



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 01:54 AM GMT

PDB ID : 2QAD
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 full wwPDB validation 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/ValidationPDFNotes.html>

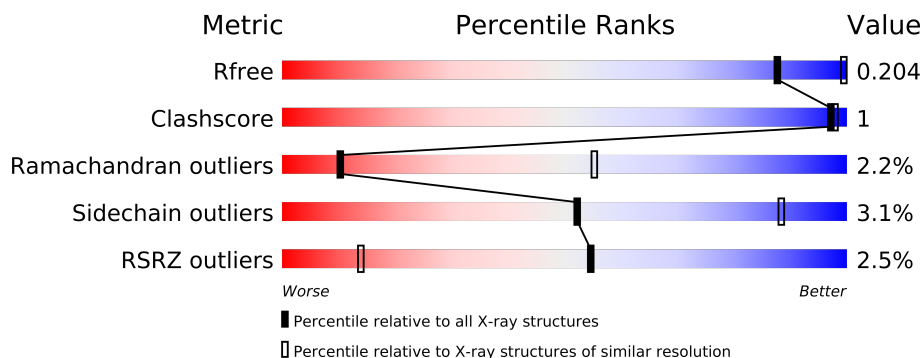
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	1341 (3.40-3.20)
Clashscore	79885	1696 (3.40-3.20)
Ramachandran outliers	78287	1664 (3.40-3.20)
Sidechain outliers	78261	1662 (3.40-3.20)
RSRZ outliers	66119	1342 (3.40-3.20)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	322	
1	E	322	
2	B	181	
2	F	181	
3	C	214	
3	G	214	
4	D	231	
4	H	231	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 14987 atoms, of which 0 are hydrogen and 0 are deuterium.

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



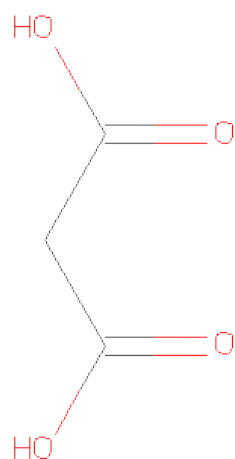
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1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

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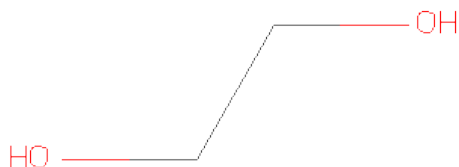
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	E	1	Total	C	N	O	0	0
			14	8	1	5		
5	E	1	Total	C	N	O	0	0
			14	8	1	5		
5	E	1	Total	C	N	O	0	0
			14	8	1	5		
5	E	1	Total	C	N	O	0	0
			14	8	1	5		
5	E	1	Total	C	N	O	0	0
			14	8	1	5		
5	E	1	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		
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 (three-letter code: MLA) (formula: C₃H₄O₄).



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

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



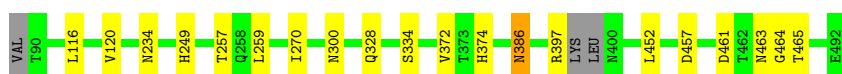
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	D	1	Total 4	C 2	O 2	0	0
7	F	1	Total 4	C 2	O 2	0	0
7	E	1	Total 4	C 2	O 2	0	0
7	A	1	Total 4	C 2	O 2	0	0
7	C	1	Total 4	C 2	O 2	0	0
7	E	1	Total 4	C 2	O 2	0	0
7	C	1	Total 4	C 2	O 2	0	0

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: Envelope glycoprotein gp160

Chain A: 



- Molecule 1: Envelope glycoprotein gp160

Chain E: 



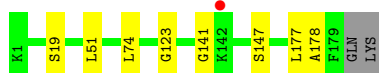
- Molecule 2: T-cell surface glycoprotein CD4

Chain B: 



- Molecule 2: T-cell surface glycoprotein CD4

Chain F: 



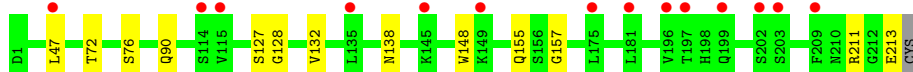
- Molecule 3: anti-HIV-1 antibody 412d light chain

Chain C: 



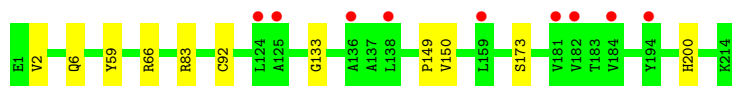
- Molecule 3: anti-HIV-1 antibody 412d light chain

Chain G: 



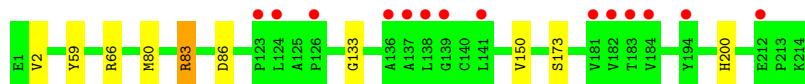
- Molecule 4: anti-HIV-1 antibody 412d heavy chain

Chain D: 



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

Chain H: 



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 49.15 – 3.31	Depositor EDS
% Data completeness (in resolution range)	66.7 (20.00-3.30) 66.4 (49.15-3.31)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.41 (at 3.33Å)	Xtriage
Refinement program	CNS/PHENIX	Depositor
R, R_{free}	0.202 , 0.269 0.205 , 0.204	Depositor DCC
R_{free} test set	1278 reflections (5.02%)	DCC
Wilson B-factor (Å ²)	93.1	Xtriage
Anisotropy	0.605	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 103.0	EDS
Estimated twinning fraction	0.034 for h,-k,-h-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 25482 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	14987	wwPDB-VP
Average B, all atoms (Å ²)	157.0	wwPDB-VP

Xtriage'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.

5 Model quality

5.1 Standard geometry

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

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	0.28	0/2546	0.47	0/3446
1	E	0.28	0/2493	0.46	0/3376
2	B	0.25	0/1402	0.44	0/1891
2	F	0.25	0/1414	0.45	0/1907
3	C	0.24	0/1677	0.41	0/2273
3	G	0.25	0/1677	0.42	0/2273
4	D	0.25	0/1757	0.43	0/2393
4	H	0.25	0/1757	0.43	0/2393
All	All	0.26	0/14723	0.44	0/19952

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2499	0	0	4	0
1	E	2445	0	0	1	0
2	B	1383	0	0	2	0
2	F	1394	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1642	0	0	0	0
3	G	1642	0	0	0	0
4	D	1746	0	0	3	0
4	H	1746	0	0	3	0
5	A	224	0	0	1	0
5	E	210	0	0	0	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	0	0
7	F	4	0	6	0	0
All	All	14987	0	54	13	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 1.

All (13) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:397:ARG:CA	1:A:397:ARG:CG	2.54	0.85
4:H:66:ARG:CZ	4:H:83:ARG:NH1	2.56	0.69
4:D:66:ARG:NH1	4:D:83:ARG:CZ	2.67	0.58
2:B:134:ARG:NH2	2:B:152:GLN:O	2.42	0.52
4:D:6:GLN:NE2	4:D:92:CYS:N	2.60	0.49
4:D:66:ARG:NH1	4:D:83:ARG:NH2	2.61	0.49
2:B:134:ARG:NH2	2:B:152:GLN:CB	2.76	0.49
1:A:257:THR:O	1:A:259:LEU:N	2.48	0.47
1:E:257:THR:O	1:E:259:LEU:N	2.47	0.47
1:A:463:ASN:OD1	5:A:963:NAG:O5	2.31	0.47
4:H:83:ARG:NH2	4:H:86:ASP:OD2	2.51	0.43
4:H:66:ARG:NE	4:H:83:ARG:NH1	2.66	0.43
1:A:457:ASP:OD1	1:A:457:ASP:N	2.54	0.41

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	315/322 (98%)	275 (87%)	34 (11%)	6 (2%)	12	60
1	E	308/322 (96%)	270 (88%)	32 (10%)	6 (2%)	12	60
2	B	176/181 (97%)	152 (86%)	20 (11%)	4 (2%)	10	54
2	F	177/181 (98%)	152 (86%)	20 (11%)	5 (3%)	8	48
3	C	211/214 (99%)	176 (83%)	30 (14%)	5 (2%)	9	53
3	G	211/214 (99%)	174 (82%)	32 (15%)	5 (2%)	9	53
4	D	227/231 (98%)	185 (82%)	37 (16%)	5 (2%)	10	55
4	H	227/231 (98%)	184 (81%)	38 (17%)	5 (2%)	10	55
All	All	1852/1896 (98%)	1568 (85%)	243 (13%)	41 (2%)	10	55

All (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
4	H	150	VAL
1	A	386	ASN
3	C	76	SER
4	D	173	SER
1	E	386	ASN
4	H	173	SER
1	A	116	LEU
1	A	374	HIS
1	A	464	GLY
2	B	19	SER
4	D	133	GLY
4	D	200	HIS
1	E	116	LEU
1	E	374	HIS

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Mol	Chain	Res	Type
1	E	464	GLY
2	F	19	SER
2	F	178	ALA
3	G	76	SER
4	H	133	GLY
4	H	200	HIS
1	A	120	VAL
3	C	127	SER
3	C	138	ASN
3	G	127	SER
3	G	138	ASN
1	A	461	ASP
3	C	128	GLY
1	E	120	VAL
1	E	461	ASP
3	G	128	GLY
2	B	141	GLY
2	F	141	GLY
2	B	123	GLY
3	C	157	GLY
2	F	123	GLY
3	G	157	GLY

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	281/285 (99%)	271 (96%)	10 (4%)	47	85
1	E	276/285 (97%)	260 (94%)	16 (6%)	28	73
2	B	161/164 (98%)	157 (98%)	4 (2%)	60	91
2	F	162/164 (99%)	159 (98%)	3 (2%)	69	93
3	C	188/189 (100%)	183 (97%)	5 (3%)	57	90
3	G	188/189 (100%)	180 (96%)	8 (4%)	40	82
4	D	192/192 (100%)	190 (99%)	2 (1%)	85	96
4	H	192/192 (100%)	189 (98%)	3 (2%)	75	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1640/1660 (99%)	1589 (97%)	51 (3%)	52 88

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	234	ASN
1	A	249	HIS
1	A	270	ILE
1	A	300	ASN
1	A	328	GLN
1	A	334	SER
1	A	372	VAL
1	A	386	ASN
1	A	452	LEU
1	A	465	THR
2	B	51	LEU
2	B	74	LEU
2	B	109	LEU
2	B	177	LEU
3	C	47	LEU
3	C	50	LYS
3	C	72	THR
3	C	132	VAL
3	C	158	ASN
4	D	59	TYR
4	D	149	PRO
1	E	119	CYS
1	E	234	ASN
1	E	243	SER
1	E	249	HIS
1	E	270	ILE
1	E	300	ASN
1	E	328	GLN
1	E	334	SER
1	E	352	GLN
1	E	393	TRP
1	E	394	ASN
1	E	416	LEU
1	E	447	SER
1	E	452	LEU
1	E	456	ARG
1	E	465	THR

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Mol	Chain	Res	Type
2	F	51	LEU
2	F	74	LEU
2	F	177	LEU
3	G	47	LEU
3	G	72	THR
3	G	90	GLN
3	G	132	VAL
3	G	148	TRP
3	G	155	GLN
3	G	211	ARG
3	G	213	GLU
4	H	59	TYR
4	H	80	MET
4	H	83	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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	D	100	4	16,16,17	4.61	4 (25%)	20,22,24	0.92	1 (5%)
4	TYS	D	100(C)	4	16,16,17	4.55	3 (18%)	20,22,24	0.99	1 (5%)
4	TYS	H	100	4	16,16,17	4.63	4 (25%)	20,22,24	0.91	1 (5%)
4	TYS	H	100(C)	4	16,16,17	4.51	3 (18%)	20,22,24	0.98	1 (5%)

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	D	100	4	-	0/9/11/13	0/1/1/1
4	TYS	D	100(C)	4	-	0/9/11/13	0/1/1/1
4	TYS	H	100	4	-	0/9/11/13	0/1/1/1
4	TYS	H	100(C)	4	-	0/9/11/13	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	100	TYS	O-C	17.71	1.23	1.11
4	D	100	TYS	O-C	17.66	1.23	1.11
4	D	100(C)	TYS	O-C	17.35	1.23	1.11
4	H	100(C)	TYS	O-C	17.19	1.23	1.11
4	D	100(C)	TYS	OH-CZ	-3.59	1.38	1.42
4	H	100(C)	TYS	OH-CZ	-3.55	1.38	1.42
4	D	100	TYS	OH-CZ	-3.25	1.38	1.42
4	H	100	TYS	OH-CZ	-3.22	1.38	1.42
4	H	100(C)	TYS	CA-C	2.78	1.53	1.48
4	D	100(C)	TYS	CA-C	2.78	1.53	1.48
4	H	100	TYS	CA-C	2.63	1.53	1.48
4	D	100	TYS	CA-C	2.58	1.53	1.48
4	D	100	TYS	O1-S	2.07	1.52	1.45
4	H	100	TYS	O1-S	2.04	1.52	1.45

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	100(C)	TYS	CZ-OH-S	-3.66	113.49	118.98
4	H	100(C)	TYS	CZ-OH-S	-3.66	113.49	118.98
4	D	100	TYS	CZ-OH-S	-3.04	114.41	118.98
4	H	100	TYS	CZ-OH-S	-3.02	114.44	118.98

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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$
6	MLA	A	3	-	6,6,6	3.28	5 (83%)	7,7,7	1.31	0
5	NAG	A	734	1	12,14,15	0.64	0	15,19,21	0.85	1 (6%)
5	NAG	A	741	1	12,14,15	0.67	1 (8%)	15,19,21	0.98	1 (6%)
5	NAG	A	762	1	12,14,15	0.61	0	15,19,21	0.90	1 (6%)
5	NAG	A	776	1	12,14,15	0.61	0	15,19,21	0.90	1 (6%)
5	NAG	A	789	1	12,14,15	0.66	1 (8%)	15,19,21	0.70	0
5	NAG	A	795	1	12,14,15	0.71	1 (8%)	15,19,21	0.83	2 (13%)
7	EDO	A	8	-	3,3,3	0.53	0	2,2,2	0.35	0
5	NAG	A	801	1	12,14,15	0.66	1 (8%)	15,19,21	0.71	0
5	NAG	A	832	1	12,14,15	0.63	0	15,19,21	0.60	0
5	NAG	A	856	1	12,14,15	0.62	0	15,19,21	0.91	1 (6%)
5	NAG	A	862	1	12,14,15	0.85	1 (8%)	15,19,21	1.38	2 (13%)
5	NAG	A	886	1	12,14,15	0.65	0	15,19,21	0.88	0
5	NAG	A	894	1	12,14,15	0.56	0	15,19,21	0.85	1 (6%)
5	NAG	A	900	1	12,14,15	0.60	0	15,19,21	1.41	4 (26%)
5	NAG	A	913	1	12,14,15	0.57	0	15,19,21	0.93	1 (6%)
5	NAG	A	948	1	12,14,15	0.67	0	15,19,21	0.83	1 (6%)
5	NAG	A	963	1	12,14,15	0.62	0	15,19,21	0.78	0
6	MLA	B	186	-	6,6,6	3.18	5 (83%)	7,7,7	1.32	0
7	EDO	C	215	-	3,3,3	0.54	0	2,2,2	0.31	0
7	EDO	C	216	-	3,3,3	0.54	0	2,2,2	0.35	0
7	EDO	D	215	-	3,3,3	0.56	0	2,2,2	0.17	0
7	EDO	E	10	-	3,3,3	0.55	0	2,2,2	0.33	0
7	EDO	E	7	-	3,3,3	0.52	0	2,2,2	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	E	734	1	12,14,15	0.66	1 (8%)	15,19,21	0.65	0
5	NAG	E	741	1	12,14,15	0.64	0	15,19,21	0.83	1 (6%)
5	NAG	E	762	1	12,14,15	0.61	0	15,19,21	0.86	0
5	NAG	E	776	1	12,14,15	0.54	0	15,19,21	1.00	1 (6%)
5	NAG	E	789	1	12,14,15	0.64	0	15,19,21	0.99	1 (6%)
5	NAG	E	795	1	12,14,15	0.70	1 (8%)	15,19,21	1.05	1 (6%)
5	NAG	E	801	1	12,14,15	0.60	0	15,19,21	0.65	0
5	NAG	E	832	1	12,14,15	0.70	1 (8%)	15,19,21	0.73	0
5	NAG	E	856	1	12,14,15	0.67	0	15,19,21	1.12	1 (6%)
5	NAG	E	862	1	12,14,15	0.55	0	15,19,21	0.99	2 (13%)
5	NAG	E	886	1	12,14,15	0.71	1 (8%)	15,19,21	0.82	0
5	NAG	E	894	1	12,14,15	0.62	0	15,19,21	0.90	1 (6%)
5	NAG	E	913	1	12,14,15	0.57	0	15,19,21	0.78	0
5	NAG	E	948	1	12,14,15	0.62	0	15,19,21	0.87	0
5	NAG	E	963	1	12,14,15	0.69	1 (8%)	15,19,21	1.36	3 (20%)
6	MLA	F	186	-	6,6,6	3.24	5 (83%)	7,7,7	1.68	1 (14%)
7	EDO	F	187	-	3,3,3	0.55	0	2,2,2	0.28	0
6	MLA	H	215	-	6,6,6	3.24	5 (83%)	7,7,7	1.33	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
6	MLA	A	3	-	-	0/4/4/4	0/0/0/0
5	NAG	A	734	1	-	0/6/23/26	0/1/1/1
5	NAG	A	741	1	-	0/6/23/26	0/1/1/1
5	NAG	A	762	1	-	0/6/23/26	0/1/1/1
5	NAG	A	776	1	-	0/6/23/26	0/1/1/1
5	NAG	A	789	1	-	1/6/23/26	0/1/1/1
5	NAG	A	795	1	-	0/6/23/26	0/1/1/1
7	EDO	A	8	-	-	0/1/1/1	0/0/0/0
5	NAG	A	801	1	-	2/6/23/26	0/1/1/1
5	NAG	A	832	1	-	1/6/23/26	0/1/1/1
5	NAG	A	856	1	-	0/6/23/26	0/1/1/1
5	NAG	A	862	1	1/1/5/7	0/6/23/26	0/1/1/1
5	NAG	A	886	1	-	0/6/23/26	0/1/1/1
5	NAG	A	894	1	1/1/5/7	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	900	1	-	1/6/23/26	0/1/1/1
5	NAG	A	913	1	-	0/6/23/26	0/1/1/1
5	NAG	A	948	1	-	0/6/23/26	0/1/1/1
5	NAG	A	963	1	-	0/6/23/26	0/1/1/1
6	MLA	B	186	-	-	0/4/4/4	0/0/0/0
7	EDO	C	215	-	-	0/1/1/1	0/0/0/0
7	EDO	C	216	-	-	0/1/1/1	0/0/0/0
7	EDO	D	215	-	-	0/1/1/1	0/0/0/0
7	EDO	E	10	-	-	0/1/1/1	0/0/0/0
7	EDO	E	7	-	-	0/1/1/1	0/0/0/0
5	NAG	E	734	1	-	0/6/23/26	0/1/1/1
5	NAG	E	741	1	-	0/6/23/26	0/1/1/1
5	NAG	E	762	1	-	0/6/23/26	0/1/1/1
5	NAG	E	776	1	-	0/6/23/26	0/1/1/1
5	NAG	E	789	1	-	0/6/23/26	0/1/1/1
5	NAG	E	795	1	-	0/6/23/26	0/1/1/1
5	NAG	E	801	1	-	0/6/23/26	0/1/1/1
5	NAG	E	832	1	-	0/6/23/26	0/1/1/1
5	NAG	E	856	1	-	0/6/23/26	0/1/1/1
5	NAG	E	862	1	1/1/5/7	0/6/23/26	0/1/1/1
5	NAG	E	886	1	-	0/6/23/26	0/1/1/1
5	NAG	E	894	1	-	0/6/23/26	0/1/1/1
5	NAG	E	913	1	-	2/6/23/26	1/1/1/1
5	NAG	E	948	1	-	0/6/23/26	0/1/1/1
5	NAG	E	963	1	1/1/5/7	0/6/23/26	0/1/1/1
6	MLA	F	186	-	-	0/4/4/4	0/0/0/0
7	EDO	F	187	-	-	0/1/1/1	0/0/0/0
6	MLA	H	215	-	-	0/4/4/4	0/0/0/0

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	215	MLA	O1B-C1	5.42	1.41	1.22
6	F	186	MLA	O1B-C1	5.41	1.41	1.22
6	A	3	MLA	O1B-C1	5.39	1.41	1.22
6	B	186	MLA	O1B-C1	5.33	1.41	1.22
6	A	3	MLA	O3B-C3	3.06	1.41	1.30
6	F	186	MLA	O3B-C3	3.03	1.41	1.30
6	B	186	MLA	O1A-C1	-3.03	1.19	1.30
6	B	186	MLA	O3B-C3	3.02	1.41	1.30
6	F	186	MLA	O1A-C1	-3.01	1.19	1.30
6	H	215	MLA	O3B-C3	2.98	1.41	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	3	MLA	O1A-C1	-2.97	1.19	1.30
6	H	215	MLA	O1A-C1	-2.97	1.19	1.30
6	A	3	MLA	C2-C1	2.95	1.55	1.51
6	A	3	MLA	C2-C3	2.86	1.55	1.51
6	H	215	MLA	C2-C1	2.83	1.55	1.51
6	F	186	MLA	C2-C1	2.80	1.55	1.51
6	H	215	MLA	C2-C3	2.69	1.55	1.51
6	F	186	MLA	C2-C3	2.68	1.55	1.51
6	B	186	MLA	C2-C1	2.67	1.55	1.51
6	B	186	MLA	C2-C3	2.50	1.54	1.51
5	A	862	NAG	O5-C5	-2.28	1.41	1.45
5	E	886	NAG	O5-C5	-2.22	1.41	1.45
5	E	832	NAG	O5-C5	-2.15	1.41	1.45
5	E	963	NAG	O5-C5	-2.12	1.41	1.45
5	E	795	NAG	O5-C5	-2.12	1.41	1.45
5	A	741	NAG	O5-C5	-2.08	1.41	1.45
5	A	789	NAG	O5-C5	-2.06	1.41	1.45
5	E	734	NAG	O5-C5	-2.03	1.41	1.45
5	A	795	NAG	O5-C5	-2.03	1.41	1.45
5	A	801	NAG	O5-C5	-2.02	1.41	1.45

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	186	MLA	O1A-C1-O1B	-3.42	114.60	123.30
5	E	856	NAG	O5-C5-C6	3.39	110.54	106.98
5	E	963	NAG	O5-C5-C6	3.38	110.53	106.98
5	A	862	NAG	O5-C5-C6	3.36	110.51	106.98
5	A	862	NAG	C3-C2-N2	-3.28	106.77	111.76
5	E	789	NAG	O5-C5-C6	3.11	110.24	106.98
5	E	795	NAG	O5-C5-C6	3.07	110.20	106.98
5	A	900	NAG	O5-C5-C6	2.98	110.11	106.98
5	A	856	NAG	O5-C5-C6	2.83	109.95	106.98
5	E	963	NAG	C3-C2-N2	-2.61	107.79	111.76
5	A	913	NAG	O5-C5-C6	2.60	109.71	106.98
5	A	741	NAG	C3-C2-N2	-2.53	107.90	111.76
5	A	948	NAG	O5-C5-C6	2.52	109.63	106.98
5	E	741	NAG	O5-C5-C6	2.50	109.61	106.98
5	A	762	NAG	O5-C5-C6	2.48	109.58	106.98
5	A	894	NAG	O5-C5-C6	2.46	109.56	106.98
5	E	862	NAG	C3-C2-N2	-2.39	108.12	111.76
5	A	734	NAG	O5-C5-C6	2.33	109.43	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	894	NAG	O5-C5-C6	2.33	109.42	106.98
5	A	776	NAG	O5-C5-C6	2.28	109.38	106.98
5	E	776	NAG	O5-C5-C6	2.28	109.37	106.98
5	A	900	NAG	C3-C2-N2	-2.25	108.34	111.76
5	A	900	NAG	C3-C4-C5	2.21	114.16	110.20
5	E	862	NAG	O5-C5-C6	2.17	109.26	106.98
5	A	900	NAG	C6-C5-C4	-2.16	107.77	113.00
5	E	963	NAG	O5-C5-C4	-2.10	107.99	110.65
5	A	795	NAG	O5-C5-C6	2.07	109.15	106.98
5	A	795	NAG	C3-C2-N2	-2.02	108.68	111.76

All (4) chirality outliers are listed below:

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

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	789	NAG	C3-C2-N2-C7
5	E	913	NAG	C8-C7-N2-C2
5	A	801	NAG	O7-C7-N2-C2
5	E	913	NAG	O7-C7-N2-C2
5	A	801	NAG	C8-C7-N2-C2
5	A	832	NAG	O7-C7-N2-C2
5	A	900	NAG	O7-C7-N2-C2

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	913	NAG	C1-C2-C3-C4-C5-O5

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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(Å²)	Q<0.9	
1	A	319/322 (99%)	-0.03	0	100	100	75, 116, 185, 255	0
1	E	312/322 (96%)	-0.05	0	100	100	81, 118, 177, 236	0
2	B	178/181 (98%)	0.02	0	100	100	95, 163, 213, 229	0
2	F	179/181 (98%)	0.08	1 (0%)	86	46	96, 163, 213, 228	0
3	C	213/214 (99%)	0.21	4 (1%)	64	20	104, 189, 260, 275	0
3	G	213/214 (99%)	0.39	14 (6%)	18	4	103, 195, 262, 275	0
4	D	231/231 (100%)	0.21	9 (3%)	37	8	92, 154, 259, 288	0
4	H	231/231 (100%)	0.24	14 (6%)	21	5	97, 157, 265, 289	0
All	All	1876/1896 (98%)	0.12	42 (2%)	54	16	75, 147, 250, 289	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	125	ALA	5.2
4	D	159	LEU	4.8
4	H	183	THR	4.1
4	H	194	TYR	4.1
3	G	197	THR	4.0
3	C	115	VAL	3.9
4	D	194	TYR	3.8
3	C	134	CYS	3.8
2	F	142	LYS	3.7
3	G	145	LYS	3.4
4	D	138	LEU	3.3
4	H	138	LEU	3.2
4	H	136	ALA	3.2
3	G	114	SER	3.1
4	H	123	PRO	3.0
4	H	137	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
3	G	115	VAL	2.9
4	D	136	ALA	2.9
4	H	124	LEU	2.8
3	G	209	PHE	2.8
4	H	126	PRO	2.7
3	G	181	LEU	2.6
4	H	212	GLU	2.5
3	G	47	LEU	2.5
4	D	184	VAL	2.4
3	G	135	LEU	2.4
4	D	182	VAL	2.3
4	H	182	VAL	2.3
4	D	124	LEU	2.3
3	G	196	VAL	2.3
3	G	149	LYS	2.3
3	C	73	LEU	2.2
4	H	141	LEU	2.2
4	H	181	VAL	2.2
3	G	203	SER	2.2
3	G	175	LEU	2.2
4	H	184	VAL	2.2
4	H	139	GLY	2.1
4	D	181	VAL	2.1
3	C	186	TYR	2.1
3	G	202	SER	2.1
3	G	199	GLN	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. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	TYS	H	100	16/17	0.18	-	129,148,162,171	0
4	TYS	H	100(C)	16/17	0.19	-	97,111,132,175	0
4	TYS	D	100	16/17	0.22	-	130,143,158,167	0
4	TYS	D	100(C)	16/17	0.19	-	94,108,129,177	0

6.3 Carbohydrates ⓘ

There are no carbohydrates 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. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	NAG	A	762	14/15	0.26	-	73,97,118,127	0
7	EDO	D	215	4/4	0.17	-	100,106,111,111	0
5	NAG	A	963	14/15	0.80	-	249,284,309,310	0
5	NAG	E	762	14/15	0.27	-	88,103,115,119	0
5	NAG	A	948	14/15	0.20	-	124,141,149,156	0
6	MLA	A	3	7/7	0.52	-	175,186,200,209	0
5	NAG	E	948	14/15	0.18	-	116,153,161,163	0
5	NAG	E	894	14/15	0.76	-	242,252,258,260	0
5	NAG	A	789	14/15	0.12	-	132,155,165,166	0
7	EDO	C	216	4/4	0.39	-	148,156,166,167	0
5	NAG	A	913	14/15	0.33	-	164,196,225,227	0
5	NAG	A	776	14/15	0.17	-	137,161,180,185	0
7	EDO	F	187	4/4	0.44	-	127,128,135,140	0
5	NAG	A	862	14/15	0.71	-	214,228,244,250	0
5	NAG	E	913	14/15	0.35	-	226,244,266,268	0
5	NAG	E	886	14/15	0.25	-	139,152,191,202	0
6	MLA	H	215	7/7	0.47	-	181,191,199,201	0
5	NAG	A	795	14/15	0.17	-	89,122,133,145	0
5	NAG	A	856	14/15	0.50	-	215,243,260,271	0
5	NAG	E	789	14/15	0.13	-	151,182,197,203	0
5	NAG	E	734	14/15	0.23	-	200,219,224,226	0
5	NAG	A	734	14/15	0.19	-	192,222,231,236	0
5	NAG	E	776	14/15	0.17	-	128,140,175,175	0
7	EDO	C	215	4/4	0.34	-	122,127,130,130	0
5	NAG	A	801	14/15	0.24	-	134,181,187,191	0
5	NAG	E	862	14/15	0.92	-	208,248,258,260	0
5	NAG	A	741	14/15	0.27	-	194,213,222,225	0
5	NAG	E	741	14/15	0.41	-	192,220,234,236	0
6	MLA	B	186	7/7	0.29	-	177,181,190,190	0
5	NAG	A	832	14/15	0.25	-	145,167,199,205	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
7	EDO	E	10	4/4	0.19	-	130,139,140,143	0
7	EDO	E	7	4/4	0.25	-	127,135,139,146	0
5	NAG	E	963	14/15	0.51	-	257,278,307,314	0
5	NAG	E	795	14/15	0.18	-	119,138,146,153	0
5	NAG	E	856	14/15	0.54	-	242,258,275,275	0
5	NAG	E	832	14/15	0.23	-	138,157,187,188	0
5	NAG	A	886	14/15	0.19	-	131,151,182,189	0
5	NAG	A	900	14/15	1.25	-	261,310,326,329	0
6	MLA	F	186	7/7	0.34	-	180,189,200,207	0
5	NAG	A	894	14/15	0.92	-	222,258,266,268	0
7	EDO	A	8	4/4	0.26	-	153,153,154,156	0
5	NAG	E	801	14/15	0.24	-	127,177,189,190	0

6.5 Other polymers

There are no such residues in this entry.