



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 11:54 PM GMT

PDB ID : 1YWH
Title : crystal structure of urokinase plasminogen activator receptor
Authors : Llinas, P.; Le Du, M.H.; Gardsvoll, H.; Dano, K.; Ploug, M.; Gilquin, B.;
Stura, E.A.; Menez, A.
Deposited on : 2005-02-18
Resolution : 2.70 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

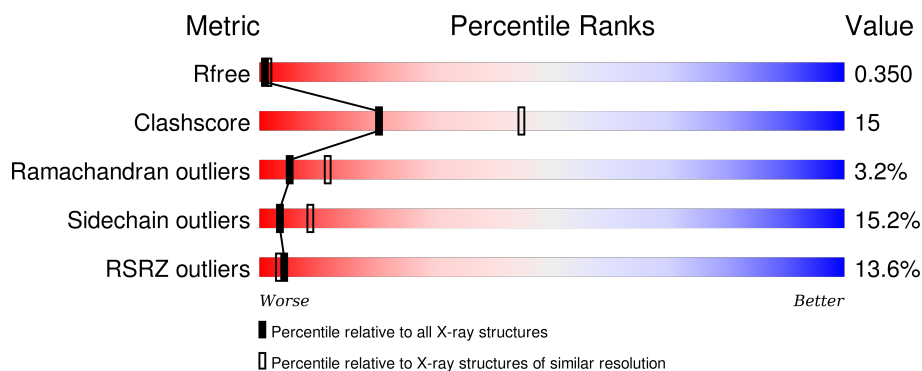
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	313	<div> <div>12%</div> <div>51% 26% 6% • 14%</div> </div>
1	C	313	<div> <div>12%</div> <div>51% 25% 6% • 17%</div> </div>
1	E	313	<div> <div>10%</div> <div>53% 25% 5% 16%</div> </div>
1	G	313	<div> <div>9%</div> <div>50% 27% 6% 18%</div> </div>
1	I	313	<div> <div>15%</div> <div>47% 29% 9% 16%</div> </div>

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Mol	Chain	Length	Quality of chain
1	K	313	
1	M	313	
1	O	313	
2	B	13	
2	D	13	
2	F	13	
2	H	13	
2	J	13	
2	L	13	
2	N	13	
2	P	13	

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
10	SO4	K	810	-	-	X	-
3	FUC	A	316	X	-	-	-
3	NAG	C	331	X	-	-	-
3	FUC	C	336	X	-	-	-
3	FUC	E	316	X	-	-	-
3	FUC	K	316	X	-	-	-
5	NAG	A	321	X	-	-	-
5	NAG	C	316	X	-	-	-
5	NAG	C	321	X	-	-	-
6	FUC	C	315	X	-	-	-
6	FUC	E	326	X	-	-	X
6	FUC	G	315	X	-	-	X
6	FUC	I	315	X	-	-	-
6	FUC	I	336	X	-	-	-
6	FUC	M	315	X	-	-	-
6	FUC	O	315	X	-	-	X
8	FUC	G	336	X	-	-	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 18552 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 Urokinase plasminogen activator surface receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	268	Total	C	N	O	S	0	0	0
			2040	1222	377	407	34			
1	C	259	Total	C	N	O	S	0	0	0
			1985	1188	368	395	34			
1	E	262	Total	C	N	O	S	0	0	0
			2006	1202	370	400	34			
1	G	258	Total	C	N	O	S	0	0	0
			1978	1186	363	395	34			
1	I	264	Total	C	N	O	S	0	0	0
			2008	1201	372	401	34			
1	K	257	Total	C	N	O	S	0	0	0
			1969	1180	363	392	34			
1	M	263	Total	C	N	O	S	0	0	0
			2016	1204	374	404	34			
1	O	258	Total	C	N	O	S	0	0	0
			1970	1180	362	394	34			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	200	GLN	ASN	CONFLICT	UNP Q9UMV0
C	200	GLN	ASN	CONFLICT	UNP Q9UMV0
E	200	GLN	ASN	CONFLICT	UNP Q9UMV0
G	200	GLN	ASN	CONFLICT	UNP Q9UMV0
I	200	GLN	ASN	CONFLICT	UNP Q9UMV0
K	200	GLN	ASN	CONFLICT	UNP Q9UMV0
M	200	GLN	ASN	CONFLICT	UNP Q9UMV0
O	200	GLN	ASN	CONFLICT	UNP Q9UMV0

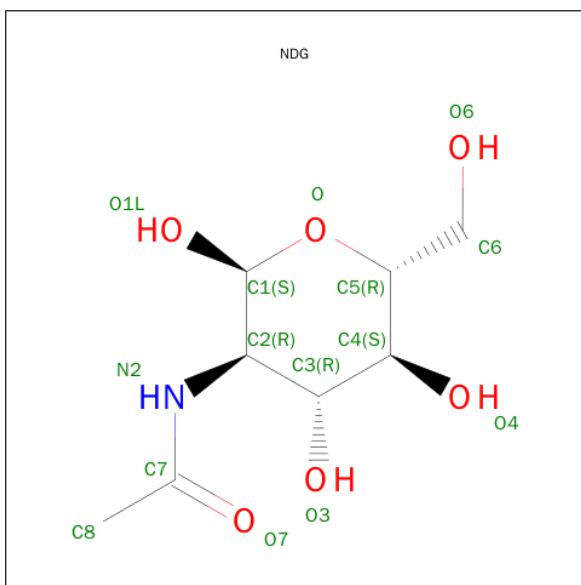
- Molecule 2 is a protein called antagonist peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	13	Total	C	N	O	0	0	0
			116	78	17	21			
2	D	13	Total	C	N	O	0	0	0
			116	78	17	21			
2	F	13	Total	C	N	O	0	0	0
			116	78	17	21			
2	H	13	Total	C	N	O	0	0	0
			116	78	17	21			
2	J	13	Total	C	N	O	0	0	0
			116	78	17	21			
2	L	13	Total	C	N	O	0	0	0
			116	78	17	21			
2	N	13	Total	C	N	O	0	0	0
			116	78	17	21			
2	P	13	Total	C	N	O	0	0	0
			116	78	17	21			

- Molecule 3 is a polymer of unknown type called SUGAR (3-MER).

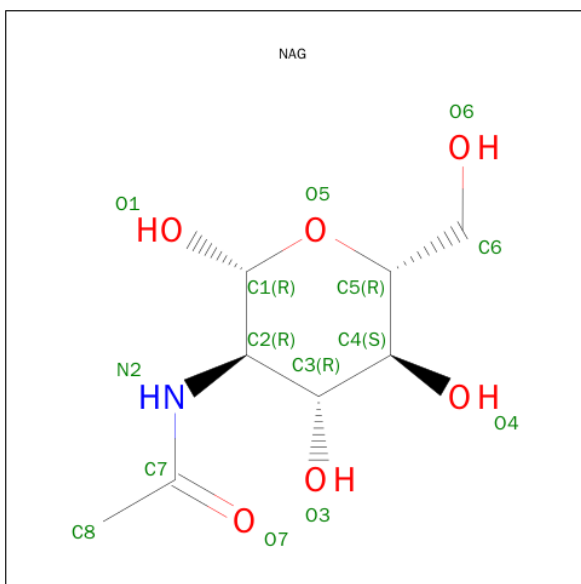
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	3	Total	C	N	O	0	0
			38	22	2	14		
3	C	3	Total	C	N	O	0	0
			38	22	2	14		
3	E	3	Total	C	N	O	0	0
			38	22	2	14		
3	K	3	Total	C	N	O	0	0
			38	22	2	14		

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NDG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 5 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: 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	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	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	G	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	K	1	Total	C	N	O	0	0
			14	8	1	5		
5	M	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	C	2	Total	C	N	O	0	0
			24	14	1	9		
6	E	2	Total	C	N	O	0	0
			24	14	1	9		
6	G	2	Total	C	N	O	0	0
			24	14	1	9		
6	I	2	Total	C	N	O	0	0
			24	14	1	9		
6	I	2	Total	C	N	O	0	0
			24	14	1	9		
6	M	2	Total	C	N	O	0	0
			24	14	1	9		
6	O	2	Total	C	N	O	0	0
			24	14	1	9		

- Molecule 7 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	G	2	Total	C	N	O	0	0
			28	16	2	10		
7	M	2	Total	C	N	O	0	0
			28	16	2	10		

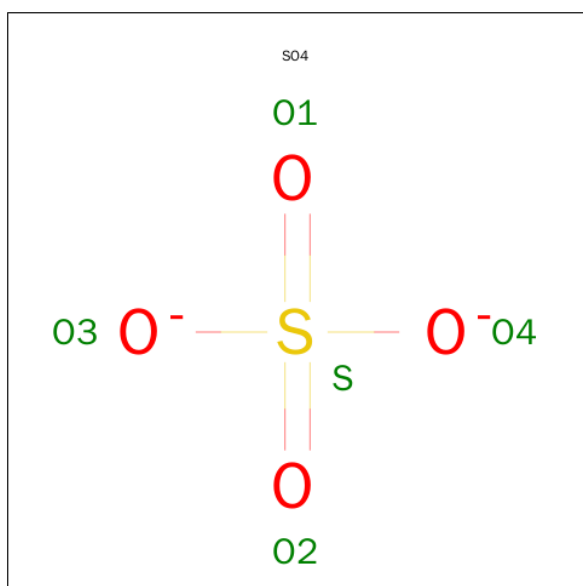
- Molecule 8 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	G	2	Total	C	N	O	0	0
			24	14	1	9		

- Molecule 9 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	I	5	Total	C	N	O	0	0
			61	34	2	25		
9	K	5	Total	C	N	O	0	0
			61	34	2	25		
9	M	5	Total	C	N	O	0	0
			61	34	2	25		
9	O	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 10 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	O	S	0	0
			5	4	1		
10	G	1	Total	O	S	0	0
			5	4	1		
10	K	1	Total	O	S	0	0
			5	4	1		
10	I	1	Total	O	S	0	0
			5	4	1		
10	A	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	C	1	Total	O	S	0	0
			5	4	1		
10	E	1	Total	O	S	0	0
			5	4	1		
10	G	1	Total	O	S	0	0
			5	4	1		
10	I	1	Total	O	S	0	0
			5	4	1		
10	K	1	Total	O	S	0	0
			5	4	1		
10	M	1	Total	O	S	0	0
			5	4	1		
10	O	1	Total	O	S	0	0
			5	4	1		
10	A	1	Total	O	S	0	0
			5	4	1		
10	C	1	Total	O	S	0	0
			5	4	1		
10	E	1	Total	O	S	0	0
			5	4	1		
10	G	1	Total	O	S	0	0
			5	4	1		
10	G	1	Total	O	S	0	0
			5	4	1		
10	C	1	Total	O	S	0	0
			5	4	1		
10	M	1	Total	O	S	0	0
			5	4	1		
10	E	1	Total	O	S	0	0
			5	4	1		
10	I	1	Total	O	S	0	0
			5	4	1		

- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	81	Total	O	0	0
			81	81		
11	B	5	Total	O	0	0
			5	5		
11	C	85	Total	O	0	0
			85	85		

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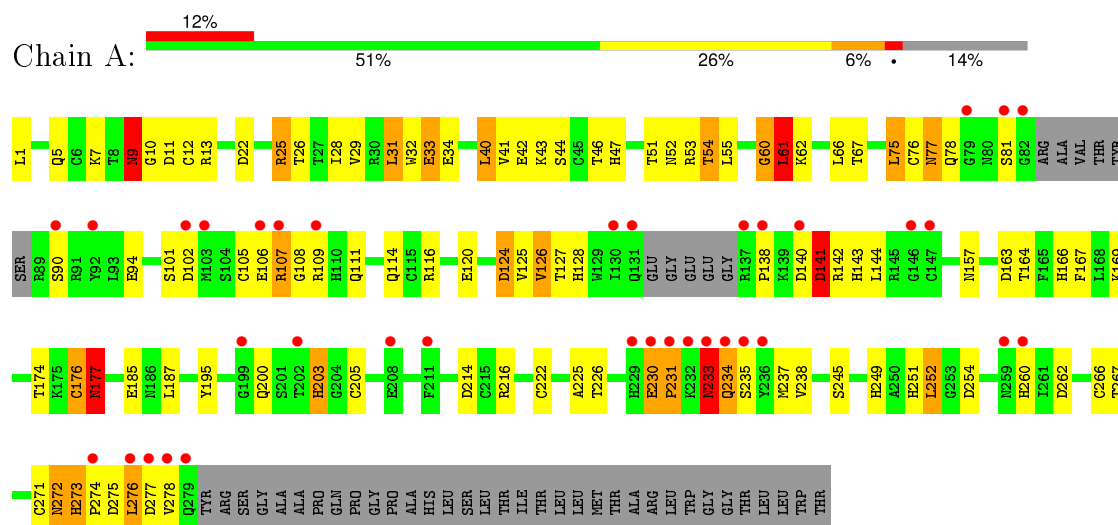
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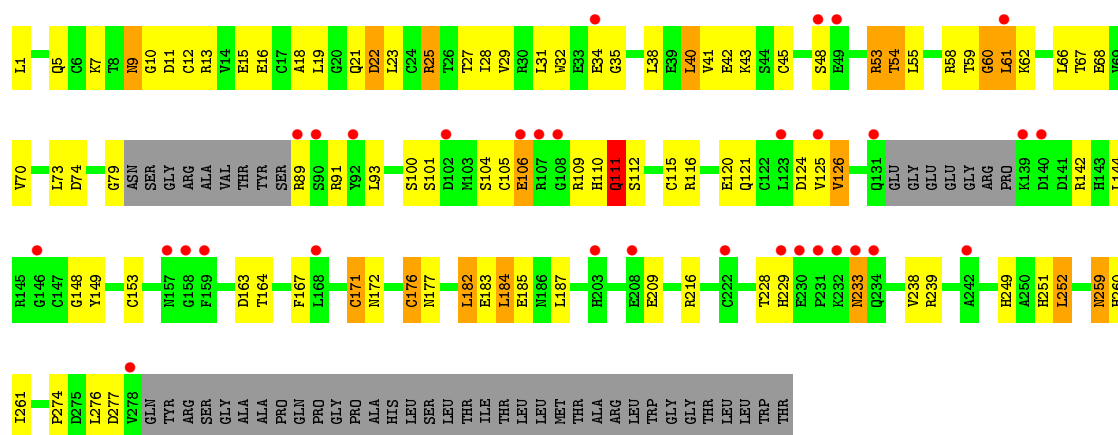
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	D	2	Total 2	O 2	0	0
11	E	98	Total 98	O 98	0	0
11	F	8	Total 8	O 8	0	0
11	G	88	Total 88	O 88	0	0
11	H	4	Total 4	O 4	0	0
11	I	87	Total 87	O 87	0	0
11	J	3	Total 3	O 3	0	0
11	K	83	Total 83	O 83	0	0
11	L	2	Total 2	O 2	0	0
11	M	91	Total 91	O 91	0	0
11	N	1	Total 1	O 1	0	0
11	O	106	Total 106	O 106	0	0
11	P	5	Total 5	O 5	0	0

3 Residue-property plots

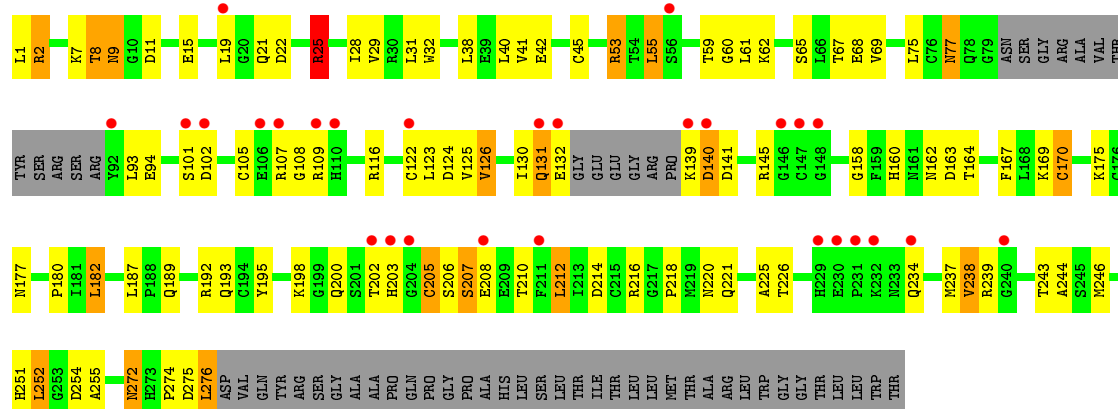
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: Urokinase plasminogen activator surface receptor

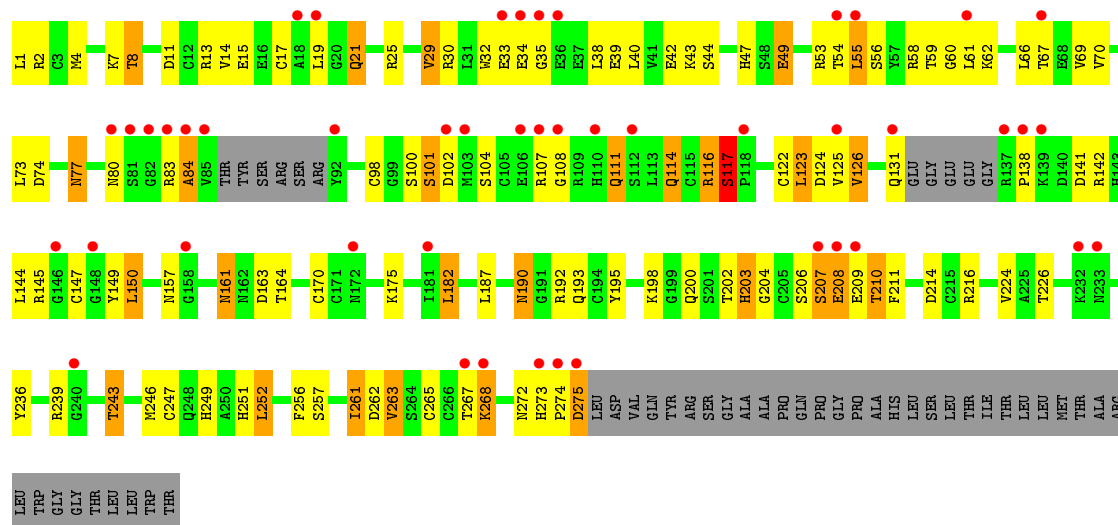




- Molecule 1: Urokinase plasminogen activator surface receptor



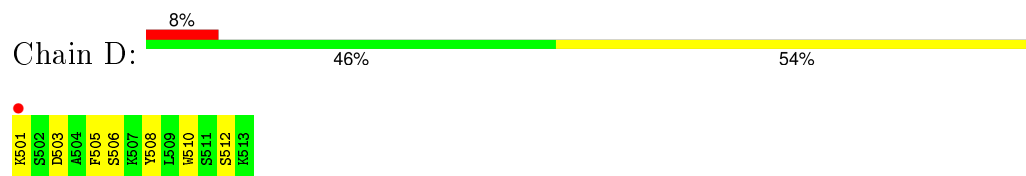
- Molecule 1: Urokinase plasminogen activator surface receptor



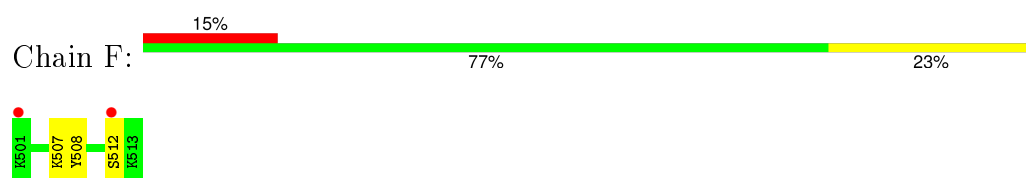
- Molecule 1: Urokinase plasminogen activator surface receptor



- Molecule 2: antagonist peptide



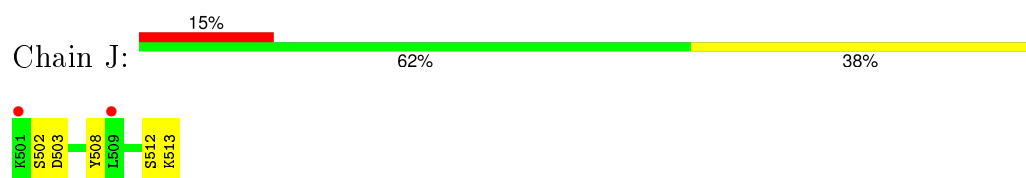
- Molecule 2: antagonist peptide



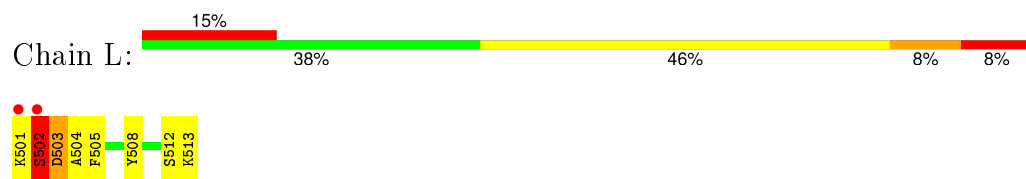
- Molecule 2: antagonist peptide



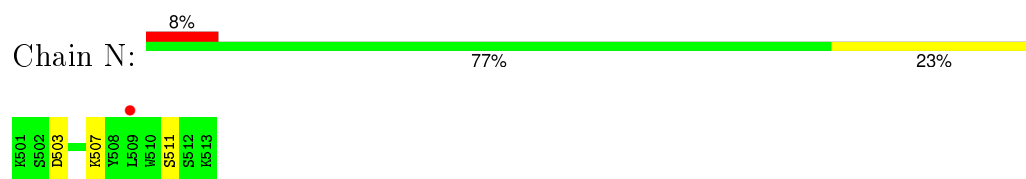
- Molecule 2: antagonist peptide



- Molecule 2: antagonist peptide



- Molecule 2: antagonist peptide



- Molecule 2: antagonist peptide



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	106.93Å 136.83Å 140.54Å 90.00° 97.27° 90.00°	Depositor
Resolution (Å)	24.85 – 2.70 24.85 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.2 (24.85-2.70) 97.2 (24.85-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.70 (at 2.72Å)	Xtriage
Refinement program	REFMAC 5.2.0003	Depositor
R, R_{free}	0.245 , 0.315 0.281 , 0.350	Depositor DCC
R_{free} test set	5332 reflections (4.99%)	DCC
Wilson B-factor (Å ²)	50.6	Xtriage
Anisotropy	0.107	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 58.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	2 of 106877 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	18552	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.00% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: BMA, NAG, ALC, NDG, DSN, SO4, DLY, MAN, FUC

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	0.55	2/2072 (0.1%)	0.87	11/2791 (0.4%)
1	C	0.62	3/2016 (0.1%)	0.87	10/2713 (0.4%)
1	E	0.54	0/2037	0.85	4/2742 (0.1%)
1	G	0.54	0/2009	0.90	10/2704 (0.4%)
1	I	0.53	1/2039 (0.0%)	0.85	9/2746 (0.3%)
1	K	0.60	1/2000 (0.1%)	0.85	6/2693 (0.2%)
1	M	0.52	0/2047	0.87	7/2755 (0.3%)
1	O	0.50	0/2001	0.82	7/2695 (0.3%)
2	B	0.63	0/91	0.86	1/116 (0.9%)
2	D	0.56	0/91	0.82	1/116 (0.9%)
2	F	0.61	0/91	0.82	0/116
2	H	0.67	0/91	0.88	1/116 (0.9%)
2	J	0.71	0/91	0.96	1/116 (0.9%)
2	L	0.54	0/91	0.86	0/116
2	N	0.56	0/91	0.92	1/116 (0.9%)
2	P	0.49	0/91	0.84	0/116
All	All	0.55	7/16949 (0.0%)	0.86	69/22767 (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	3
1	E	0	1
1	G	0	1
1	I	0	1
1	K	0	2
3	A	2	0
3	C	3	0

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	E	2	0
3	K	2	0
6	C	2	0
6	E	2	0
6	G	2	0
6	I	4	0
6	M	2	0
6	O	2	0
8	G	2	0
All	All	25	8

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	268	LYS	CE-NZ	14.47	1.85	1.49
1	C	273	HIS	CE1-NE2	13.68	1.64	1.32
1	C	273	HIS	CG-ND1	11.19	1.63	1.38
1	A	233	ASN	CG-ND2	6.80	1.49	1.32
1	I	268	LYS	CE-NZ	5.75	1.63	1.49

The worst 5 of 69 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	141	ASP	CB-CG-OD2	7.49	125.04	118.30
1	A	102	ASP	CB-CG-OD2	6.97	124.57	118.30
1	A	262	ASP	CB-CG-OD2	6.68	124.31	118.30
1	I	141	ASP	CB-CG-OD2	6.54	124.19	118.30
2	H	503	ASP	CB-CG-OD2	6.45	124.10	118.30

5 of 25 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	316	FUC	C5,C1
6	C	315	FUC	C5,C1
3	C	331	NAG	C1
3	C	336	FUC	C5,C1
3	E	316	FUC	C5,C1

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	230	GLU	Peptide

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Mol	Chain	Res	Type	Group
1	A	272	ASN	Peptide
1	A	61	LEU	Peptide
1	E	61	LEU	Peptide
1	G	208	GLU	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2040	0	1885	59	0
1	C	1985	0	1840	72	0
1	E	2006	0	1864	66	0
1	G	1978	0	1836	62	0
1	I	2008	0	1850	67	0
1	K	1969	0	1825	65	0
1	M	2016	0	1868	56	0
1	O	1970	0	1823	55	0
2	B	116	0	112	9	0
2	D	116	0	112	7	0
2	F	116	0	112	3	0
2	H	116	0	112	3	0
2	J	116	0	112	2	0
2	L	116	0	112	7	0
2	N	116	0	112	2	0
2	P	116	0	112	6	0
3	A	38	0	34	0	0
3	C	38	0	34	0	0
3	E	38	0	34	0	0
3	K	38	0	34	0	0
4	A	14	0	13	0	0
4	K	14	0	13	0	0
4	O	14	0	13	0	0
5	A	14	0	13	0	0
5	C	28	0	26	0	0
5	E	14	0	13	0	0
5	G	14	0	13	0	0
5	I	14	0	13	0	0
5	K	14	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	M	14	0	13	0	0
6	C	24	0	22	0	0
6	E	24	0	22	1	0
6	G	24	0	22	0	0
6	I	48	0	44	1	0
6	M	24	0	22	1	0
6	O	24	0	22	0	0
7	G	28	0	25	2	0
7	M	28	0	25	0	0
8	G	24	0	22	0	0
9	I	61	0	52	1	0
9	K	61	0	52	1	0
9	M	61	0	52	1	0
9	O	61	0	52	1	0
10	A	15	0	0	1	0
10	C	15	0	0	1	0
10	E	15	0	0	0	0
10	G	20	0	0	1	0
10	I	15	0	0	1	0
10	K	10	0	0	3	0
10	M	10	0	0	1	0
10	O	5	0	0	0	0
11	A	81	0	0	2	0
11	B	5	0	0	0	0
11	C	85	0	0	1	0
11	D	2	0	0	1	0
11	E	98	0	0	4	0
11	F	8	0	0	1	0
11	G	88	0	0	3	0
11	H	4	0	0	0	0
11	I	87	0	0	1	0
11	J	3	0	0	0	0
11	K	83	0	0	4	0
11	L	2	0	0	1	0
11	M	91	0	0	4	0
11	N	1	0	0	0	0
11	O	106	0	0	5	0
11	P	5	0	0	1	0
All	All	18552	0	16400	500	0

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 15.

The worst 5 of 500 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)
1:K:268:LYS:NZ	1:K:268:LYS:CE	1.85	1.38
1:C:273:HIS:HB3	1:C:274:PRO:HD3	1.11	1.10
1:C:273:HIS:HB3	1:C:274:PRO:CD	1.86	1.05
1:C:55:LEU:HB3	1:C:66:LEU:HD23	1.35	1.04
1:G:55:LEU:HD23	1:G:123:LEU:HD12	1.46	0.97

There are no symmetry-related clashes.

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	262/313 (84%)	231 (88%)	16 (6%)	15 (6%)	2	3
1	C	253/313 (81%)	226 (89%)	16 (6%)	11 (4%)	3	7
1	E	256/313 (82%)	229 (90%)	22 (9%)	5 (2%)	9	24
1	G	252/313 (80%)	233 (92%)	16 (6%)	3 (1%)	16	39
1	I	258/313 (82%)	228 (88%)	23 (9%)	7 (3%)	6	16
1	K	251/313 (80%)	227 (90%)	20 (8%)	4 (2%)	12	30
1	M	257/313 (82%)	230 (90%)	15 (6%)	12 (5%)	3	5
1	O	252/313 (80%)	223 (88%)	20 (8%)	9 (4%)	4	9
2	B	8/13 (62%)	7 (88%)	1 (12%)	0	100	100
2	D	8/13 (62%)	7 (88%)	1 (12%)	0	100	100
2	F	8/13 (62%)	7 (88%)	1 (12%)	0	100	100
2	H	8/13 (62%)	7 (88%)	1 (12%)	0	100	100
2	J	8/13 (62%)	7 (88%)	0	1 (12%)	0	0
2	L	8/13 (62%)	7 (88%)	0	1 (12%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	N	8/13 (62%)	7 (88%)	1 (12%)	0	100	100
2	P	8/13 (62%)	8 (100%)	0	0	100	100
All	All	2105/2608 (81%)	1884 (90%)	153 (7%)	68 (3%)	5	12

5 of 68 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	138	PRO
1	A	231	PRO
1	A	276	LEU
1	C	208	GLU
1	C	273	HIS

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	234/273 (86%)	208 (89%)	26 (11%)	8	17
1	C	229/273 (84%)	192 (84%)	37 (16%)	3	7
1	E	232/273 (85%)	200 (86%)	32 (14%)	4	10
1	G	229/273 (84%)	188 (82%)	41 (18%)	2	5
1	I	230/273 (84%)	183 (80%)	47 (20%)	1	4
1	K	228/273 (84%)	194 (85%)	34 (15%)	4	9
1	M	234/273 (86%)	196 (84%)	38 (16%)	3	7
1	O	228/273 (84%)	198 (87%)	30 (13%)	5	12
2	B	10/10 (100%)	8 (80%)	2 (20%)	1	4
2	D	10/10 (100%)	10 (100%)	0	100	100
2	F	10/10 (100%)	10 (100%)	0	100	100
2	H	10/10 (100%)	8 (80%)	2 (20%)	1	4
2	J	10/10 (100%)	9 (90%)	1 (10%)	9	22
2	L	10/10 (100%)	8 (80%)	2 (20%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	N	10/10 (100%)	10 (100%)	0	100	100
2	P	10/10 (100%)	10 (100%)	0	100	100
All	All	1924/2264 (85%)	1632 (85%)	292 (15%)	3	9

5 of 292 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	226	THR
1	I	125	VAL
1	O	63	ILE
1	G	252	LEU
1	I	53	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 79 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	200	GLN
1	I	193	GLN
1	O	157	ASN
1	G	251	HIS
1	I	121	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
2	ALC	B	504	2	10,11,12	0.41	0	10,13,15	1.48	2 (20%)
2	DSN	B	506	2	4,5,6	0.66	0	2,5,7	1.25	0
2	DLY	B	507	2	7,8,9	0.47	0	6,8,10	0.90	0
2	ALC	D	504	2	10,11,12	0.52	0	10,13,15	1.70	2 (20%)
2	DSN	D	506	2	4,5,6	0.67	0	2,5,7	1.42	1 (50%)
2	DLY	D	507	2	7,8,9	0.47	0	6,8,10	0.75	0
2	ALC	F	504	2	10,11,12	0.43	0	10,13,15	1.40	2 (20%)
2	DSN	F	506	2	4,5,6	0.58	0	2,5,7	1.07	0
2	DLY	F	507	2	7,8,9	0.51	0	6,8,10	0.87	0
2	ALC	H	504	2	10,11,12	0.50	0	10,13,15	1.88	3 (30%)
2	DSN	H	506	2	4,5,6	0.64	0	2,5,7	1.43	0
2	DLY	H	507	2	7,8,9	0.59	0	6,8,10	0.69	0
2	ALC	J	504	2	10,11,12	0.49	0	10,13,15	2.27	6 (60%)
2	DSN	J	506	2	4,5,6	0.65	0	2,5,7	1.58	0
2	DLY	J	507	2	7,8,9	0.52	0	6,8,10	0.88	0
2	ALC	L	504	2	10,11,12	0.53	0	10,13,15	1.17	2 (20%)
2	DSN	L	506	2	4,5,6	0.42	0	2,5,7	1.85	0
2	DLY	L	507	2	7,8,9	0.42	0	6,8,10	1.00	1 (16%)
2	ALC	N	504	2	10,11,12	0.47	0	10,13,15	2.18	4 (40%)
2	DSN	N	506	2	4,5,6	0.60	0	2,5,7	1.51	0
2	DLY	N	507	2	7,8,9	0.39	0	6,8,10	0.70	0
2	ALC	P	504	2	10,11,12	0.52	0	10,13,15	1.02	0
2	DSN	P	506	2	4,5,6	0.43	0	2,5,7	1.62	0
2	DLY	P	507	2	7,8,9	0.48	0	6,8,10	0.90	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
2	ALC	B	504	2	-	0/4/14/16	0/1/1/1
2	DSN	B	506	2	-	0/2/4/6	0/0/0/0
2	DLY	B	507	2	-	0/5/7/9	0/0/0/0
2	ALC	D	504	2	-	0/4/14/16	0/1/1/1
2	DSN	D	506	2	-	0/2/4/6	0/0/0/0
2	DLY	D	507	2	-	0/5/7/9	0/0/0/0
2	ALC	F	504	2	-	0/4/14/16	0/1/1/1
2	DSN	F	506	2	-	0/2/4/6	0/0/0/0
2	DLY	F	507	2	-	0/5/7/9	0/0/0/0
2	ALC	H	504	2	-	0/4/14/16	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DSN	H	506	2	-	0/2/4/6	0/0/0/0
2	DLY	H	507	2	-	0/5/7/9	0/0/0/0
2	ALC	J	504	2	-	0/4/14/16	0/1/1/1
2	DSN	J	506	2	-	0/2/4/6	0/0/0/0
2	DLY	J	507	2	-	0/5/7/9	0/0/0/0
2	ALC	L	504	2	-	0/4/14/16	0/1/1/1
2	DSN	L	506	2	-	0/2/4/6	0/0/0/0
2	DLY	L	507	2	-	0/5/7/9	0/0/0/0
2	ALC	N	504	2	-	0/4/14/16	0/1/1/1
2	DSN	N	506	2	-	0/2/4/6	0/0/0/0
2	DLY	N	507	2	-	0/5/7/9	0/0/0/0
2	ALC	P	504	2	-	0/4/14/16	0/1/1/1
2	DSN	P	506	2	-	0/2/4/6	0/0/0/0
2	DLY	P	507	2	-	0/5/7/9	0/0/0/0

There are no bond length outliers.

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	504	ALC	CB-CG-CD1	-4.15	101.82	111.67
2	J	504	ALC	CB-CG-CD1	-3.28	103.90	111.67
2	N	504	ALC	CB-CG-CD1	-3.16	104.18	111.67
2	B	504	ALC	CB-CG-CD2	-2.76	105.13	111.67
2	D	504	ALC	CB-CG-CD1	-2.71	105.24	111.67

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	504	ALC	2	0
2	B	506	DSN	1	0
2	D	506	DSN	1	0
2	F	507	DLY	1	0
2	L	504	ALC	1	0
2	N	507	DLY	2	0
2	P	504	ALC	1	0
2	P	507	DLY	1	0

5.5 Carbohydrates ⓘ

52 carbohydrates 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	NAG	A	314	1,3	14,14,15	0.54	0	15,19,21	1.32	3 (20%)
3	NAG	A	315	3	14,14,15	0.60	0	15,19,21	1.79	1 (6%)
3	FUC	A	316	3	10,10,11	0.64	0	14,14,16	1.21	1 (7%)
6	NAG	C	314	1,6	14,14,15	0.52	0	15,19,21	1.62	2 (13%)
6	FUC	C	315	6	10,10,11	0.57	0	14,14,16	1.05	2 (14%)
3	NAG	C	331	1,3	14,14,15	0.50	0	15,19,21	2.48	2 (13%)
3	NAG	C	332	3	14,14,15	0.67	0	15,19,21	1.36	2 (13%)
3	FUC	C	336	3	10,10,11	0.59	0	14,14,16	1.21	2 (14%)
3	NAG	E	314	1,3	14,14,15	0.55	0	15,19,21	1.53	2 (13%)
3	NAG	E	315	3	14,14,15	0.55	0	15,19,21	1.55	1 (6%)
3	FUC	E	316	3	10,10,11	0.66	0	14,14,16	1.65	4 (28%)
6	NAG	E	321	1,6	14,14,15	0.55	0	15,19,21	1.97	4 (26%)
6	FUC	E	326	6	10,10,11	0.88	0	14,14,16	2.04	4 (28%)
6	NAG	G	314	1,6	14,14,15	0.52	0	15,19,21	1.74	3 (20%)
6	FUC	G	315	6	10,10,11	0.53	0	14,14,16	1.38	2 (14%)
7	NAG	G	316	1,7	14,14,15	0.63	0	15,19,21	1.11	2 (13%)
7	NAG	G	317	7	14,14,15	0.57	0	15,19,21	1.51	3 (20%)
8	NDG	G	331	1,8	14,14,15	0.55	0	15,19,21	1.59	2 (13%)
8	FUC	G	336	8	10,10,11	0.67	0	14,14,16	1.59	2 (14%)
6	NAG	I	314	1,6	14,14,15	0.41	0	15,19,21	1.69	3 (20%)
6	FUC	I	315	6	10,10,11	0.72	0	14,14,16	1.92	3 (21%)
9	NDG	I	316	9,1	14,14,15	0.44	0	15,19,21	1.14	1 (6%)
9	NAG	I	317	9	14,14,15	0.59	0	15,19,21	1.04	1 (6%)
9	BMA	I	318	9	11,11,12	0.47	0	14,15,17	3.15	5 (35%)
9	MAN	I	319	9	11,11,12	0.62	0	14,15,17	2.28	3 (21%)
9	MAN	I	320	9	11,11,12	0.72	0	14,15,17	1.24	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	I	331	1,6	14,14,15	0.46	0	15,19,21	1.90	2 (13%)
6	FUC	I	336	6	10,10,11	0.60	0	14,14,16	1.42	2 (14%)
3	NAG	K	314	1,3	14,14,15	0.59	0	15,19,21	1.61	3 (20%)
3	NAG	K	315	3	14,14,15	0.61	0	15,19,21	2.66	2 (13%)
3	FUC	K	316	3	10,10,11	0.60	0	14,14,16	1.09	1 (7%)
9	NDG	K	317	9,1	14,14,15	0.64	0	15,19,21	1.57	3 (20%)
9	NAG	K	318	9	14,14,15	0.66	0	15,19,21	1.20	2 (13%)
9	BMA	K	319	9	11,11,12	0.89	1 (9%)	14,15,17	2.02	3 (21%)
9	MAN	K	320	9	11,11,12	0.71	0	14,15,17	2.15	4 (28%)
9	MAN	K	321	9	11,11,12	0.68	0	14,15,17	1.34	3 (21%)
6	NAG	M	314	1,6	14,14,15	0.40	0	15,19,21	1.81	3 (20%)
6	FUC	M	315	6	10,10,11	0.67	0	14,14,16	1.48	2 (14%)
9	NDG	M	316	9,1	14,14,15	0.59	0	15,19,21	1.79	2 (13%)
9	NAG	M	317	9	14,14,15	0.58	0	15,19,21	1.22	1 (6%)
9	BMA	M	318	9	11,11,12	0.55	0	14,15,17	2.12	3 (21%)
9	MAN	M	319	9	11,11,12	0.75	0	14,15,17	2.94	5 (35%)
9	MAN	M	320	9	11,11,12	0.66	0	14,15,17	1.45	2 (14%)
7	NAG	M	321	1,7	14,14,15	0.64	0	15,19,21	1.37	1 (6%)
7	NAG	M	322	7	14,14,15	0.52	0	15,19,21	1.77	3 (20%)
6	NAG	O	314	1,6	14,14,15	0.50	0	15,19,21	1.29	2 (13%)
6	FUC	O	315	6	10,10,11	0.69	0	14,14,16	1.59	4 (28%)
9	NDG	O	316	9,1	14,14,15	0.66	0	15,19,21	1.82	3 (20%)
9	NAG	O	317	9	14,14,15	0.51	0	15,19,21	0.88	0
9	BMA	O	318	9	11,11,12	0.92	1 (9%)	14,15,17	1.78	3 (21%)
9	MAN	O	319	9	11,11,12	0.74	0	14,15,17	1.78	3 (21%)
9	MAN	O	320	9	11,11,12	0.61	0	14,15,17	1.83	3 (21%)

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
3	NAG	A	314	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	315	3	-	0/6/23/26	0/1/1/1
3	FUC	A	316	3	2/2/4/5	0/0/17/20	0/1/1/1
6	NAG	C	314	1,6	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	FUC	C	315	6	2/2/4/5	0/0/17/20	0/1/1/1
3	NAG	C	331	1,3	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	C	332	3	-	0/6/23/26	0/1/1/1
3	FUC	C	336	3	2/2/4/5	0/0/17/20	0/1/1/1
3	NAG	E	314	1,3	-	0/6/23/26	0/1/1/1
3	NAG	E	315	3	-	0/6/23/26	0/1/1/1
3	FUC	E	316	3	2/2/4/5	0/0/17/20	0/1/1/1
6	NAG	E	321	1,6	-	0/6/23/26	0/1/1/1
6	FUC	E	326	6	2/2/4/5	0/0/17/20	0/1/1/1
6	NAG	G	314	1,6	-	0/6/23/26	0/1/1/1
6	FUC	G	315	6	2/2/4/5	0/0/17/20	0/1/1/1
7	NAG	G	316	1,7	-	0/6/23/26	0/1/1/1
7	NAG	G	317	7	-	0/6/23/26	0/1/1/1
8	NDG	G	331	1,8	-	1/6/23/26	0/1/1/1
8	FUC	G	336	8	2/2/4/5	0/0/17/20	0/1/1/1
6	NAG	I	314	1,6	-	0/6/23/26	0/1/1/1
6	FUC	I	315	6	2/2/4/5	0/0/17/20	0/1/1/1
9	NDG	I	316	9,1	-	0/6/23/26	0/1/1/1
9	NAG	I	317	9	-	0/6/23/26	0/1/1/1
9	BMA	I	318	9	-	0/2/19/22	0/1/1/1
9	MAN	I	319	9	-	0/2/19/22	0/1/1/1
9	MAN	I	320	9	-	0/2/19/22	1/1/1/1
6	NAG	I	331	1,6	-	0/6/23/26	0/1/1/1
6	FUC	I	336	6	2/2/4/5	0/0/17/20	0/1/1/1
3	NAG	K	314	1,3	-	0/6/23/26	0/1/1/1
3	NAG	K	315	3	-	2/6/23/26	0/1/1/1
3	FUC	K	316	3	2/2/4/5	0/0/17/20	0/1/1/1
9	NDG	K	317	9,1	-	0/6/23/26	0/1/1/1
9	NAG	K	318	9	-	0/6/23/26	0/1/1/1
9	BMA	K	319	9	-	0/2/19/22	0/1/1/1
9	MAN	K	320	9	-	0/2/19/22	0/1/1/1
9	MAN	K	321	9	-	0/2/19/22	0/1/1/1
6	NAG	M	314	1,6	-	0/6/23/26	0/1/1/1
6	FUC	M	315	6	2/2/4/5	0/0/17/20	0/1/1/1
9	NDG	M	316	9,1	-	0/6/23/26	0/1/1/1
9	NAG	M	317	9	-	0/6/23/26	0/1/1/1
9	BMA	M	318	9	-	0/2/19/22	0/1/1/1
9	MAN	M	319	9	-	0/2/19/22	1/1/1/1
9	MAN	M	320	9	-	0/2/19/22	0/1/1/1
7	NAG	M	321	1,7	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	M	322	7	-	0/6/23/26	0/1/1/1
6	NAG	O	314	1,6	-	0/6/23/26	0/1/1/1
6	FUC	O	315	6	2/2/4/5	0/0/17/20	0/1/1/1
9	NDG	O	316	9,1	-	0/6/23/26	0/1/1/1
9	NAG	O	317	9	-	0/6/23/26	0/1/1/1
9	BMA	O	318	9	-	0/2/19/22	0/1/1/1
9	MAN	O	319	9	-	0/2/19/22	0/1/1/1
9	MAN	O	320	9	-	0/2/19/22	1/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	O	318	BMA	O5-C1	-2.32	1.39	1.43
9	K	319	BMA	O5-C1	-2.17	1.40	1.43

The worst 5 of 126 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	M	319	MAN	C1-C2-C3	-7.88	100.22	109.54
9	I	319	MAN	C1-C2-C3	-6.74	101.56	109.54
9	K	320	MAN	C1-C2-C3	-6.02	102.42	109.54
9	O	319	MAN	C1-C2-C3	-4.58	104.12	109.54
9	M	319	MAN	C1-O5-C5	-4.12	107.02	112.25

5 of 25 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	C	315	FUC	C5
6	C	315	FUC	C1
3	K	316	FUC	C5
3	K	316	FUC	C1
6	M	315	FUC	C5

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	K	315	NAG	C8-C7-N2-C2
8	G	331	NDG	O7-C7-N2-C2
3	K	315	NAG	O7-C7-N2-C2

All (3) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	O	320	MAN	C1-C2-C3-C4-C5-O5
9	M	319	MAN	C1-C2-C3-C4-C5-O5
9	I	320	MAN	C1-C2-C3-C4-C5-O5

9 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	E	321	NAG	1	0
7	G	316	NAG	2	0
7	G	317	NAG	1	0
6	I	314	NAG	1	0
9	I	316	NDG	1	0
9	K	317	NDG	1	0
6	M	314	NAG	1	0
9	M	316	NDG	1	0
9	O	319	MAN	1	0

5.6 Ligand geometry [i](#)

32 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	$\# Z > 2$
4	NDG	A	317	1	14,14,15	0.45	0	15,19,21	1.79	2 (13%)
5	NAG	A	321	1	14,14,15	0.66	0	15,19,21	2.19	4 (26%)
10	SO4	A	801	-	4,4,4	0.23	0	6,6,6	0.36	0
10	SO4	A	805	-	4,4,4	0.22	0	6,6,6	0.13	0
10	SO4	A	813	-	4,4,4	0.21	0	6,6,6	0.34	0
5	NAG	C	316	1	14,14,15	0.42	0	15,19,21	1.09	1 (6%)
5	NAG	C	321	1	14,14,15	0.62	0	15,19,21	0.96	1 (6%)
10	SO4	C	806	-	4,4,4	0.11	0	6,6,6	0.19	0
10	SO4	C	814	-	4,4,4	0.14	0	6,6,6	0.31	0
10	SO4	C	818	-	4,4,4	0.20	0	6,6,6	0.25	0
5	NAG	E	317	1	14,14,15	0.55	0	15,19,21	1.45	1 (6%)
10	SO4	E	807	-	4,4,4	0.24	0	6,6,6	0.15	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	SO4	E	815	-	4,4,4	0.25	0	6,6,6	0.51	0
10	SO4	E	820	-	4,4,4	0.11	0	6,6,6	0.13	0
5	NAG	G	321	1	14,14,15	0.66	0	15,19,21	1.30	2 (13%)
10	SO4	G	802	-	4,4,4	0.20	0	6,6,6	0.22	0
10	SO4	G	808	-	4,4,4	0.15	0	6,6,6	0.35	0
10	SO4	G	816	-	4,4,4	0.26	0	6,6,6	0.42	0
10	SO4	G	817	-	4,4,4	0.25	0	6,6,6	0.17	0
5	NAG	I	321	1	14,14,15	0.68	1 (7%)	15,19,21	1.07	0
10	SO4	I	804	-	4,4,4	0.21	0	6,6,6	0.17	0
10	SO4	I	809	-	4,4,4	0.20	0	6,6,6	0.07	0
10	SO4	I	821	-	4,4,4	0.15	0	6,6,6	0.09	0
5	NAG	K	322	1	14,14,15	0.80	0	15,19,21	1.38	2 (13%)
4	NDG	K	331	1	14,14,15	0.51	0	15,19,21	1.68	3 (20%)
10	SO4	K	803	-	4,4,4	0.16	0	6,6,6	0.15	0
10	SO4	K	810	-	4,4,4	0.21	0	6,6,6	0.14	0
5	NAG	M	331	1	14,14,15	0.39	0	15,19,21	1.70	1 (6%)
10	SO4	M	811	-	4,4,4	0.10	0	6,6,6	0.28	0
10	SO4	M	819	-	4,4,4	0.15	0	6,6,6	0.06	0
4	NDG	O	321	1	14,14,15	0.69	0	15,19,21	0.83	1 (6%)
10	SO4	O	812	-	4,4,4	0.10	0	6,6,6	0.19	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	NDG	A	317	1	-	0/6/23/26	0/1/1/1
5	NAG	A	321	1	1/1/5/7	0/6/23/26	0/1/1/1
10	SO4	A	801	-	-	0/0/0/0	0/0/0/0
10	SO4	A	805	-	-	0/0/0/0	0/0/0/0
10	SO4	A	813	-	-	0/0/0/0	0/0/0/0
5	NAG	C	316	1	1/1/5/7	0/6/23/26	0/1/1/1
5	NAG	C	321	1	1/1/5/7	0/6/23/26	0/1/1/1
10	SO4	C	806	-	-	0/0/0/0	0/0/0/0
10	SO4	C	814	-	-	0/0/0/0	0/0/0/0
10	SO4	C	818	-	-	0/0/0/0	0/0/0/0
5	NAG	E	317	1	-	0/6/23/26	0/1/1/1
10	SO4	E	807	-	-	0/0/0/0	0/0/0/0
10	SO4	E	815	-	-	0/0/0/0	0/0/0/0
10	SO4	E	820	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	G	321	1	-	0/6/23/26	0/1/1/1
10	SO4	G	802	-	-	0/0/0/0	0/0/0/0
10	SO4	G	808	-	-	0/0/0/0	0/0/0/0
10	SO4	G	816	-	-	0/0/0/0	0/0/0/0
10	SO4	G	817	-	-	0/0/0/0	0/0/0/0
5	NAG	I	321	1	-	0/6/23/26	0/1/1/1
10	SO4	I	804	-	-	0/0/0/0	0/0/0/0
10	SO4	I	809	-	-	0/0/0/0	0/0/0/0
10	SO4	I	821	-	-	0/0/0/0	0/0/0/0
5	NAG	K	322	1	-	1/6/23/26	0/1/1/1
4	NDG	K	331	1	-	0/6/23/26	0/1/1/1
10	SO4	K	803	-	-	0/0/0/0	0/0/0/0
10	SO4	K	810	-	-	0/0/0/0	0/0/0/0
5	NAG	M	331	1	-	0/6/23/26	0/1/1/1
10	SO4	M	811	-	-	0/0/0/0	0/0/0/0
10	SO4	M	819	-	-	0/0/0/0	0/0/0/0
4	NDG	O	321	1	-	0/6/23/26	0/1/1/1
10	SO4	O	812	-	-	0/0/0/0	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	I	321	NAG	C1-C2	2.05	1.55	1.52

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	321	NAG	C4-C3-C2	-2.32	107.63	111.23
5	A	321	NAG	C2-N2-C7	2.04	125.66	123.04
5	G	321	NAG	C4-C3-C2	2.05	114.42	111.23
5	A	321	NAG	C8-C7-N2	2.10	120.12	116.11
4	O	321	NDG	C4-C3-C2	2.19	114.63	111.23

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	C	321	NAG	C1
5	C	316	NAG	C1
5	A	321	NAG	C1

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	K	322	NAG	O7-C7-N2-C2

There are no ring outliers.

7 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	801	SO4	1	0
10	C	818	SO4	1	0
10	G	817	SO4	1	0
10	I	804	SO4	1	0
10	K	803	SO4	1	0
10	K	810	SO4	2	0
10	M	811	SO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	268/313 (85%)	1.00	36 (13%) 4 3	45, 57, 69, 98	0
1	C	259/313 (82%)	0.89	37 (14%) 4 3	48, 58, 66, 76	0
1	E	262/313 (83%)	0.84	32 (12%) 5 4	46, 56, 64, 72	0
1	G	258/313 (82%)	0.78	28 (10%) 7 5	46, 57, 67, 69	0
1	I	264/313 (84%)	0.98	46 (17%) 2 1	44, 58, 69, 89	0
1	K	257/313 (82%)	0.93	34 (13%) 4 4	45, 58, 67, 78	0
1	M	263/313 (84%)	0.89	35 (13%) 4 3	43, 57, 66, 83	0
1	O	258/313 (82%)	0.97	34 (13%) 4 4	47, 58, 68, 87	0
2	B	10/13 (76%)	0.91	1 (10%) 9 7	53, 60, 69, 71	0
2	D	10/13 (76%)	1.12	1 (10%) 9 7	50, 57, 64, 66	0
2	F	10/13 (76%)	1.24	2 (20%) 1 1	51, 63, 71, 71	0
2	H	10/13 (76%)	1.02	1 (10%) 9 7	52, 56, 65, 69	0
2	J	10/13 (76%)	1.33	2 (20%) 1 1	47, 54, 64, 70	0
2	L	10/13 (76%)	1.11	2 (20%) 1 1	50, 56, 72, 75	0
2	N	10/13 (76%)	1.17	1 (10%) 9 7	49, 55, 66, 71	0
2	P	10/13 (76%)	1.10	2 (20%) 1 1	52, 58, 72, 74	0
All	All	2169/2608 (83%)	0.92	294 (13%) 4 3	43, 57, 67, 98	0

The worst 5 of 294 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	278	VAL	10.0
1	E	231	PRO	8.8
1	A	138	PRO	8.3
1	I	275	ASP	8.1
1	A	279	GLN	8.0

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
2	DSN	P	506	6/7	0.94	0.17	-	56,56,56,57	0
2	DLY	H	507	9/10	0.97	0.22	-	50,50,51,51	0
2	DLY	L	507	9/10	0.94	0.23	-	51,52,59,61	0
2	DLY	N	507	9/10	0.95	0.32	-	47,50,50,51	0
2	DSN	B	506	6/7	0.97	0.16	-	52,54,54,54	0
2	DLY	D	507	9/10	0.94	0.29	-	51,52,53,53	0
2	DSN	N	506	6/7	0.96	0.28	-	51,51,52,53	0
2	DSN	L	506	6/7	0.98	0.16	-	53,54,54,55	0
2	ALC	P	504	11/12	0.96	0.26	-	59,60,61,63	0
2	ALC	H	504	11/12	0.93	0.27	-	54,56,61,61	0
2	ALC	J	504	11/12	0.94	0.28	-	55,56,57,57	0
2	ALC	L	504	11/12	0.96	0.23	-	60,61,63,63	0
2	DSN	H	506	6/7	0.97	0.24	-	48,50,50,50	0
2	ALC	F	504	11/12	0.96	0.25	-	54,54,56,58	0
2	DLY	P	507	9/10	0.87	0.27	-	54,55,61,63	0
2	ALC	D	504	11/12	0.94	0.27	-	53,54,55,56	0
2	DLY	J	507	9/10	0.96	0.30	-	49,50,50,51	0
2	DLY	B	507	9/10	0.89	0.26	-	53,54,58,58	0
2	ALC	N	504	11/12	0.93	0.28	-	55,56,57,58	0
2	DSN	F	506	6/7	0.97	0.22	-	49,50,50,50	0
2	DLY	F	507	9/10	0.93	0.22	-	51,52,57,57	0
2	DSN	D	506	6/7	0.96	0.23	-	51,52,52,52	0
2	DSN	J	506	6/7	0.97	0.27	-	52,52,52,54	0
2	ALC	B	504	11/12	0.96	0.25	-	56,57,58,60	0

6.3 Carbohydrates ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
6	FUC	E	326	10/11	0.67	0.42	3.25	84,85,86,86	0
6	FUC	G	315	10/11	0.87	0.35	2.31	71,73,74,75	0
6	FUC	O	315	10/11	0.90	0.35	2.18	71,72,73,73	0
6	FUC	C	315	10/11	0.82	0.34	1.56	71,72,73,73	0
3	FUC	E	316	10/11	0.72	0.30	1.26	84,85,85,85	0
3	FUC	A	316	10/11	0.94	0.28	0.40	81,82,82,83	0
9	NDG	O	316	14/15	0.88	0.21	-0.00	61,65,67,67	0
9	NAG	I	317	14/15	0.92	0.18	-0.09	60,61,63,64	0
9	NDG	M	316	14/15	0.93	0.15	-0.42	44,47,48,49	0
3	FUC	K	316	10/11	0.90	0.23	-0.44	76,77,77,78	0
9	NDG	K	317	14/15	0.94	0.16	-0.52	45,51,53,53	0
9	MAN	K	321	11/12	0.91	0.18	-0.70	45,47,48,49	0
9	NDG	I	316	14/15	0.93	0.16	-0.79	57,58,61,63	0
9	MAN	M	320	11/12	0.93	0.17	-0.89	43,45,46,48	0
6	FUC	I	315	10/11	0.85	0.23	-1.35	73,75,76,76	0
3	NAG	A	314	14/15	0.92	0.17	-1.54	68,73,79,80	0
6	NAG	I	314	14/15	0.90	0.19	-	58,61,67,71	0
3	NAG	C	332	14/15	0.68	0.46	-	99,101,101,102	0
7	NAG	M	321	14/15	0.57	0.48	-	82,86,88,92	0
8	NDG	G	331	14/15	0.73	0.45	-	80,84,89,92	0
3	FUC	C	336	10/11	0.84	0.47	-	96,97,97,98	0
6	NAG	M	314	14/15	0.87	0.26	-	57,59,61,64	0
9	MAN	K	320	11/12	0.75	0.21	-	55,57,59,59	0
6	NAG	I	331	14/15	0.78	0.28	-	76,79,81,82	0
9	NAG	M	317	14/15	0.96	0.17	-	47,48,48,50	0
3	NAG	E	315	14/15	0.75	0.40	-	89,91,92,93	0
6	NAG	C	314	14/15	0.93	0.21	-	62,65,66,68	0
6	FUC	M	315	10/11	0.83	0.33	-	66,68,69,69	0
9	MAN	O	319	11/12	0.74	0.39	-	74,76,77,77	0
9	BMA	M	318	11/12	0.92	0.16	-	47,49,51,54	0
3	NAG	K	314	14/15	0.88	0.17	-	68,72,74,78	0
9	BMA	I	318	11/12	0.83	0.16	-	64,66,68,71	0
6	NAG	O	314	14/15	0.86	0.21	-	63,65,67,70	0
7	NAG	M	322	14/15	0.69	0.48	-	95,96,98,99	0
6	NAG	E	321	14/15	0.67	0.51	-	76,79,82,83	0
7	NAG	G	317	14/15	0.72	0.41	-	91,92,93,93	0
9	MAN	O	320	11/12	0.81	0.20	-	65,69,71,72	0
3	NAG	A	315	14/15	0.74	0.35	-	83,84,86,86	0
9	NAG	K	318	14/15	0.93	0.19	-	50,52,54,54	0
9	MAN	I	320	11/12	0.84	0.17	-	67,68,71,72	0
9	BMA	K	319	11/12	0.90	0.18	-	48,50,52,52	0
9	MAN	I	319	11/12	0.74	0.31	-	73,75,77,77	0
6	FUC	I	336	10/11	0.71	0.41	-	83,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	NAG	G	314	14/15	0.96	0.16	-	57,60,63,67	0
3	NAG	K	315	14/15	0.76	0.45	-	81,83,86,86	0
8	FUC	G	336	10/11	0.55	0.54	-	94,95,96,96	0
3	NAG	C	331	14/15	0.79	0.33	-	85,91,95,96	0
9	BMA	O	318	11/12	0.89	0.28	-	70,71,72,73	0
9	NAG	O	317	14/15	0.87	0.24	-	66,69,71,71	0
9	MAN	M	319	11/12	0.83	0.29	-	54,58,62,63	0
7	NAG	G	316	14/15	0.79	0.46	-	80,86,87,90	0
3	NAG	E	314	14/15	0.77	0.19	-	74,77,83,86	0

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
10	SO4	A	805	5/5	0.82	0.28	0.98	132,132,133,133	0
10	SO4	E	807	5/5	0.87	0.34	0.91	125,125,125,125	0
10	SO4	O	812	5/5	0.92	0.26	0.31	79,79,80,80	0
10	SO4	K	810	5/5	0.90	0.21	-0.15	84,85,86,86	0
10	SO4	E	820	5/5	0.93	0.21	-0.49	86,87,87,87	0
10	SO4	I	809	5/5	0.98	0.16	-0.77	64,65,65,65	0
10	SO4	G	816	5/5	0.92	0.20	-0.80	61,62,63,63	0
10	SO4	C	806	5/5	0.92	0.17	-0.83	79,80,81,81	0
10	SO4	I	821	5/5	0.97	0.18	-1.37	71,72,72,73	0
10	SO4	G	808	5/5	0.97	0.16	-1.56	58,58,60,60	0
10	SO4	A	813	5/5	0.96	0.12	-1.68	64,66,66,67	0
10	SO4	M	811	5/5	0.97	0.10	-1.81	63,63,63,64	0
10	SO4	C	814	5/5	0.93	0.16	-1.91	65,67,68,69	0
10	SO4	C	818	5/5	0.95	0.13	-1.96	75,75,76,77	0
10	SO4	M	819	5/5	0.94	0.16	-2.30	79,79,80,80	0
10	SO4	G	817	5/5	0.97	0.12	-2.78	67,69,69,70	0
10	SO4	E	815	5/5	0.96	0.11	-3.04	56,57,58,58	0
10	SO4	G	802	5/5	0.92	0.16	-	56,57,58,58	0
5	NAG	I	321	14/15	0.77	0.49	-	76,79,80,80	0
5	NAG	C	316	14/15	0.86	0.52	-	77,80,84,84	0
5	NAG	E	317	14/15	0.83	0.38	-	72,75,80,80	0
10	SO4	I	804	5/5	0.94	0.20	-	58,58,59,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
10	SO4	K	803	5/5	0.96	0.12	-	61,61,61,62	0
5	NAG	A	321	14/15	0.52	0.50	-	75,78,80,80	0
4	NDG	O	321	14/15	0.74	0.37	-	78,82,82,83	0
4	NDG	A	317	14/15	0.79	0.36	-	78,82,85,85	0
4	NDG	K	331	14/15	0.39	0.51	-	84,86,88,88	0
5	NAG	K	322	14/15	0.68	0.41	-	76,79,80,81	0
5	NAG	G	321	14/15	0.67	0.52	-	76,80,82,83	0
5	NAG	M	331	14/15	0.77	0.33	-	72,75,76,76	0
10	SO4	A	801	5/5	0.94	0.13	-	70,70,72,72	0
5	NAG	C	321	14/15	0.85	0.49	-	78,82,83,84	0

6.5 Other polymers [i](#)

There are no such residues in this entry.