Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2023 – 12:06 AM EDT

PDB ID	:	7LPW
Title	:	Crystal Structure of HIV-1 RT in Complex with NBD-14189
Authors	:	Losada, N.; Ruiz, F.X.; Arnold, E.
Deposited on	:	2021-02-12
Resolution	:	2.32 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1
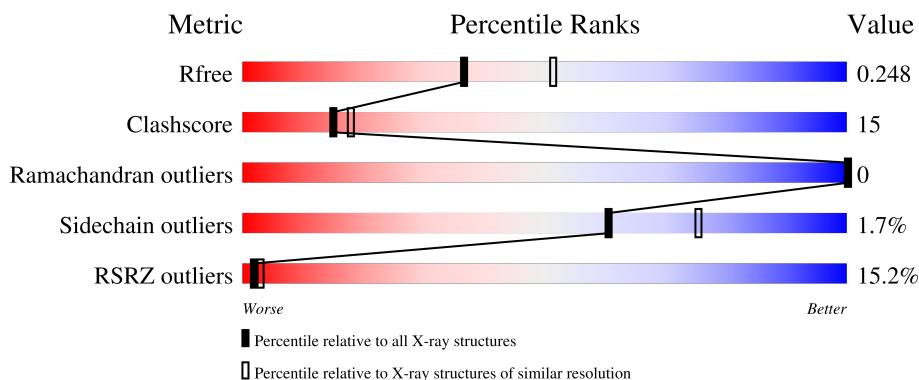
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION
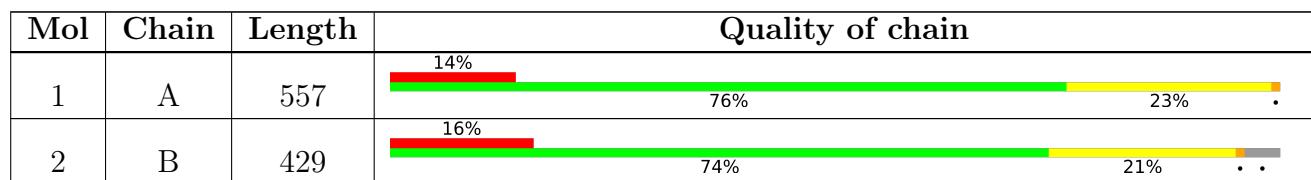
The reported resolution of this entry is 2.32 Å.

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}	130704	5974 (2.34-2.30)
Clashscore	141614	6604 (2.34-2.30)
Ramachandran outliers	138981	6523 (2.34-2.30)
Sidechain outliers	138945	6523 (2.34-2.30)
RSRZ outliers	127900	5855 (2.34-2.30)

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 <=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	557	14% ... 76% 23% ·
2	B	429	16% ... 74% 21% · ·

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	A	601	-	-	X	-
3	SO4	B	501	-	-	X	-
3	SO4	B	502	-	-	X	-

2 Entry composition ⓘ

There are 7 unique types of molecules in this entry. The entry contains 8129 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 Reverse transcriptase p66.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	556	4512	2920	749	835	8	0	0	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	initiating methionine	UNP P03366
A	0	VAL	-	expression tag	UNP P03366
A	172	ALA	LYS	engineered mutation	UNP P03366
A	173	ALA	LYS	engineered mutation	UNP P03366
A	280	SER	CYS	engineered mutation	UNP P03366
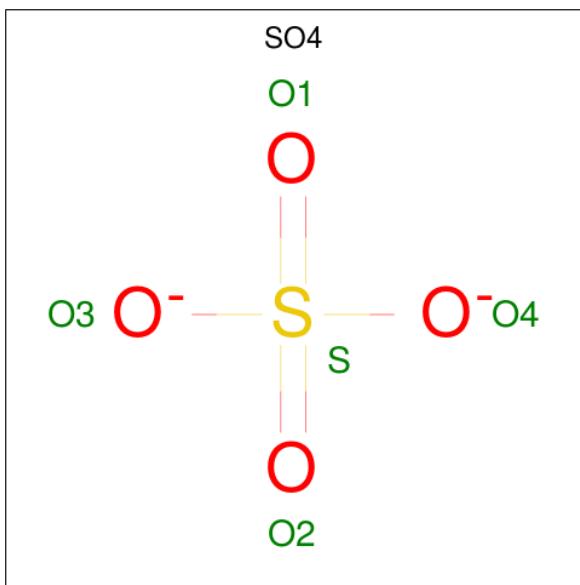
- Molecule 2 is a protein called Reverse transcriptase p51.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	412	3409	2220	564	618	7	0	0	0

There are 2 discrepancies between the modelled and reference sequences:
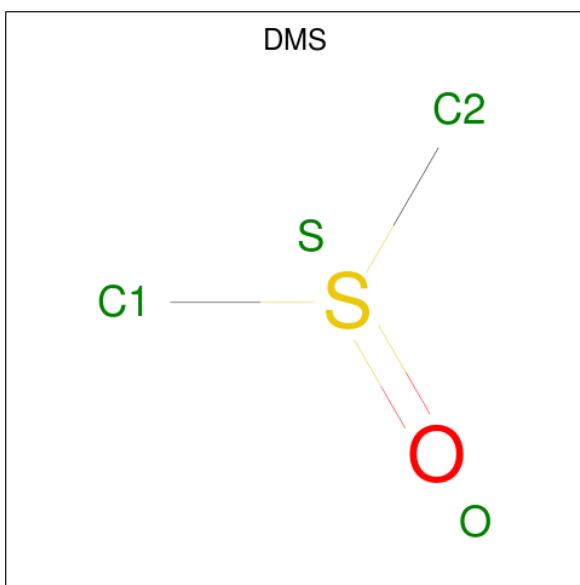
Chain	Residue	Modelled	Actual	Comment	Reference
B	0	GLY	-	expression tag	UNP P03366
B	280	SER	CYS	engineered mutation	UNP P03366

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

SO4

O1

O

O3 O⁻ — S — O⁻ O4

S

O

O2
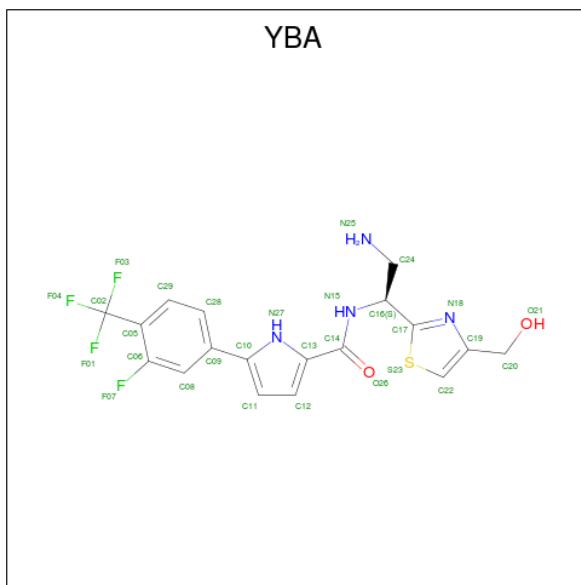
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 5	O 4	S 1	0	0
3	A	1	Total 5	O 4	S 1	0	0
3	B	1	Total 5	O 4	S 1	0	0
3	B	1	Total 5	O 4	S 1	0	0

- Molecule 4 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).

DMS

C2

S

C1 — S

O

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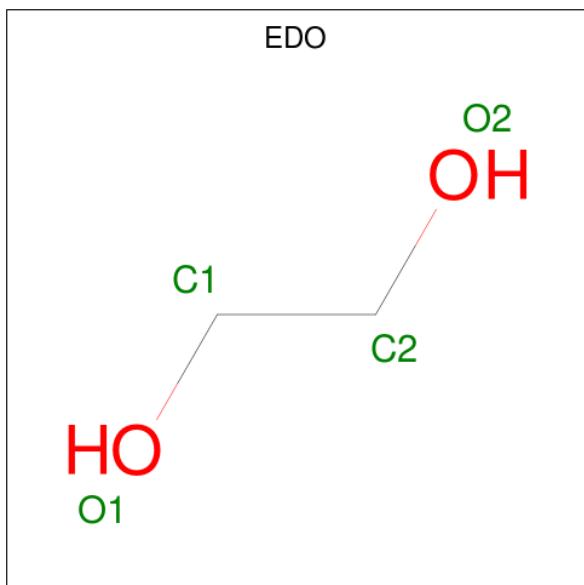
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total 4	C 2	O 1	S 1	0	0
4	A	1	Total 4	C 2	O 1	S 1	0	0
4	B	1	Total 4	C 2	O 1	S 1	0	0

- Molecule 5 is {N}-[(1 {S})-2-azanyl-1-[4-(hydroxymethyl)-1,3-thiazol-2-yl]ethyl]-5-[3-fluoranyl-4-(trifluoromethyl)phenyl]-1 {H}-pyrrole-2-carboxamide (three-letter code: YBA) (formula: $C_{18}H_{16}F_4N_4O_2S$) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total 29	C 18	F 4	N 4	O 2	S 1	0	0

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).

EDO

O2

OH

C1

C2

HO

O1

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total 4	C 2	O 2	0	0
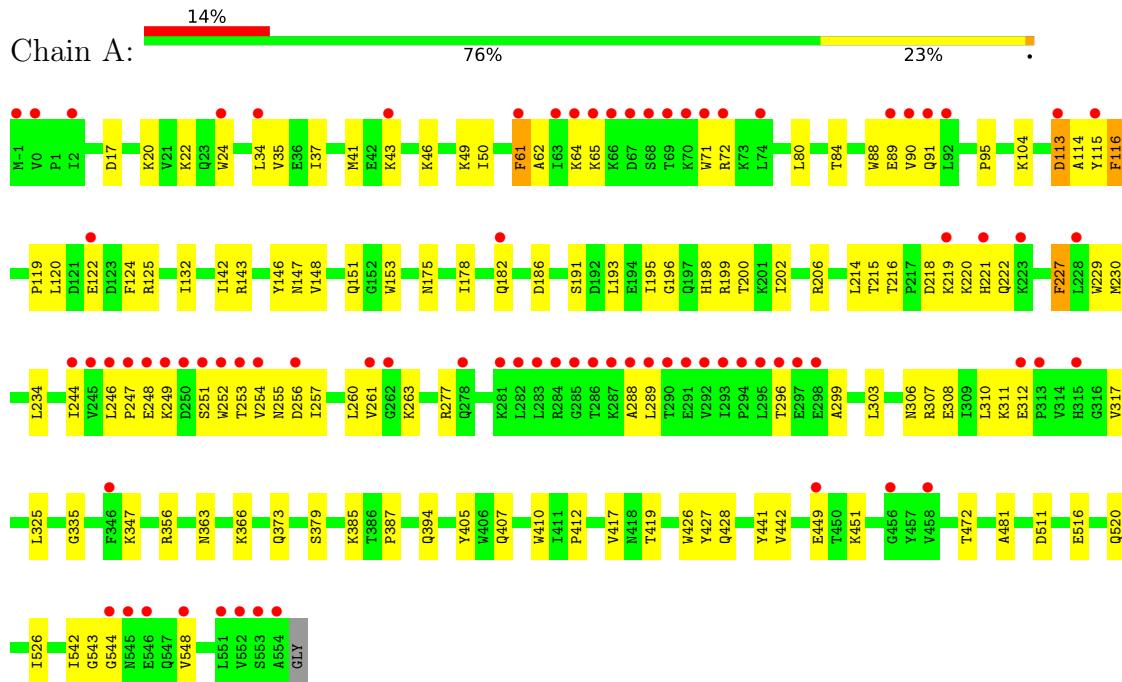
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	71	Total 71	O 71	0	0
7	B	72	Total 72	O 72	0	0
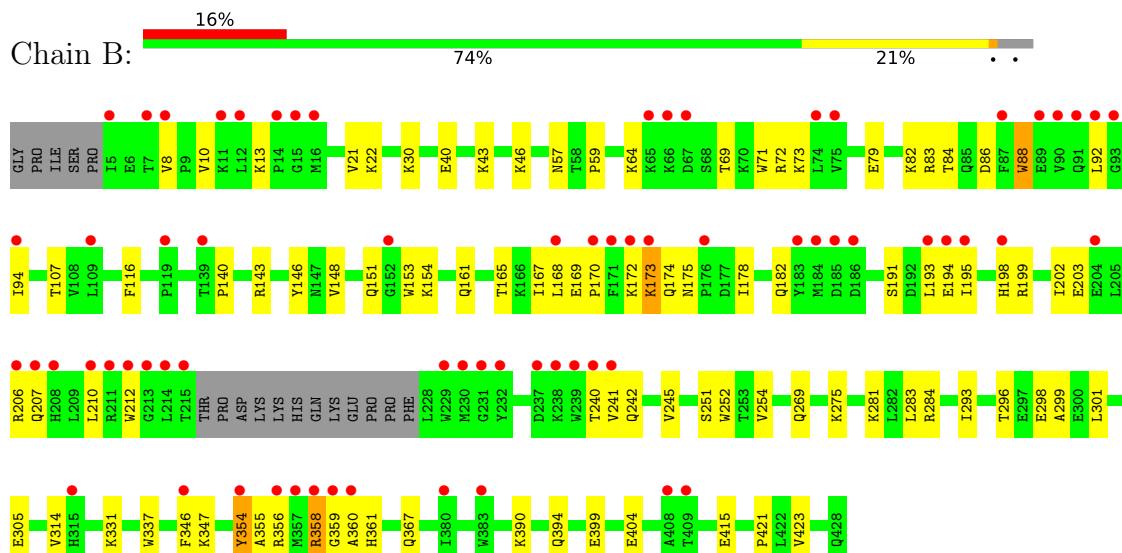
3 Residue-property plots ⓘ

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: Reverse transcriptase p66

Chain A:

• Molecule 2: Reverse transcriptase p51

Chain B:

4   Data and refinement statistics   ⓘ

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	161.43Å 72.95Å 107.75Å 90.00° 99.87° 90.00°	Depositor
Resolution (Å)	34.82 – 2.32 34.82 – 2.32	Depositor EDS
% Data completeness (in resolution range)	98.7 (34.82-2.32) 98.7 (34.82-2.32)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.08 (at 2.31Å)	Xtriage
Refinement program	PHENIX dev_3051	Depositor
R, R_{free}	0.215 , 0.248 0.215 , 0.248	Depositor DCC
R_{free} test set	2000 reflections (3.76%)	wwPDB-VP
Wilson B-factor (Å^2)	63.7	Xtriage
Anisotropy	0.166	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 63.0	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8129	wwPDB-VP
Average B, all atoms (Å^2)	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.44% of the height of the origin peak. No significant pseudotranslation is detected.*

---

[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, EDO, YBA, DMS

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	0.33	0/4630	0.53	0/6295
2	B	0.32	0/3506	0.52	0/4762
All	All	0.33	0/8136	0.53	0/11057

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4512	0	4561	120	0
2	B	3409	0	3441	126	0
3	A	10	0	0	3	0
3	B	10	0	0	4	0
4	A	8	0	12	0	0
4	B	4	0	6	2	0
5	A	29	0	0	3	0
6	B	4	0	6	2	0
7	A	71	0	0	5	0
7	B	72	0	0	30	0
All	All	8129	0	8026	241	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.

All (241) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:354:TYR:O	2:B:354:TYR:CD1	1.76	1.35
2:B:354:TYR:HD1	2:B:354:TYR:C	1.25	1.27
2:B:354:TYR:O	2:B:354:TYR:HD1	0.91	1.23
1:A:65:LYS:CE	1:A:72:ARG:HD3	1.78	1.14
1:A:65:LYS:HE3	1:A:72:ARG:HB2	1.31	1.10
2:B:354:TYR:CD1	2:B:354:TYR:C	2.00	1.09
2:B:423:VAL:HG12	7:B:637:HOH:O	1.55	1.07
2:B:358:ARG:H	2:B:358:ARG:HD2	1.22	1.00
1:A:90:VAL:HG22	7:B:659:HOH:O	1.61	1.00
2:B:399:GLU:OE1	6:B:504:EDO:H22	1.64	0.98
2:B:88:TRP:HB3	2:B:92:LEU:HG	1.43	0.97
1:A:244:ILE:HG22	1:A:263:LYS:HE3	1.47	0.97
2:B:251:SER:HA	7:B:603:HOH:O	1.67	0.94
2:B:404:GLU:HG2	3:B:501:SO4:O4	1.69	0.92
2:B:30:LYS:HE2	7:B:635:HOH:O	1.69	0.90
2:B:358:ARG:HD2	2:B:358:ARG:N	1.85	0.88
1:A:65:LYS:HE3	1:A:72:ARG:CB	2.04	0.86
2:B:314:VAL:HG12	7:B:605:HOH:O	1.73	0.86
1:A:220:LYS:HG2	1:A:221:HIS:H	1.41	0.85
1:A:410:TRP:CZ2	7:A:720:HOH:O	2.31	0.84
1:A:246:LEU:HD21	1:A:310:LEU:HD12	1.61	0.83
1:A:206:ARG:NH2	1:A:218:ASP:HB2	1.93	0.83
1:A:89:GLU:HB2	7:B:601:HOH:O	1.79	0.82
2:B:88:TRP:HB3	2:B:92:LEU:CG	2.10	0.82
2:B:88:TRP:CB	2:B:92:LEU:HG	2.12	0.80
1:A:65:LYS:NZ	1:A:72:ARG:HD3	1.95	0.80
1:A:88:TRP:HZ2	7:B:638:HOH:O	1.64	0.80
2:B:281:LYS:HD3	7:B:611:HOH:O	1.83	0.79
1:A:410:TRP:HZ2	7:A:720:HOH:O	1.64	0.77
1:A:65:LYS:HE2	1:A:72:ARG:HD3	1.67	0.77
1:A:114:ALA:HB1	1:A:214:LEU:HD22	1.66	0.76
2:B:399:GLU:OE1	6:B:504:EDO:C2	2.33	0.76
4:B:503:DMS:H22	7:B:637:HOH:O	1.85	0.76
1:A:61:PHE:HD2	1:A:62:ALA:H	1.32	0.75
2:B:245:VAL:HG22	7:B:606:HOH:O	1.85	0.75
2:B:73:LYS:NZ	2:B:146:TYR:OH	2.21	0.74
2:B:240:THR:O	2:B:242:GLN:NE2	2.21	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:LYS:NZ	1:A:24:TRP:HA	2.03	0.73
2:B:88:TRP:CG	2:B:92:LEU:HG	2.24	0.72
1:A:84:THR:HG22	1:A:124:PHE:HZ	1.54	0.72
2:B:167:ILE:HA	2:B:212:TRP:CZ3	2.24	0.72
2:B:296:THR:HG21	7:B:611:HOH:O	1.88	0.72
1:A:65:LYS:HE3	1:A:72:ARG:HD3	1.70	0.71
2:B:22:LYS:NZ	7:B:601:HOH:O	2.22	0.71
2:B:69:THR:HG23	2:B:69:THR:O	1.91	0.71
1:A:116:PHE:CE2	7:A:757:HOH:O	2.44	0.70
1:A:441:TYR:CD1	1:A:544:GLY:HA3	2.26	0.70
2:B:269:GLN:HB3	2:B:346:PHE:CE2	2.27	0.70
2:B:358:ARG:CD	2:B:359:GLY:N	2.54	0.70
1:A:543:GLY:HA3	2:B:284:ARG:HA	1.72	0.69
2:B:241:VAL:HG12	2:B:242:GLN:N	2.06	0.69
1:A:116:PHE:HE2	7:A:757:HOH:O	1.76	0.69
2:B:296:THR:CB	7:B:611:HOH:O	2.40	0.69
2:B:360:ALA:HB3	2:B:367:GLN:HG2	1.75	0.69
2:B:358:ARG:HD3	2:B:359:GLY:N	2.08	0.69
2:B:86:ASP:HB3	2:B:88:TRP:NE1	2.07	0.68
2:B:358:ARG:HD3	2:B:360:ALA:H	1.57	0.68
1:A:49:LYS:HD3	1:A:142:ILE:HD11	1.76	0.67
1:A:254:VAL:HG23	1:A:255:ASN:H	1.59	0.67
2:B:203:GLU:OE2	2:B:203:GLU:N	2.25	0.66
1:A:220:LYS:HG2	1:A:221:HIS:N	2.09	0.66
2:B:347:LYS:NZ	7:B:605:HOH:O	2.29	0.66
2:B:170:PRO:O	2:B:173:LYS:HG2	1.96	0.65
2:B:88:TRP:HB3	2:B:92:LEU:HA	1.78	0.65
2:B:46:LYS:HE2	2:B:116:PHE:HB3	1.80	0.64
2:B:358:ARG:CD	2:B:359:GLY:H	2.10	0.63
1:A:116:PHE:HZ	1:A:146:TYR:HE2	1.47	0.63
2:B:241:VAL:HG12	2:B:242:GLN:H	1.65	0.62
1:A:229:TRP:CE2	1:A:230:MET:HG2	2.35	0.62
2:B:245:VAL:CG2	7:B:606:HOH:O	2.46	0.62
1:A:254:VAL:HG11	1:A:288:ALA:O	2.00	0.60
1:A:80:LEU:O	1:A:84:THR:HG23	2.00	0.60
2:B:254:VAL:HG23	2:B:293:ILE:HD11	1.83	0.60
1:A:202:ILE:O	1:A:206:ARG:HG3	2.02	0.60
2:B:22:LYS:HE3	7:B:649:HOH:O	2.00	0.60
2:B:275:LYS:HD2	3:B:502:SO4:O4	2.01	0.60
2:B:88:TRP:HA	2:B:92:LEU:HA	1.83	0.59
1:A:84:THR:HG21	1:A:153:TRP:HE1	1.67	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:LEU:HD12	1:A:260:LEU:HD11	1.84	0.59
2:B:22:LYS:CE	7:B:601:HOH:O	2.51	0.58
1:A:206:ARG:CZ	1:A:218:ASP:HB2	2.33	0.58
1:A:206:ARG:HH22	1:A:218:ASP:HB2	1.67	0.58
2:B:354:TYR:CD1	2:B:355:ALA:N	2.68	0.58
2:B:169:GLU:O	2:B:173:LYS:HB3	2.04	0.58
1:A:90:VAL:HG11	2:B:140:PRO:HB3	1.86	0.57
2:B:88:TRP:HB3	2:B:92:LEU:CB	2.35	0.57
2:B:356:ARG:HG2	2:B:358:ARG:NH2	2.19	0.57
1:A:206:ARG:NE	1:A:216:THR:OG1	2.35	0.57
2:B:269:GLN:CB	2:B:346:PHE:CE2	2.88	0.57
1:A:125:ARG:HB3	1:A:146:TYR:O	2.04	0.57
1:A:249:LYS:O	1:A:252:TRP:NE1	2.37	0.57
2:B:30:LYS:CE	7:B:613:HOH:O	2.52	0.57
2:B:94:ILE:HG13	2:B:94:ILE:O	2.05	0.56
2:B:22:LYS:HE2	7:B:601:HOH:O	2.05	0.56
2:B:296:THR:CG2	7:B:611:HOH:O	2.49	0.56
1:A:104:LYS:N	1:A:104:LYS:HD2	2.20	0.55
2:B:212:TRP:CD1	2:B:212:TRP:N	2.75	0.55
2:B:107:THR:HG21	2:B:202:ILE:CD1	2.36	0.55
2:B:195:ILE:HD12	2:B:195:ILE:H	1.73	0.54
2:B:358:ARG:HD2	2:B:359:GLY:H	1.72	0.54
2:B:358:ARG:HD3	2:B:359:GLY:H	1.71	0.54
1:A:218:ASP:OD2	1:A:219:LYS:HG3	2.07	0.54
1:A:257:ILE:HA	1:A:260:LEU:HB3	1.89	0.54
1:A:543:GLY:CA	2:B:284:ARG:HA	2.37	0.54
1:A:17:ASP:OD2	1:A:20:LYS:NZ	2.41	0.54
2:B:88:TRP:CD2	2:B:92:LEU:HG	2.43	0.54
2:B:241:VAL:CG1	2:B:242:GLN:N	2.71	0.54
2:B:269:GLN:CD	2:B:346:PHE:CE2	2.81	0.54
1:A:35:VAL:HG23	1:A:132:ILE:HG21	1.90	0.54
2:B:269:GLN:HB3	2:B:346:PHE:CD2	2.43	0.54
1:A:451:LYS:HE3	1:A:451:LYS:HA	1.89	0.53
1:A:253:THR:HG22	1:A:254:VAL:H	1.72	0.53
2:B:10:VAL:HG11	2:B:153:TRP:HH2	1.73	0.53
1:A:90:VAL:CG2	7:B:659:HOH:O	2.35	0.53
2:B:394:GLN:HG3	7:B:624:HOH:O	2.09	0.53
1:A:22:LYS:HZ1	1:A:24:TRP:HA	1.74	0.52
1:A:65:LYS:CE	1:A:72:ARG:CD	2.69	0.52
1:A:227:PHE:N	1:A:227:PHE:CD1	2.78	0.52
1:A:417:VAL:HG22	1:A:419:THR:HG23	1.91	0.52

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:22:LYS:N	2:B:22:LYS:HD2	2.23	0.52
2:B:30:LYS:HE3	7:B:613:HOH:O	2.08	0.52
1:A:428:GLN:N	3:A:601:SO4:O3	2.36	0.52
2:B:94:ILE:HD11	2:B:182:GLN:O	2.09	0.52
2:B:269:GLN:NE2	2:B:346:PHE:CZ	2.78	0.52
1:A:91:GLN:N	1:A:91:GLN:OE1	2.42	0.51
2:B:170:PRO:O	2:B:174:GLN:HG2	2.11	0.51
2:B:10:VAL:HG11	2:B:153:TRP:CH2	2.45	0.51
2:B:241:VAL:CG1	2:B:242:GLN:H	2.24	0.51
1:A:218:ASP:CG	1:A:219:LYS:N	2.61	0.51
1:A:220:LYS:C	1:A:222:GLN:H	2.14	0.51
2:B:421:PRO:HD2	7:B:616:HOH:O	2.10	0.51
1:A:516:GLU:HB3	3:A:602:SO4:O2	2.11	0.51
1:A:120:LEU:O	1:A:125:ARG:NH2	2.44	0.51
2:B:30:LYS:HE2	7:B:613:HOH:O	2.11	0.51
2:B:207:GLN:HA	2:B:210:LEU:HD12	1.93	0.51
2:B:252:TRP:N	7:B:603:HOH:O	2.26	0.51
2:B:358:ARG:HD3	2:B:360:ALA:N	2.24	0.50
1:A:405:TYR:CE2	1:A:407:GLN:HB2	2.45	0.50
2:B:167:ILE:HG12	2:B:212:TRP:CE3	2.46	0.50
2:B:269:GLN:CD	2:B:346:PHE:CZ	2.85	0.50
1:A:311:LYS:HG3	1:A:312:GLU:HG3	1.92	0.50
1:A:247:PRO:HD3	1:A:263:LYS:HZ3	1.76	0.50
1:A:257:ILE:CG2	1:A:261:VAL:HG13	2.41	0.50
1:A:246:LEU:HD22	1:A:246:LEU:H	1.76	0.50
1:A:116:PHE:CZ	1:A:146:TYR:HE2	2.28	0.50
1:A:191:SER:OG	1:A:198:HIS:ND1	2.35	0.49
1:A:113:ASP:OD2	1:A:215:THR:OG1	2.29	0.49
5:A:605:YBA:C14	5:A:605:YBA:S23	3.00	0.49
2:B:191:SER:OG	2:B:198:HIS:ND1	2.38	0.49
1:A:544:GLY:O	1:A:548:VAL:HG12	2.12	0.49
2:B:168:LEU:O	2:B:172:LYS:HG2	2.12	0.49
2:B:40:GLU:OE1	2:B:43:LYS:HD2	2.13	0.49
1:A:37:ILE:HG22	1:A:41:MET:SD	2.53	0.49
1:A:366:LYS:HE2	1:A:405:TYR:OH	2.13	0.48
1:A:88:TRP:CZ3	2:B:57:ASN:HB2	2.48	0.48
2:B:84:THR:HB	2:B:154:LYS:HE2	1.95	0.48
2:B:254:VAL:CG2	2:B:293:ILE:HD11	2.42	0.48
2:B:360:ALA:HB3	2:B:367:GLN:CG	2.42	0.48
1:A:95:PRO:HG2	5:A:605:YBA:F03	2.03	0.48
1:A:115:TYR:OH	1:A:151:GLN:HB3	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:167:ILE:HA	2:B:212:TRP:CH2	2.47	0.48
2:B:88:TRP:HB3	2:B:92:LEU:CA	2.42	0.48
1:A:175:ASN:O	1:A:178:ILE:HG12	2.14	0.47
1:A:426:TRP:HB3	1:A:526:ILE:HG12	1.96	0.47
1:A:516:GLU:O	1:A:520:GLN:HG3	2.14	0.47
1:A:50:ILE:HG13	1:A:143:ARG:HB3	1.96	0.47
2:B:356:ARG:HG2	2:B:358:ARG:HH21	1.78	0.47
2:B:301:LEU:O	2:B:305:GLU:HG3	2.14	0.47
2:B:64:LYS:HE2	2:B:71:TRP:CE2	2.49	0.47
2:B:269:GLN:OE1	2:B:346:PHE:CE2	2.67	0.47
2:B:296:THR:HB	7:B:611:HOH:O	2.12	0.47
1:A:88:TRP:NE1	2:B:143:ARG:HD3	2.30	0.47
1:A:220:LYS:O	1:A:221:HIS:HB2	2.14	0.47
2:B:296:THR:HG22	2:B:299:ALA:H	1.79	0.47
1:A:196:GLY:O	1:A:200:THR:HG23	2.15	0.47
1:A:248:GLU:HG2	1:A:307:ARG:NH2	2.29	0.47
2:B:82:LYS:NZ	7:B:614:HOH:O	2.48	0.47
2:B:358:ARG:HD2	2:B:359:GLY:N	2.29	0.47
1:A:88:TRP:CH2	2:B:22:LYS:NZ	2.80	0.46
1:A:182:GLN:CG	2:B:140:PRO:HD3	2.45	0.46
1:A:84:THR:HG22	1:A:124:PHE:CZ	2.43	0.46
2:B:275:LYS:HD2	3:B:502:SO4:S	2.56	0.46
1:A:317:VAL:HG21	1:A:347:LYS:HB3	1.98	0.46
1:A:119:PRO:HA	1:A:148:VAL:HG12	1.97	0.46
2:B:21:VAL:HB	2:B:59:PRO:HD3	1.97	0.46
2:B:8:VAL:O	2:B:10:VAL:HG23	2.15	0.46
1:A:122:GLU:HA	1:A:125:ARG:HG3	1.97	0.46
2:B:269:GLN:OE1	2:B:346:PHE:HE2	1.99	0.46
1:A:72:ARG:HH11	1:A:72:ARG:HG2	1.81	0.45
1:A:132:ILE:HB	1:A:142:ILE:HG22	1.98	0.45
1:A:254:VAL:HG23	1:A:255:ASN:N	2.30	0.45
1:A:412:PRO:HB2	7:A:740:HOH:O	2.16	0.45
1:A:451:LYS:HE3	1:A:472:THR:O	2.17	0.45
2:B:203:GLU:HA	2:B:206:ARG:HB2	1.99	0.44
1:A:253:THR:HG22	1:A:254:VAL:N	2.32	0.44
1:A:379:SER:CB	1:A:387:PRO:HD3	2.48	0.44
2:B:390:LYS:NZ	2:B:415:GLU:OE2	2.49	0.44
1:A:296:THR:HG22	1:A:299:ALA:HB2	2.00	0.44
1:A:34:LEU:HD21	1:A:62:ALA:HB2	2.00	0.44
1:A:335:GLY:HA3	1:A:356:ARG:HD3	2.00	0.44
1:A:363:ASN:HA	1:A:511:ASP:OD1	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:314:VAL:CG1	7:B:605:HOH:O	2.49	0.44
2:B:404:GLU:CG	3:B:501:SO4:O4	2.53	0.44
2:B:173:LYS:HG2	2:B:174:GLN:HG2	1.99	0.43
2:B:331:LYS:HB2	2:B:337:TRP:CZ3	2.53	0.43
1:A:46:LYS:HB3	1:A:46:LYS:HE3	1.68	0.43
2:B:296:THR:HG22	2:B:298:GLU:N	2.33	0.43
1:A:64:LYS:N	1:A:71:TRP:CZ3	2.87	0.43
1:A:72:ARG:HG2	1:A:72:ARG:NH1	2.33	0.43
1:A:229:TRP:CE3	1:A:234:LEU:HD11	2.53	0.43
1:A:91:GLN:N	1:A:91:GLN:CD	2.72	0.43
1:A:303:LEU:HD22	1:A:306:ASN:HB2	2.00	0.43
1:A:249:LYS:HG3	1:A:256:ASP:OD2	2.18	0.42
2:B:79:GLU:OE2	2:B:83:ARG:NH2	2.45	0.42
1:A:442:VAL:HB	1:A:481:ALA:HB1	2.01	0.42
1:A:449:GLU:OE2	1:A:449:GLU:N	2.51	0.42
1:A:125:ARG:HD3	1:A:147:ASN:HA	2.01	0.42
1:A:229:TRP:NE1	1:A:230:MET:HG2	2.34	0.42
1:A:195:ILE:HG13	1:A:199:ARG:HE	1.84	0.42
1:A:253:THR:H	1:A:256:ASP:HB2	1.84	0.42
1:A:254:VAL:HG21	1:A:289:LEU:C	2.39	0.42
1:A:308:GLU:O	1:A:311:LYS:HD2	2.20	0.42
2:B:88:TRP:CB	2:B:92:LEU:HA	2.47	0.42
1:A:427:TYR:HA	3:A:601:SO4:O3	2.19	0.42
1:A:132:ILE:HB	1:A:142:ILE:CG2	2.50	0.42
2:B:275:LYS:HA	2:B:275:LYS:HD3	1.78	0.41
1:A:325:LEU:HB2	1:A:385:LYS:HE2	2.02	0.41
1:A:542:ILE:HG23	2:B:283:LEU:HB3	2.02	0.41
2:B:69:THR:O	2:B:69:THR:CG2	2.61	0.41
2:B:72:ARG:NH2	2:B:151:GLN:OE1	2.54	0.41
4:B:503:DMS:C2	7:B:637:HOH:O	2.53	0.41
2:B:199:ARG:O	2:B:203:GLU:OE2	2.39	0.41
1:A:186:ASP:OD2	5:A:605:YBA:N15	2.54	0.41
1:A:251:SER:O	1:A:251:SER:OG	2.39	0.41
2:B:193:LEU:HD12	2:B:194:GLU:H	1.85	0.41
1:A:247:PRO:HD3	1:A:263:LYS:NZ	2.35	0.40
1:A:61:PHE:CD2	1:A:62:ALA:N	2.87	0.40
2:B:116:PHE:C	2:B:148:VAL:HG21	2.42	0.40
2:B:161:GLN:O	2:B:165:THR:HG23	2.21	0.40
2:B:175:ASN:HB3	2:B:178:ILE:HD12	2.04	0.40
2:B:212:TRP:N	2:B:212:TRP:HD1	2.19	0.40

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	554/557 (100%)	522 (94%)	32 (6%)	0	100	100
2	B	408/429 (95%)	388 (95%)	20 (5%)	0	100	100
All	All	962/986 (98%)	910 (95%)	52 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	494/495 (100%)	485 (98%)	9 (2%)	59	74
2	B	374/390 (96%)	368 (98%)	6 (2%)	62	77
All	All	868/885 (98%)	853 (98%)	15 (2%)	60	75

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	LYS
1	A	61	PHE
1	A	113	ASP
1	A	116	PHE
1	A	193	LEU
1	A	227	PHE
1	A	277	ARG
1	A	373	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	394	GLN
2	B	13	LYS
2	B	88	TRP
2	B	173	LYS
2	B	354	TYR
2	B	358	ARG
2	B	361	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	197	GLN
2	B	242	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

9 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths				Bond angles			
					Counts	RMSZ	#$|Z| > 2$		Counts	RMSZ	#$|Z| > 2$	
4	DMS	B	503	-	3,3,3	0.66	0		3,3,3	0.52	0	
3	SO4	A	601	-	4,4,4	0.32	0		6,6,6	0.05	0	
4	DMS	A	604	-	3,3,3	0.85	0		3,3,3	0.56	0	
3	SO4	A	602	-	4,4,4	0.33	0		6,6,6	0.05	0	
3	SO4	B	502	-	4,4,4	0.32	0		6,6,6	0.05	0	
3	SO4	B	501	-	4,4,4	0.32	0		6,6,6	0.05	0	
6	EDO	B	504	-	3,3,3	0.46	0		2,2,2	0.34	0	
5	YBA	A	605	-	26,31,31	2.01	5 (19%)		28,45,45	1.75	6 (21%)	
4	DMS	A	603	-	3,3,3	0.66	0		3,3,3	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
6	EDO	B	504	-	-	1/1/1/1	-
5	YBA	A	605	-	-	3/16/26/26	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	605	YBA	C22-S23	-6.19	1.60	1.70
5	A	605	YBA	C14-N15	5.28	1.45	1.34
5	A	605	YBA	C17-S23	-3.36	1.63	1.73
5	A	605	YBA	C09-C10	2.59	1.53	1.48
5	A	605	YBA	O26-C14	-2.11	1.19	1.23

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	605	YBA	C08-C06-C05	-3.68	120.00	124.00
5	A	605	YBA	C09-C10-N27	3.18	126.13	120.78
5	A	605	YBA	C29-C05-C06	3.14	120.01	116.10
5	A	605	YBA	C20-C19-C22	-3.06	124.92	130.00
5	A	605	YBA	C11-C10-C09	-2.67	126.28	128.77
5	A	605	YBA	C13-C14-N15	2.54	119.92	115.20

There are no chirality outliers.

All (4) torsion outliers are listed below:
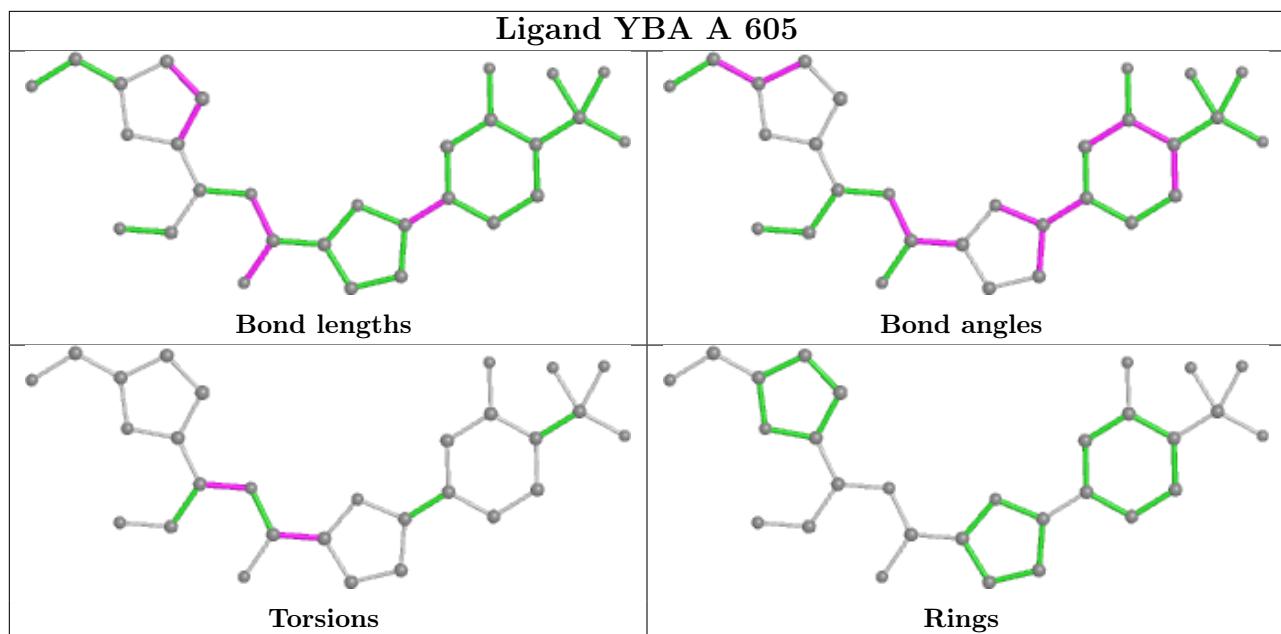
Mol	Chain	Res	Type	Atoms
5	A	605	YBA	C17-C16-N15-C14
6	B	504	EDO	O1-C1-C2-O2
5	A	605	YBA	C24-C16-N15-C14
5	A	605	YBA	C12-C13-C14-O26

There are no ring outliers.

7 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	503	DMS	2	0
3	A	601	SO4	2	0
3	A	602	SO4	1	0
3	B	502	SO4	2	0
3	B	501	SO4	2	0
6	B	504	EDO	2	0
5	A	605	YBA	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand YBA A 605

Bond lengths

Bond angles

Torsions

Rings

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(Å^2)	Q<0.9
1	A	556/557 (99%)	0.87	78 (14%)	2	4	49, 88, 169, 204	0
2	B	412/429 (96%)	0.92	69 (16%)	1	2	48, 81, 161, 223	0
All	All	968/986 (98%)	0.89	147 (15%)	2	3	48, 84, 166, 223	0

All (147) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	289	LEU	13.3
2	B	214	LEU	12.6
1	A	554	ALA	12.0
2	B	229	TRP	9.1
2	B	90	VAL	9.0
2	B	230	MET	8.9
1	A	284	ARG	8.5
2	B	231	GLY	8.1
1	A	290	THR	8.0
1	A	249	LYS	7.9
2	B	66	LYS	7.7
2	B	92	LEU	7.5
1	A	247	PRO	7.5
2	B	93	GLY	7.2
1	A	67	ASP	7.0
1	A	66	LYS	7.0
2	B	215	THR	6.9
1	A	552	VAL	6.8
2	B	91	GLN	6.7
1	A	252	TRP	6.6
2	B	89	GLU	6.6
1	A	254	VAL	6.5
1	A	251	SER	6.5
1	A	90	VAL	6.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	67	ASP	5.9
1	A	92	LEU	5.7
1	A	292	VAL	5.5
1	A	283	LEU	5.5
2	B	354	TYR	5.4
1	A	291	GLU	5.3
1	A	69	THR	5.3
2	B	5	ILE	5.3
2	B	237	ASP	5.1
1	A	544	GLY	5.0
2	B	210	LEU	5.0
1	A	548	VAL	5.0
1	A	295	LEU	4.9
2	B	212	TRP	4.8
1	A	293	ILE	4.8
2	B	94	ILE	4.6
2	B	241	VAL	4.5
1	A	115	TYR	4.5
2	B	357	MET	4.4
2	B	87	PHE	4.4
1	A	288	ALA	4.3
1	A	246	LEU	4.3
1	A	65	LYS	4.2
2	B	195	ILE	4.2
2	B	346	PHE	4.1
2	B	359	GLY	4.1
1	A	250	ASP	4.1
1	A	285	GLY	4.0
2	B	184	MET	4.0
1	A	287	LYS	4.0
2	B	232	TYR	4.0
2	B	186	ASP	3.9
1	A	219	LYS	3.9
2	B	168	LEU	3.8
2	B	14	PRO	3.8
1	A	2	ILE	3.7
1	A	70	LYS	3.7
1	A	546	GLU	3.6
1	A	68	SER	3.5
2	B	239	TRP	3.5
2	B	211	ARG	3.5
1	A	63	ILE	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	282	LEU	3.4
1	A	244	ILE	3.4
2	B	240	THR	3.4
1	A	72	ARG	3.3
1	A	261	VAL	3.3
1	A	545	ASN	3.3
2	B	173	LYS	3.3
2	B	238	LYS	3.1
1	A	0	VAL	3.0
2	B	183	TYR	3.0
1	A	61	PHE	3.0
2	B	409	THR	3.0
1	A	553	SER	3.0
2	B	194	GLU	2.9
1	A	71	TRP	2.9
1	A	24	TRP	2.9
1	A	286	THR	2.9
2	B	172	LYS	2.8
2	B	358	ARG	2.8
2	B	185	ASP	2.8
1	A	315	HIS	2.8
1	A	248	GLU	2.8
2	B	176	PRO	2.7
2	B	74	LEU	2.7
1	A	-1	MET	2.6
2	B	15	GLY	2.6
1	A	245	VAL	2.5
2	B	213	GLY	2.5
1	A	551	LEU	2.5
1	A	298	GLU	2.5
1	A	223	LYS	2.5
2	B	206	ARG	2.5
1	A	182	GLN	2.5
2	B	171	PHE	2.5
1	A	228	LEU	2.5
2	B	75	VAL	2.4
2	B	360	ALA	2.4
2	B	170	PRO	2.4
1	A	262	GLY	2.4
1	A	346	PHE	2.4
1	A	278	GLN	2.4
1	A	74	LEU	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	193	LEU	2.4
2	B	7	THR	2.4
2	B	16	MET	2.3
2	B	65	LYS	2.3
2	B	315	HIS	2.3
1	A	43	LYS	2.3
1	A	281	LYS	2.3
2	B	198	HIS	2.3
1	A	253	THR	2.3
1	A	296	THR	2.3
2	B	208	HIS	2.3
1	A	313	PRO	2.3
2	B	207	GLN	2.3
2	B	383	TRP	2.2
2	B	356	ARG	2.2
1	A	256	ASP	2.2
1	A	312	GLU	2.2
1	A	113	ASP	2.2
2	B	152	GLY	2.2
2	B	119	PRO	2.2
2	B	8	VAL	2.1
1	A	122	GLU	2.1
1	A	297	GLU	2.1
2	B	380	ILE	2.1
1	A	294	PRO	2.1
1	A	458	VAL	2.1
2	B	408	ALA	2.1
1	A	449	GLU	2.1
2	B	109	LEU	2.1
1	A	64	LYS	2.1
1	A	91	GLN	2.1
2	B	11	LYS	2.1
1	A	221	HIS	2.1
2	B	12	LEU	2.1
2	B	139	THR	2.1
2	B	204	GLU	2.0
1	A	34	LEU	2.0
1	A	456	GLY	2.0
1	A	89	GLU	2.0

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

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

6.3 Carbohydrates ⓘ
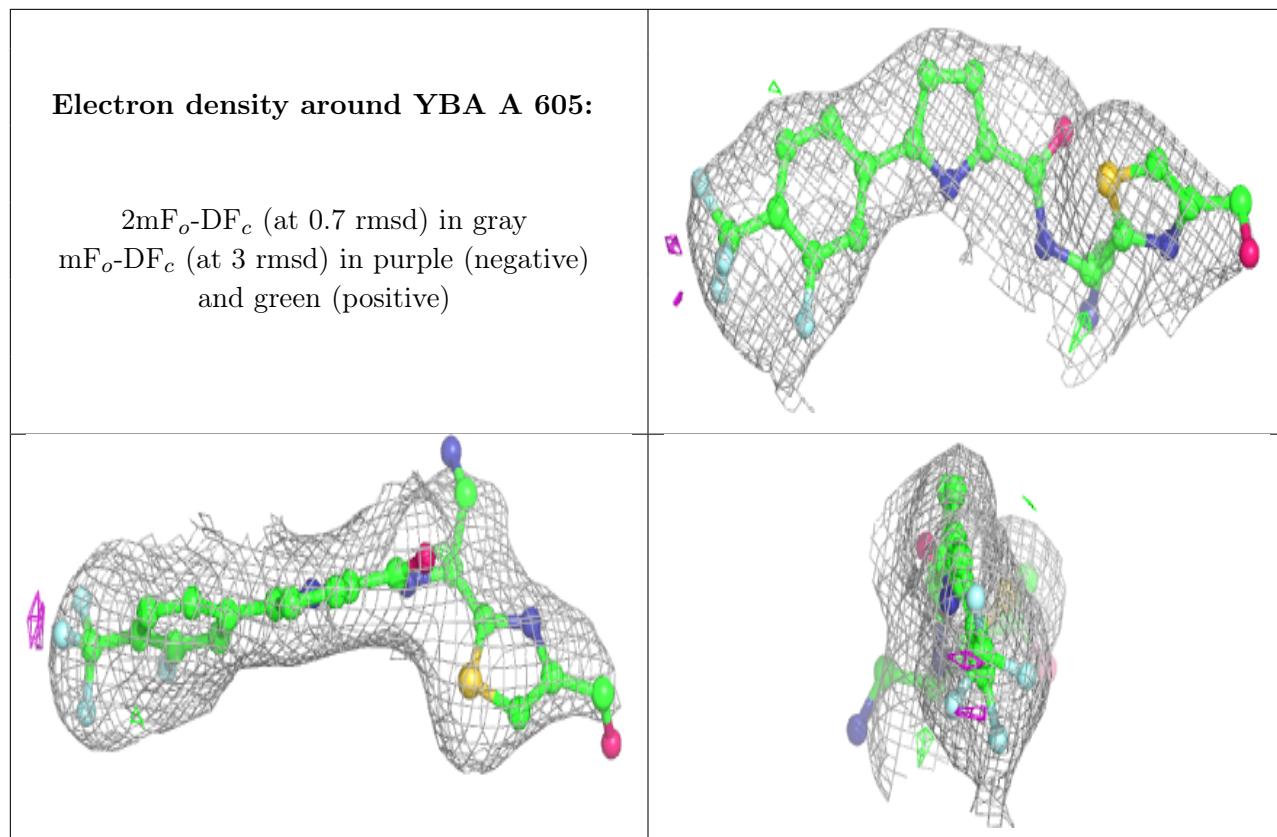
There are no monosaccharides in this entry.

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
3	SO4	B	502	5/5	0.81	0.29	178,179,179,179	0
5	YBA	A	605	29/29	0.83	0.19	100,108,120,122	0
3	SO4	A	601	5/5	0.87	0.25	136,136,136,139	0
3	SO4	B	501	5/5	0.90	0.31	147,147,149,150	0
6	EDO	B	504	4/4	0.91	0.20	71,72,76,80	0
4	DMS	A	603	4/4	0.92	0.12	98,102,105,107	0
3	SO4	A	602	5/5	0.93	0.14	129,129,133,133	0
4	DMS	A	604	4/4	0.93	0.09	98,100,101,103	0
4	DMS	B	503	4/4	0.95	0.20	102,102,105,106	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around YBA A 605:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

6.5 Other polymers ⓘ

There are no such residues in this entry.