71	1.43	1.38
2	e	23	U2X	CE1-CZ	2.71	1.43	1.38
2	b	23	U2X	CE1-CZ	2.69	1.43	1.38
2	v	23	U2X	CE1-CZ	2.69	1.43	1.38
2	a	23	U2X	CE1-CZ	2.68	1.43	1.38
2	p	23	U2X	CE1-CZ	2.68	1.43	1.38
2	s	23	U2X	CE1-CZ	2.68	1.43	1.38
2	i	23	U2X	CE1-CZ	2.68	1.43	1.38
2	p	23	U2X	C4-C3	2.19	1.58	1.52
2	s	23	U2X	C4-C3	2.19	1.58	1.52
2	m	23	U2X	C4-C3	2.18	1.58	1.52
2	a	23	U2X	C4-C3	2.18	1.58	1.52
2	v	23	U2X	C4-C3	2.18	1.58	1.52
2	b	23	U2X	C4-C3	2.18	1.58	1.52
2	i	23	U2X	C4-C3	2.17	1.58	1.52
2	e	23	U2X	C4-C3	2.16	1.58	1.52
2	e	23	U2X	CB-CA	-2.14	1.49	1.53
2	p	23	U2X	CB-CA	-2.14	1.49	1.53
2	b	23	U2X	CB-CA	-2.14	1.49	1.53
2	a	23	U2X	CB-CA	-2.13	1.49	1.53
2	i	23	U2X	CB-CA	-2.12	1.49	1.53
2	m	23	U2X	CB-CA	-2.12	1.49	1.53
2	s	23	U2X	CB-CA	-2.12	1.49	1.53
2	v	23	U2X	CB-CA	-2.11	1.49	1.53

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	m	23	U2X	C2-C3-C7	3.84	121.66	111.42
2	e	23	U2X	C2-C3-C7	3.84	121.66	111.42
2	p	23	U2X	C2-C3-C7	3.83	121.65	111.42
2	i	23	U2X	C2-C3-C7	3.83	121.64	111.42
2	a	23	U2X	C2-C3-C7	3.83	121.63	111.42
2	v	23	U2X	C2-C3-C7	3.83	121.63	111.42
2	s	23	U2X	C2-C3-C7	3.82	121.63	111.42
2	b	23	U2X	C2-C3-C7	3.81	121.59	111.42
2	s	23	U2X	C4-C3-C7	2.60	118.37	111.42
2	i	23	U2X	C4-C3-C7	2.60	118.36	111.42
2	e	23	U2X	C4-C3-C7	2.60	118.35	111.42
2	b	23	U2X	C4-C3-C7	2.59	118.34	111.42
2	v	23	U2X	C4-C3-C7	2.59	118.34	111.42
2	m	23	U2X	C4-C3-C7	2.59	118.34	111.42
2	a	23	U2X	C4-C3-C7	2.59	118.33	111.42
2	p	23	U2X	C4-C3-C7	2.59	118.32	111.42
4	Q	30	OAS	CB-CA-C	-2.56	105.73	111.35
4	F	30	OAS	CB-CA-C	-2.49	105.86	111.35
2	b	23	U2X	C1-C2-C3	-2.45	106.92	112.08
2	i	23	U2X	C1-C2-C3	-2.44	106.94	112.08
2	e	23	U2X	C1-C2-C3	-2.44	106.95	112.08
2	p	23	U2X	C1-C2-C3	-2.44	106.96	112.08
2	a	23	U2X	C1-C2-C3	-2.43	106.96	112.08
2	s	23	U2X	C1-C2-C3	-2.43	106.97	112.08
2	v	23	U2X	C1-C2-C3	-2.43	106.97	112.08
2	m	23	U2X	C1-C2-C3	-2.42	106.98	112.08
2	b	23	U2X	CD2-CG-CD1	2.30	121.64	118.23
2	s	23	U2X	CD2-CG-CD1	2.29	121.63	118.23
2	i	23	U2X	CD2-CG-CD1	2.28	121.62	118.23
2	p	23	U2X	CD2-CG-CD1	2.26	121.60	118.23
2	a	23	U2X	CD2-CG-CD1	2.26	121.59	118.23
2	m	23	U2X	CD2-CG-CD1	2.25	121.58	118.23
2	e	23	U2X	CD2-CG-CD1	2.25	121.58	118.23
2	v	23	U2X	CD2-CG-CD1	2.24	121.56	118.23
2	v	23	U2X	C5-C4-C3	-2.05	107.78	112.08
2	a	23	U2X	C5-C4-C3	-2.04	107.80	112.08
2	p	23	U2X	C5-C4-C3	-2.04	107.80	112.08
2	b	23	U2X	C5-C4-C3	-2.04	107.80	112.08
2	m	23	U2X	C5-C4-C3	-2.03	107.81	112.08
2	e	23	U2X	C5-C4-C3	-2.03	107.82	112.08
2	s	23	U2X	C5-C4-C3	-2.03	107.82	112.08
2	i	23	U2X	C5-C4-C3	-2.02	107.83	112.08

There are no chirality outliers.

All (55) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	a	23	U2X	C2-C3-C7-OH
4	H	30	OAS	N-CA-CB-OG
4	H	30	OAS	C-CA-CB-OG
4	H	30	OAS	CA-CB-OG-C1A
2	b	23	U2X	C2-C3-C7-OH
4	C	30	OAS	C-CA-CB-OG
2	e	23	U2X	C2-C3-C7-OH
2	i	23	U2X	C2-C3-C7-OH
2	m	23	U2X	C2-C3-C7-OH
2	p	23	U2X	C2-C3-C7-OH
2	s	23	U2X	C2-C3-C7-OH
4	T	30	OAS	C-CA-CB-OG
2	v	23	U2X	C2-C3-C7-OH
4	H	30	OAS	C2A-C1A-OG-CB
4	T	30	OAS	C2A-C1A-OG-CB
4	H	30	OAS	OAC-C1A-OG-CB
4	T	30	OAS	OAC-C1A-OG-CB
4	W	30	OAS	OAC-C1A-OG-CB
4	W	30	OAS	C2A-C1A-OG-CB
4	C	30	OAS	C2A-C1A-OG-CB
4	C	30	OAS	OAC-C1A-OG-CB
2	a	23	U2X	C3-C7-OH-CZ
2	b	23	U2X	C3-C7-OH-CZ
2	e	23	U2X	C3-C7-OH-CZ
2	i	23	U2X	C3-C7-OH-CZ
2	m	23	U2X	C3-C7-OH-CZ
2	p	23	U2X	C3-C7-OH-CZ
2	s	23	U2X	C3-C7-OH-CZ
2	v	23	U2X	C3-C7-OH-CZ
4	C	30	OAS	N-CA-CB-OG
4	T	30	OAS	N-CA-CB-OG
2	a	23	U2X	CE2-CZ-OH-C7
2	b	23	U2X	CE2-CZ-OH-C7
2	i	23	U2X	CE2-CZ-OH-C7
2	m	23	U2X	CE2-CZ-OH-C7
2	p	23	U2X	CE2-CZ-OH-C7
2	s	23	U2X	CE2-CZ-OH-C7
2	v	23	U2X	CE2-CZ-OH-C7
2	e	23	U2X	CE2-CZ-OH-C7
2	e	23	U2X	CE1-CZ-OH-C7
2	m	23	U2X	CE1-CZ-OH-C7
2	p	23	U2X	CE1-CZ-OH-C7

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Mol	Chain	Res	Type	Atoms
2	s	23	U2X	CE1-CZ-OH-C7
2	v	23	U2X	CE1-CZ-OH-C7
2	a	23	U2X	CE1-CZ-OH-C7
2	b	23	U2X	CE1-CZ-OH-C7
2	i	23	U2X	CE1-CZ-OH-C7
2	a	23	U2X	C4-C3-C7-OH
2	b	23	U2X	C4-C3-C7-OH
2	e	23	U2X	C4-C3-C7-OH
2	i	23	U2X	C4-C3-C7-OH
2	m	23	U2X	C4-C3-C7-OH
2	p	23	U2X	C4-C3-C7-OH
2	s	23	U2X	C4-C3-C7-OH
2	v	23	U2X	C4-C3-C7-OH

There are no ring outliers.

9 monomers are involved in 54 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	b	23	U2X	13	0
2	i	23	U2X	3	0
4	H	30	OAS	1	0
2	p	23	U2X	7	0
2	e	23	U2X	5	0
2	s	23	U2X	8	0
2	m	23	U2X	4	0
2	a	23	U2X	5	0
2	v	23	U2X	8	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

19 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	$\# Z > 2$
5	NAG	B	502	1	14,14,15	0.35	0	17,19,21	1.30	1 (5%)
5	NAG	I	503	1	14,14,15	0.23	0	17,19,21	0.43	0
5	NAG	A	503	1	14,14,15	0.21	0	17,19,21	0.45	0
5	NAG	V	501	1	14,14,15	0.34	0	17,19,21	0.40	0
5	NAG	S	503	1	14,14,15	0.27	0	17,19,21	0.39	0
5	NAG	A	501	1	14,14,15	0.45	0	17,19,21	0.41	0
5	NAG	I	501	1	14,14,15	0.28	0	17,19,21	0.51	0
5	NAG	A	504	1	14,14,15	0.19	0	17,19,21	0.42	0
5	NAG	S	502	1	14,14,15	0.52	0	17,19,21	0.84	1 (5%)
5	NAG	S	501	1	14,14,15	0.23	0	17,19,21	0.41	0
5	NAG	A	502	1	14,14,15	0.27	0	17,19,21	0.43	0
5	NAG	P	501	1	14,14,15	0.24	0	17,19,21	0.36	0
5	NAG	E	502	1	14,14,15	0.26	0	17,19,21	0.45	0
5	NAG	P	502	1	14,14,15	0.33	0	17,19,21	0.52	0
5	NAG	I	502	1	14,14,15	0.37	0	17,19,21	0.47	0
5	NAG	B	501	1	14,14,15	0.23	0	17,19,21	0.43	0
5	NAG	M	501	1	14,14,15	0.27	0	17,19,21	0.47	0
5	NAG	E	501	1	14,14,15	0.28	0	17,19,21	0.41	0
5	NAG	I	504	1	14,14,15	0.51	0	17,19,21	0.36	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
5	NAG	B	502	1	-	3/6/23/26	0/1/1/1
5	NAG	I	503	1	-	4/6/23/26	0/1/1/1
5	NAG	A	503	1	-	4/6/23/26	0/1/1/1
5	NAG	V	501	1	-	3/6/23/26	0/1/1/1
5	NAG	S	503	1	-	4/6/23/26	0/1/1/1
5	NAG	A	501	1	-	2/6/23/26	0/1/1/1
5	NAG	I	501	1	-	1/6/23/26	0/1/1/1
5	NAG	A	504	1	-	2/6/23/26	0/1/1/1
5	NAG	S	502	1	-	0/6/23/26	0/1/1/1
5	NAG	S	501	1	-	2/6/23/26	0/1/1/1
5	NAG	A	502	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	P	501	1	-	2/6/23/26	0/1/1/1
5	NAG	E	502	1	-	0/6/23/26	0/1/1/1
5	NAG	P	502	1	-	1/6/23/26	0/1/1/1
5	NAG	I	502	1	-	3/6/23/26	0/1/1/1
5	NAG	B	501	1	-	2/6/23/26	0/1/1/1
5	NAG	M	501	1	-	2/6/23/26	0/1/1/1
5	NAG	E	501	1	-	2/6/23/26	0/1/1/1
5	NAG	I	504	1	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	502	NAG	C1-O5-C5	4.35	118.01	112.19
5	S	502	NAG	C1-C2-N2	2.39	114.20	110.43

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	P	501	NAG	O5-C5-C6-O6
5	S	501	NAG	O5-C5-C6-O6
5	A	503	NAG	C4-C5-C6-O6
5	I	503	NAG	O5-C5-C6-O6
5	I	504	NAG	O5-C5-C6-O6
5	B	501	NAG	O5-C5-C6-O6
5	E	501	NAG	O5-C5-C6-O6
5	B	501	NAG	C4-C5-C6-O6
5	A	501	NAG	O5-C5-C6-O6
5	P	501	NAG	C4-C5-C6-O6
5	B	502	NAG	O5-C5-C6-O6
5	I	504	NAG	C4-C5-C6-O6
5	S	501	NAG	C4-C5-C6-O6
5	A	502	NAG	O5-C5-C6-O6
5	A	503	NAG	O5-C5-C6-O6
5	A	501	NAG	C4-C5-C6-O6
5	I	503	NAG	C4-C5-C6-O6
5	I	502	NAG	O5-C5-C6-O6
5	E	501	NAG	C4-C5-C6-O6
5	A	503	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
5	A	503	NAG	O7-C7-N2-C2
5	A	504	NAG	C8-C7-N2-C2
5	A	504	NAG	O7-C7-N2-C2
5	I	503	NAG	C8-C7-N2-C2
5	I	503	NAG	O7-C7-N2-C2
5	S	503	NAG	C8-C7-N2-C2
5	S	503	NAG	O7-C7-N2-C2
5	A	502	NAG	C4-C5-C6-O6
5	S	503	NAG	O5-C5-C6-O6
5	S	503	NAG	C4-C5-C6-O6
5	M	501	NAG	C4-C5-C6-O6
5	M	501	NAG	O5-C5-C6-O6
5	I	502	NAG	C4-C5-C6-O6
5	B	502	NAG	C4-C5-C6-O6
5	I	501	NAG	C3-C2-N2-C7
5	P	502	NAG	O5-C5-C6-O6
5	V	501	NAG	C4-C5-C6-O6
5	I	502	NAG	C3-C2-N2-C7
5	B	502	NAG	C3-C2-N2-C7
5	I	504	NAG	C3-C2-N2-C7
5	V	501	NAG	C3-C2-N2-C7
5	V	501	NAG	O5-C5-C6-O6

There are no ring outliers.

16 monomers are involved in 49 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	502	NAG	7	0
5	A	503	NAG	1	0
5	V	501	NAG	3	0
5	A	501	NAG	2	0
5	I	501	NAG	6	0
5	A	504	NAG	2	0
5	S	502	NAG	11	0
5	S	501	NAG	2	0
5	A	502	NAG	3	0
5	P	501	NAG	2	0
5	E	502	NAG	1	0
5	P	502	NAG	3	0
5	B	501	NAG	3	0
5	M	501	NAG	1	0
5	E	501	NAG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	I	504	NAG	3	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, 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	333/352 (94%)	-0.64	4 (1%) 76 49	81, 166, 250, 287	0
1	B	342/352 (97%)	-0.70	1 (0%) 90 74	86, 198, 304, 339	0
1	E	329/352 (93%)	-0.69	5 (1%) 72 44	114, 219, 296, 332	0
1	I	341/352 (96%)	-0.75	0 100 100	96, 176, 261, 296	0
1	M	339/352 (96%)	-0.63	2 (0%) 85 63	112, 198, 283, 342	0
1	P	338/352 (96%)	-0.62	2 (0%) 85 63	77, 180, 284, 316	0
1	S	339/352 (96%)	-0.72	0 100 100	83, 187, 293, 330	0
1	V	338/352 (96%)	-0.68	1 (0%) 90 74	105, 199, 292, 332	0
2	a	24/28 (85%)	-0.77	0 100 100	141, 188, 204, 208	0
2	b	24/28 (85%)	-0.59	0 100 100	161, 195, 225, 229	0
2	e	24/28 (85%)	-0.52	0 100 100	171, 198, 220, 223	0
2	i	24/28 (85%)	-0.58	0 100 100	140, 189, 200, 204	0
2	m	24/28 (85%)	-0.50	0 100 100	171, 209, 228, 233	0
2	p	24/28 (85%)	-0.71	0 100 100	118, 160, 181, 188	0
2	s	24/28 (85%)	-0.58	0 100 100	149, 202, 226, 231	0
2	v	24/28 (85%)	-0.61	0 100 100	170, 213, 220, 221	0
3	D	210/210 (100%)	-0.64	0 100 100	65, 228, 330, 356	0
3	G	210/210 (100%)	-0.76	1 (0%) 87 66	135, 250, 329, 358	0
3	K	210/210 (100%)	-0.77	0 100 100	166, 322, 361, 379	0
3	L	210/210 (100%)	-0.90	0 100 100	116, 227, 301, 336	0
3	O	210/210 (100%)	-0.82	0 100 100	167, 254, 309, 337	0
3	R	210/210 (100%)	-0.81	0 100 100	144, 244, 325, 347	0
3	U	210/210 (100%)	-0.73	1 (0%) 87 66	72, 236, 305, 332	0
3	X	210/210 (100%)	-0.85	0 100 100	155, 247, 314, 354	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
4	C	219/220 (99%)	-0.70	3 (1%) 73 45	70, 188, 337, 371	0
4	F	219/220 (99%)	-0.80	0 100 100	162, 234, 298, 345	0
4	H	219/220 (99%)	-0.86	0 100 100	100, 196, 291, 329	0
4	J	219/220 (99%)	-0.90	0 100 100	182, 295, 372, 404	0
4	N	219/220 (99%)	-0.88	0 100 100	160, 240, 298, 322	0
4	Q	219/220 (99%)	-0.82	1 (0%) 87 66	155, 236, 294, 326	0
4	T	219/220 (99%)	-0.78	2 (0%) 81 56	69, 208, 310, 369	0
4	W	219/220 (99%)	-0.84	0 100 100	130, 226, 290, 334	0
All	All	6323/6480 (97%)	-0.75	23 (0%) 88 70	65, 217, 320, 404	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	P	284	ILE	4.3
4	T	99	PRO	3.5
1	P	454	LEU	3.1
1	E	259	LEU	3.0
1	A	338	TRP	3.0
1	E	284	ILE	2.8
1	M	259	LEU	2.8
1	E	423	ILE	2.7
4	Q	207	VAL	2.4
4	T	100(A)	LEU	2.3
4	C	100(A)	LEU	2.3
1	M	452	LEU	2.3
3	G	12	SER	2.3
1	A	286	VAL	2.2
1	B	284	ILE	2.2
1	E	453	ILE	2.2
1	A	346	VAL	2.1
1	A	451	GLY	2.1
1	V	284	ILE	2.1
4	C	207	VAL	2.1
1	E	454	LEU	2.1
4	C	99	PRO	2.0
3	U	25	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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(Å ²)	Q<0.9
4	OAS	H	30	9/10	0.08	0.12	172,176,180,182	0
4	OAS	J	30	6/10	0.38	0.09	164,236,245,246	0
4	OAS	W	30	9/10	0.43	0.07	201,211,216,219	0
4	OAS	N	30	6/10	0.55	0.05	179,233,246,251	0
4	OAS	Q	30	6/10	0.67	0.07	246,262,273,274	0
2	U2X	p	23	19/20	0.69	0.21	106,113,127,130	0
4	OAS	F	30	6/10	0.77	0.04	248,273,281,281	0
4	OAS	C	30	9/10	0.79	0.05	155,165,179,180	0
2	U2X	b	23	19/20	0.83	0.11	131,154,176,177	0
4	OAS	T	30	9/10	0.86	0.06	156,170,195,200	0
2	DPR	s	21	7/8	0.86	0.10	151,152,155,158	0
2	DPR	v	21	7/8	0.87	0.20	170,171,176,180	0
2	DPR	i	21	7/8	0.88	0.13	136,137,141,144	0
2	DPR	p	21	7/8	0.88	0.06	123,126,133,136	0
2	U2X	a	23	19/20	0.88	0.16	130,136,145,145	0
2	U2X	i	23	19/20	0.88	0.14	133,139,150,152	0
2	U2X	e	23	19/20	0.89	0.10	175,179,184,185	0
2	U2X	v	23	19/20	0.90	0.12	146,156,181,182	0
2	U2X	m	23	19/20	0.90	0.10	155,164,181,184	0
2	DPR	m	21	7/8	0.92	0.08	173,175,182,187	0
2	U2X	s	23	19/20	0.92	0.12	146,152,160,160	0
2	DPR	a	21	7/8	0.93	0.07	146,147,150,151	0
2	DPR	b	21	7/8	0.94	0.05	165,166,170,173	0
2	DPR	e	21	7/8	0.96	0.10	176,177,180,182	0

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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($\text{\AA}^2$)	Q<0.9
5	NAG	A	504	14/15	0.34	0.05	184,188,192,195	0
5	NAG	I	504	14/15	0.44	0.06	176,180,185,186	0
5	NAG	I	503	14/15	0.47	0.05	194,202,208,209	0
5	NAG	P	502	14/15	0.54	0.06	208,216,230,231	0
5	NAG	I	502	14/15	0.61	0.07	183,189,198,199	0
5	NAG	B	502	14/15	0.69	0.04	219,232,245,249	0
5	NAG	E	502	14/15	0.76	0.07	190,201,211,212	0
5	NAG	S	503	14/15	0.76	0.04	202,210,214,216	0
5	NAG	A	502	14/15	0.77	0.05	184,189,200,200	0
5	NAG	A	503	14/15	0.78	0.05	152,167,177,182	0
5	NAG	I	501	14/15	0.81	0.08	161,165,172,173	0
5	NAG	S	502	14/15	0.84	0.04	230,238,252,259	0
5	NAG	V	501	14/15	0.87	0.10	153,158,163,165	0
5	NAG	B	501	14/15	0.89	0.06	152,161,168,170	0
5	NAG	P	501	14/15	0.91	0.08	153,165,177,177	0
5	NAG	M	501	14/15	0.93	0.11	178,180,182,185	0
5	NAG	A	501	14/15	0.93	0.10	127,136,143,144	0
5	NAG	E	501	14/15	0.95	0.09	204,207,209,209	0
5	NAG	S	501	14/15	0.97	0.07	154,162,168,171	0

6.5 Other polymers [i](#)

There are no such residues in this entry.