



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 08:46 AM UTC

PDB ID : 2QAD / pdb_00002qad
Title : Structure of tyrosine-sulfated 412d antibody complexed with HIV-1 YU2 gp120 and CD4
Authors : Huang, C.-C.; Tang, M.; Robinson, J.; Wyatt, R.; Kwong, P.D.
Deposited on : 2007-06-14
Resolution : 3.30 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The 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

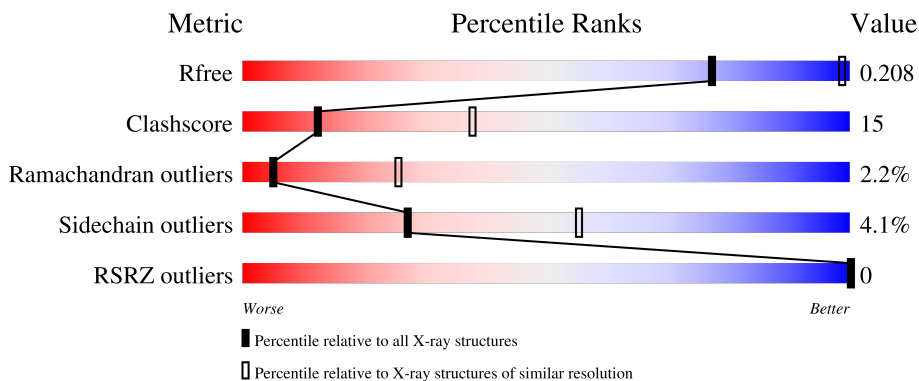
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	322	63% 33% ..
1	E	322	60% 33% . . .
2	B	181	63% 33% . .
2	F	181	65% 31% . .
3	C	214	62% 35% .

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Mol	Chain	Length	Quality of chain	
3	G	214	57%	40%
4	D	231	66%	32%
4	H	231	74%	25%

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
5	NAG	A	862	X	-	-	-
5	NAG	A	894	X	-	-	-
5	NAG	E	862	X	-	-	-
5	NAG	E	963	X	-	-	-
6	MLA	A	3	-	X	-	-
6	MLA	B	186	-	X	-	-
6	MLA	F	186	-	X	-	-
6	MLA	H	215	-	X	-	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 14987 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 Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	319	Total	C	N	O	S	0	0	0
			2499	1562	445	474	18			
1	E	312	Total	C	N	O	S	0	0	0
			2445	1533	430	464	18			

- Molecule 2 is a protein called T-cell surface glycoprotein CD4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	178	Total	C	N	O	S	0	0	0
			1383	865	242	272	4			
2	F	179	Total	C	N	O	S	0	0	0
			1394	874	243	273	4			

- Molecule 3 is a protein called anti-HIV-1 antibody 412d light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	213	Total	C	N	O	S	0	0	0
			1642	1024	278	334	6			
3	G	213	Total	C	N	O	S	0	0	0
			1642	1024	278	334	6			

- Molecule 4 is a protein called anti-HIV-1 antibody 412d heavy chain.

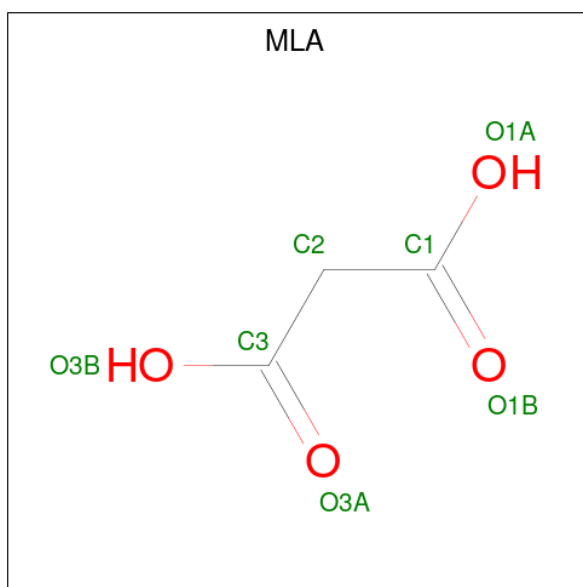
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	231	Total	C	N	O	S	0	0	0
			1746	1101	286	350	9			
4	H	231	Total	C	N	O	S	0	0	0
			1746	1101	286	350	9			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).

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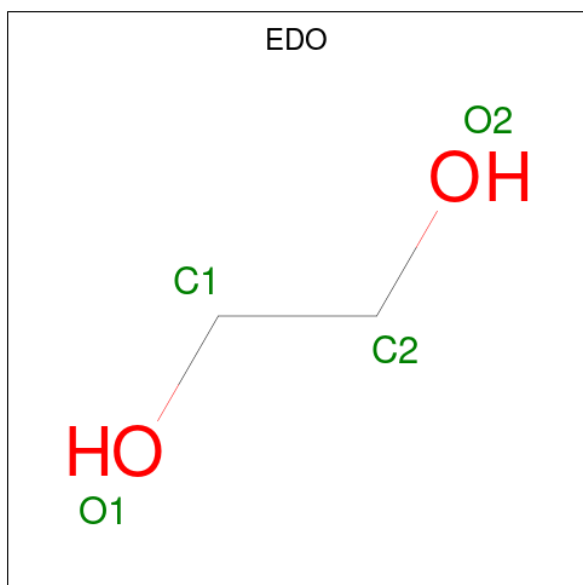
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	E	1	Total	C	N	O	0	0
			14	8	1	5		
5	E	1	Total	C	N	O	0	0
			14	8	1	5		
5	E	1	Total	C	N	O	0	0
			14	8	1	5		
5	E	1	Total	C	N	O	0	0
			14	8	1	5		
5	E	1	Total	C	N	O	0	0
			14	8	1	5		
5	E	1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

- Molecule 6 is MALONIC ACID (CCD ID: MLA) (formula: C₃H₄O₄).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 7 3 4	0	0
6	B	1	Total C O 7 3 4	0	0
6	F	1	Total C O 7 3 4	0	0
6	H	1	Total C O 7 3 4	0	0

- Molecule 7 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).

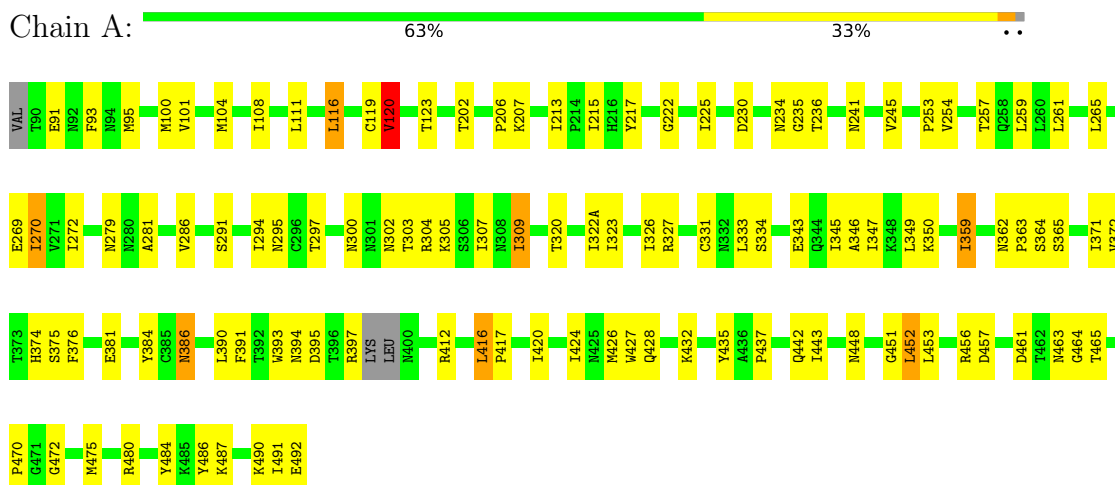


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total 4	C 2	O 2	0	0
7	C	1	Total 4	C 2	O 2	0	0
7	C	1	Total 4	C 2	O 2	0	0
7	D	1	Total 4	C 2	O 2	0	0
7	E	1	Total 4	C 2	O 2	0	0
7	E	1	Total 4	C 2	O 2	0	0
7	F	1	Total 4	C 2	O 2	0	0

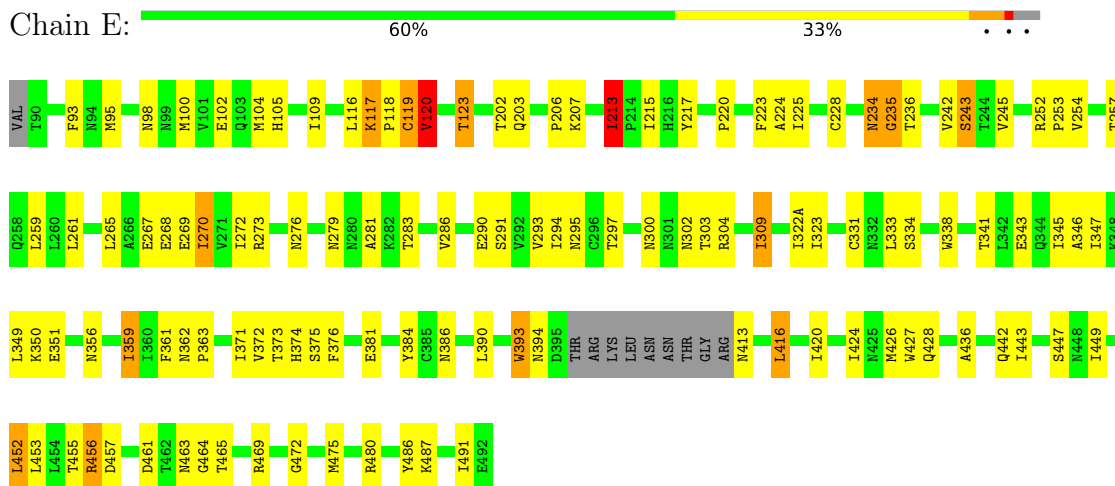
3 Residue-property plots

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: Envelope glycoprotein gp160



- Molecule 1: Envelope glycoprotein gp160

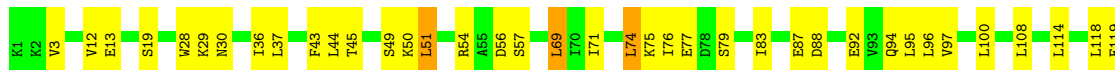


- Molecule 2: T-cell surface glycoprotein CD4

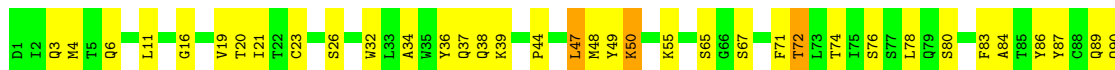




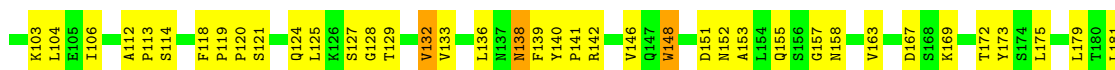
• Molecule 2: T-cell surface glycoprotein CD4



• Molecule 3: anti-HIV-1 antibody 412d light chain

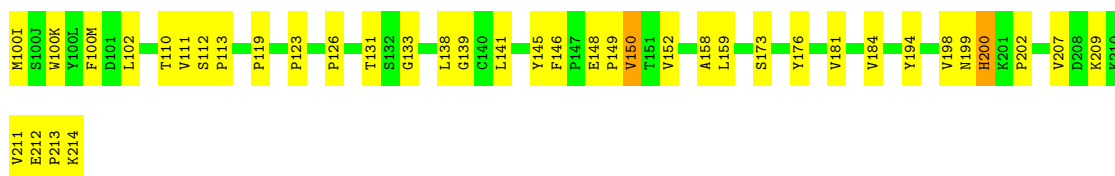


• Molecule 3: anti-HIV-1 antibody 412d light chain



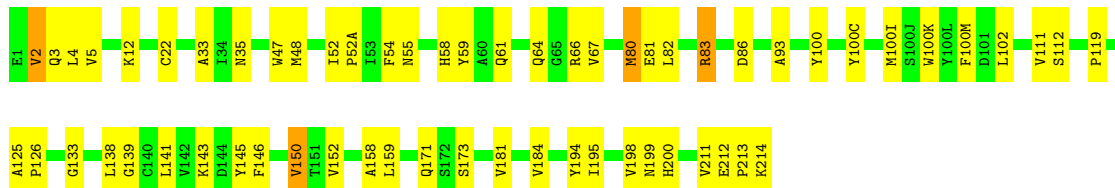
• Molecule 4: anti-HIV-1 antibody 412d heavy chain





- Molecule 4: anti-HIV-1 antibody 412d heavy chain

Chain H: 74% 25%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	109.60Å 53.02Å 225.33Å 90.00° 104.64° 90.00°	Depositor
Resolution (Å)	20.00 – 3.30 20.00 – 3.31	Depositor EDS
% Data completeness (in resolution range)	66.7 (20.00-3.30) 65.9 (20.00-3.31)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.41 (at 3.33Å)	Xtrriage
Refinement program	PHENIX, CNS	Depositor
R, R_{free}	0.202 , 0.269 0.206 , 0.208	Depositor DCC
R_{free} test set	1280 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	93.1	Xtrriage
Anisotropy	0.605	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 88.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.034 for h,-k,-h-l	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14987	wwPDB-VP
Average B, all atoms (Å ²)	157.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.47% 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: MLA, TYS, NAG, EDO

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.34	0/2546	0.81	5/3446 (0.1%)
1	E	0.34	0/2493	0.80	6/3376 (0.2%)
2	B	0.29	0/1402	0.72	0/1891
2	F	0.29	0/1414	0.72	0/1907
3	C	0.28	0/1677	0.73	0/2273
3	G	0.29	0/1677	0.74	0/2273
4	D	0.31	0/1757	0.74	2/2393 (0.1%)
4	H	0.32	0/1757	0.74	0/2393
All	All	0.31	0/14723	0.76	13/19952 (0.1%)

There are no bond length outliers.

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	213	ILE	CA-C-N	6.93	128.51	119.84
1	A	213	ILE	C-N-CA	6.93	128.51	119.84
1	E	213	ILE	CA-C-N	6.53	128.00	119.84
1	E	213	ILE	C-N-CA	6.53	128.00	119.84
1	A	416	LEU	CA-C-N	5.75	125.51	119.76

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2499	0	2443	102	0
1	E	2445	0	2394	90	0
2	B	1383	0	1414	42	0
2	F	1394	0	1423	39	0
3	C	1642	0	1596	54	0
3	G	1642	0	1596	68	0
4	D	1746	0	1684	53	0
4	H	1746	0	1684	43	0
5	A	224	0	208	12	0
5	E	210	0	195	6	0
6	A	7	0	3	0	0
6	B	7	0	3	0	0
6	F	7	0	3	0	0
6	H	7	0	3	0	0
7	A	4	0	6	0	0
7	C	8	0	12	0	0
7	D	4	0	6	0	0
7	E	8	0	12	1	0
7	F	4	0	6	0	0
All	All	14987	0	14691	457	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 457 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:A:95:MET:HE2	1:A:484:TYR:HB2	1.33	1.05
2:B:134:ARG:HH22	2:B:152:GLN:HB3	1.22	1.02
1:A:272:ILE:HG22	1:A:286:VAL:HG22	1.47	0.96
2:F:79:SER:HB3	2:F:97:VAL:HG23	1.52	0.92
1:A:95:MET:HE3	1:A:235:GLY:HA3	1.55	0.89

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	315/322 (98%)	275 (87%)	34 (11%)	6 (2%)	6	28
1	E	308/322 (96%)	270 (88%)	32 (10%)	6 (2%)	6	28
2	B	176/181 (97%)	152 (86%)	20 (11%)	4 (2%)	5	25
2	F	177/181 (98%)	152 (86%)	20 (11%)	5 (3%)	4	21
3	C	211/214 (99%)	176 (83%)	30 (14%)	5 (2%)	4	24
3	G	211/214 (99%)	174 (82%)	32 (15%)	5 (2%)	4	24
4	D	227/231 (98%)	185 (82%)	37 (16%)	5 (2%)	5	26
4	H	227/231 (98%)	184 (81%)	38 (17%)	5 (2%)	5	26
All	All	1852/1896 (98%)	1568 (85%)	243 (13%)	41 (2%)	5	26

5 of 41 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	147	SER
4	D	2	VAL
4	D	150	VAL
2	F	147	SER
4	H	2	VAL

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	281/285 (99%)	267 (95%)	14 (5%)	22	50
1	E	276/285 (97%)	255 (92%)	21 (8%)	12	37
2	B	161/164 (98%)	154 (96%)	7 (4%)	26	54
2	F	162/164 (99%)	156 (96%)	6 (4%)	30	58
3	C	188/189 (100%)	183 (97%)	5 (3%)	39	63
3	G	188/189 (100%)	181 (96%)	7 (4%)	30	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	D	192/192 (100%)	188 (98%)	4 (2%)	47 67
4	H	192/192 (100%)	189 (98%)	3 (2%)	55 72
All	All	1640/1660 (99%)	1573 (96%)	67 (4%)	27 55

5 of 67 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	G	47	LEU
3	G	90	GLN
4	H	80	MET
3	C	132	VAL
3	C	72	THR

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

Mol	Chain	Res	Type
2	F	52	ASN
3	G	124	GLN
2	F	66	ASN
3	G	38	GLN
4	H	58	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

4 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	TYS	H	100	4	15,16,17	1.01	1 (6%)	15,22,24	0.53	0
4	TYS	D	100(C)	4	15,16,17	1.04	1 (6%)	15,22,24	0.38	0
4	TYS	H	100(C)	4	15,16,17	1.03	1 (6%)	15,22,24	0.38	0
4	TYS	D	100	4	15,16,17	1.01	1 (6%)	15,22,24	0.53	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	TYS	H	100	4	-	1/10/11/13	0/1/1/1
4	TYS	D	100(C)	4	-	1/10/11/13	0/1/1/1
4	TYS	H	100(C)	4	-	1/10/11/13	0/1/1/1
4	TYS	D	100	4	-	1/10/11/13	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	100(C)	TYS	OH-CZ	-2.79	1.38	1.42
4	H	100(C)	TYS	OH-CZ	-2.76	1.38	1.42
4	D	100	TYS	OH-CZ	-2.55	1.38	1.42
4	H	100	TYS	OH-CZ	-2.53	1.38	1.42

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	100(C)	TYS	O-C-CA-CB
4	H	100(C)	TYS	O-C-CA-CB
4	D	100	TYS	C-CA-CB-CG
4	H	100	TYS	C-CA-CB-CG

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	100(C)	TYS	2	0
4	D	100	TYS	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

42 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	E	832	1	14,14,15	0.56	0	17,19,21	0.73	0
7	EDO	C	215	-	3,3,3	0.42	0	2,2,2	0.32	0
7	EDO	C	216	-	3,3,3	0.43	0	2,2,2	0.35	0
5	NAG	E	734	1	14,14,15	0.52	0	17,19,21	0.71	1 (5%)
5	NAG	E	795	1	14,14,15	0.52	0	17,19,21	0.69	0
5	NAG	A	862	1	14,14,15	0.70	0	17,19,21	1.53	3 (17%)
5	NAG	A	762	1	14,14,15	0.48	0	17,19,21	1.14	1 (5%)
5	NAG	A	894	1	14,14,15	0.42	0	17,19,21	1.10	1 (5%)
5	NAG	A	963	1	14,14,15	0.47	0	17,19,21	1.30	2 (11%)
5	NAG	E	948	1	14,14,15	0.49	0	17,19,21	0.73	0
7	EDO	F	187	-	3,3,3	0.43	0	2,2,2	0.29	0
6	MLA	A	3	-	6,6,6	3.48	5 (83%)	7,7,7	1.47	2 (28%)
5	NAG	A	886	1	14,14,15	0.47	0	17,19,21	1.22	3 (17%)
5	NAG	A	801	1	14,14,15	0.50	0	17,19,21	0.63	0
5	NAG	A	795	1	14,14,15	0.54	0	17,19,21	0.57	0
5	NAG	E	913	1	14,14,15	0.52	0	17,19,21	1.09	1 (5%)
5	NAG	A	832	1	14,14,15	0.50	0	17,19,21	1.01	1 (5%)
5	NAG	E	894	1	14,14,15	0.56	0	17,19,21	1.34	2 (11%)
5	NAG	A	741	1	14,14,15	0.63	0	17,19,21	1.42	2 (11%)
7	EDO	A	8	-	3,3,3	0.42	0	2,2,2	0.36	0
5	NAG	A	856	1	14,14,15	0.48	0	17,19,21	0.73	0
5	NAG	E	741	1	14,14,15	0.49	0	17,19,21	0.64	0
5	NAG	E	963	1	14,14,15	0.60	0	17,19,21	1.31	2 (11%)
5	NAG	E	856	1	14,14,15	0.52	0	17,19,21	0.82	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	A	776	1	14,14,15	0.48	0	17,19,21	0.92	1 (5%)
5	NAG	A	948	1	14,14,15	0.52	0	17,19,21	0.54	0
5	NAG	E	762	1	14,14,15	0.46	0	17,19,21	1.01	1 (5%)
5	NAG	E	789	1	14,14,15	0.49	0	17,19,21	0.63	0
6	MLA	F	186	-	6,6,6	3.45	5 (83%)	7,7,7	1.79	2 (28%)
5	NAG	A	734	1	14,14,15	0.51	0	17,19,21	0.65	0
7	EDO	E	7	-	3,3,3	0.41	0	2,2,2	0.42	0
5	NAG	E	776	1	14,14,15	0.49	0	17,19,21	1.54	1 (5%)
5	NAG	A	789	1	14,14,15	0.52	0	17,19,21	0.86	1 (5%)
7	EDO	E	10	-	3,3,3	0.44	0	2,2,2	0.33	0
5	NAG	E	886	1	14,14,15	0.53	0	17,19,21	0.93	0
7	EDO	D	215	-	3,3,3	0.45	0	2,2,2	0.19	0
5	NAG	E	862	1	14,14,15	0.49	0	17,19,21	1.05	1 (5%)
6	MLA	H	215	-	6,6,6	3.45	5 (83%)	7,7,7	1.49	2 (28%)
5	NAG	A	900	1	14,14,15	0.47	0	17,19,21	1.04	2 (11%)
5	NAG	A	913	1	14,14,15	0.50	0	17,19,21	1.12	2 (11%)
6	MLA	B	186	-	6,6,6	3.40	5 (83%)	7,7,7	1.49	2 (28%)
5	NAG	E	801	1	14,14,15	0.49	0	17,19,21	1.27	2 (11%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	E	832	1	-	4/6/23/26	0/1/1/1
7	EDO	C	215	-	-	0/1/1/1	-
7	EDO	C	216	-	-	0/1/1/1	-
5	NAG	E	734	1	-	5/6/23/26	0/1/1/1
5	NAG	E	795	1	-	2/6/23/26	0/1/1/1
5	NAG	A	862	1	1/1/5/7	3/6/23/26	0/1/1/1
5	NAG	A	894	1	1/1/5/7	3/6/23/26	0/1/1/1
5	NAG	A	762	1	-	2/6/23/26	0/1/1/1
5	NAG	A	963	1	-	4/6/23/26	0/1/1/1
5	NAG	E	948	1	-	2/6/23/26	0/1/1/1
7	EDO	F	187	-	-	0/1/1/1	-
6	MLA	A	3	-	-	0/4/4/4	-
5	NAG	A	886	1	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	801	1	-	2/6/23/26	0/1/1/1
5	NAG	A	795	1	-	3/6/23/26	0/1/1/1
5	NAG	E	913	1	-	3/6/23/26	0/1/1/1
5	NAG	A	832	1	-	3/6/23/26	0/1/1/1
5	NAG	E	894	1	-	3/6/23/26	0/1/1/1
5	NAG	A	741	1	-	4/6/23/26	0/1/1/1
7	EDO	A	8	-	-	0/1/1/1	-
5	NAG	A	856	1	-	4/6/23/26	0/1/1/1
5	NAG	E	741	1	-	2/6/23/26	0/1/1/1
5	NAG	E	963	1	1/1/5/7	5/6/23/26	0/1/1/1
5	NAG	E	856	1	-	4/6/23/26	0/1/1/1
5	NAG	A	776	1	-	4/6/23/26	0/1/1/1
5	NAG	A	948	1	-	2/6/23/26	0/1/1/1
5	NAG	E	762	1	-	4/6/23/26	0/1/1/1
5	NAG	E	789	1	-	4/6/23/26	0/1/1/1
6	MLA	F	186	-	-	1/4/4/4	-
5	NAG	A	734	1	-	3/6/23/26	0/1/1/1
7	EDO	E	7	-	-	0/1/1/1	-
5	NAG	E	776	1	-	2/6/23/26	0/1/1/1
5	NAG	A	789	1	-	3/6/23/26	0/1/1/1
7	EDO	E	10	-	-	0/1/1/1	-
5	NAG	E	886	1	-	3/6/23/26	0/1/1/1
7	EDO	D	215	-	-	0/1/1/1	-
5	NAG	E	862	1	1/1/5/7	3/6/23/26	0/1/1/1
6	MLA	H	215	-	-	2/4/4/4	-
5	NAG	A	900	1	-	4/6/23/26	0/1/1/1
5	NAG	A	913	1	-	2/6/23/26	0/1/1/1
6	MLA	B	186	-	-	2/4/4/4	-
5	NAG	E	801	1	-	4/6/23/26	0/1/1/1

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	215	MLA	O1B-C1	5.95	1.41	1.22
6	F	186	MLA	O1B-C1	5.94	1.41	1.22
6	A	3	MLA	O1B-C1	5.92	1.41	1.22
6	B	186	MLA	O1B-C1	5.85	1.41	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	186	MLA	O1A-C1	-3.42	1.19	1.30

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	776	NAG	C1-O5-C5	5.27	119.25	112.19
5	A	741	NAG	C1-O5-C5	4.94	118.81	112.19
5	E	801	NAG	C1-O5-C5	4.24	117.86	112.19
5	A	862	NAG	C1-O5-C5	4.22	117.84	112.19
5	E	894	NAG	C1-O5-C5	4.21	117.83	112.19

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	862	NAG	C1
5	A	894	NAG	C1
5	E	862	NAG	C1
5	E	963	NAG	C1

5 of 104 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	734	NAG	C8-C7-N2-C2
5	A	734	NAG	O7-C7-N2-C2
5	A	741	NAG	O7-C7-N2-C2
5	A	762	NAG	C8-C7-N2-C2
5	A	762	NAG	O7-C7-N2-C2

There are no ring outliers.

13 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	862	NAG	2	0
5	A	894	NAG	4	0
5	A	963	NAG	1	0
5	E	913	NAG	1	0
5	A	832	NAG	1	0
5	A	776	NAG	2	0
5	E	762	NAG	1	0
5	E	789	NAG	3	0
5	A	734	NAG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	E	7	EDO	1	0
5	A	789	NAG	1	0
5	E	862	NAG	1	0
5	A	913	NAG	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	319/322 (99%)	-0.82	0 100 100	75, 116, 185, 255	0
1	E	312/322 (96%)	-0.84	0 100 100	81, 118, 177, 236	0
2	B	178/181 (98%)	-0.77	0 100 100	95, 163, 213, 229	0
2	F	179/181 (98%)	-0.77	0 100 100	96, 163, 213, 228	0
3	C	213/214 (99%)	-0.64	0 100 100	104, 189, 260, 275	0
3	G	213/214 (99%)	-0.64	0 100 100	103, 195, 262, 275	0
4	D	229/231 (99%)	-0.68	0 100 100	92, 157, 259, 288	0
4	H	229/231 (99%)	-0.61	0 100 100	97, 157, 265, 289	0
All	All	1872/1896 (98%)	-0.73	0 100 100	75, 147, 250, 289	0

There are no RSRZ outliers to report.

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	TYS	H	100	16/17	0.90	0.07	129,148,162,171	0
4	TYS	D	100	16/17	0.93	0.08	130,143,158,167	0
4	TYS	H	100(C)	16/17	0.96	0.06	97,111,132,175	0
4	TYS	D	100(C)	16/17	0.97	0.05	94,108,129,177	0

6.3 Carbohydrates [i](#)

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(Å ²)	Q<0.9
5	NAG	A	963	14/15	0.15	0.12	249,284,309,310	0
7	EDO	C	216	4/4	0.30	0.09	148,156,166,167	0
5	NAG	E	856	14/15	0.38	0.11	242,258,275,275	0
5	NAG	A	856	14/15	0.39	0.10	215,243,260,271	0
7	EDO	E	10	4/4	0.42	0.11	130,139,140,143	0
5	NAG	E	862	14/15	0.43	0.09	208,248,258,260	0
5	NAG	E	963	14/15	0.47	0.08	257,278,307,314	0
5	NAG	E	741	14/15	0.50	0.07	192,220,234,236	0
5	NAG	A	862	14/15	0.52	0.08	214,228,244,250	0
6	MLA	F	186	7/7	0.53	0.07	180,189,200,207	0
5	NAG	A	894	14/15	0.54	0.09	222,258,266,268	0
7	EDO	F	187	4/4	0.54	0.08	127,128,135,140	0
5	NAG	E	913	14/15	0.60	0.09	226,244,266,268	0
6	MLA	A	3	7/7	0.63	0.08	175,186,200,209	0
5	NAG	A	734	14/15	0.65	0.09	192,222,231,236	0
5	NAG	A	900	14/15	0.68	0.10	261,310,326,329	0
6	MLA	H	215	7/7	0.70	0.08	181,191,199,201	0
5	NAG	E	734	14/15	0.72	0.09	200,219,224,226	0
7	EDO	D	215	4/4	0.73	0.06	100,106,111,111	0
6	MLA	B	186	7/7	0.74	0.05	177,181,190,190	0
5	NAG	E	894	14/15	0.75	0.07	242,252,258,260	0
5	NAG	A	913	14/15	0.77	0.08	164,196,225,227	0
5	NAG	A	789	14/15	0.78	0.08	132,155,165,166	0
5	NAG	A	741	14/15	0.80	0.06	194,213,222,225	0
5	NAG	E	789	14/15	0.82	0.07	151,182,197,203	0
5	NAG	E	886	14/15	0.83	0.09	139,152,191,202	0
5	NAG	E	795	14/15	0.83	0.10	119,138,146,153	0
5	NAG	E	801	14/15	0.85	0.07	127,177,189,190	0
7	EDO	E	7	4/4	0.86	0.06	127,135,139,146	0
5	NAG	A	801	14/15	0.86	0.07	134,181,187,191	0
7	EDO	C	215	4/4	0.86	0.05	122,127,130,130	0
5	NAG	A	886	14/15	0.87	0.07	131,151,182,189	0
5	NAG	A	776	14/15	0.88	0.05	137,161,180,185	0
5	NAG	E	776	14/15	0.89	0.06	128,140,175,175	0
7	EDO	A	8	4/4	0.90	0.05	153,153,154,156	0
5	NAG	E	948	14/15	0.91	0.05	116,153,161,163	0
5	NAG	A	948	14/15	0.92	0.06	124,141,149,156	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	NAG	A	795	14/15	0.92	0.06	89,122,133,145	0
5	NAG	E	832	14/15	0.92	0.09	138,157,187,188	0
5	NAG	A	832	14/15	0.94	0.09	145,167,199,205	0
5	NAG	A	762	14/15	0.96	0.06	73,97,118,127	0
5	NAG	E	762	14/15	0.97	0.05	88,103,115,119	0

6.5 Other polymers [i](#)

There are no such residues in this entry.