WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Apr 24, 2025 – 02:11 PM EDT

PDB ID	:	8VUM / pdb_00008vum
Title	:	Crystal structure of GH9 (K101P, K103N, V108I) HIV-1 reverse transcriptase in complex with non-nucleoside inhibitor 5e2
Authors	:	Rumrill, S.; Ruiz, F.X.; Arnold, E.
Deposited on	:	2024-01-29
Resolution	:	2.15 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

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 2.15 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	Percentile Ranks	Value
Rfree		0.262
Clashscore		6
Ramachandran outliers		0.1%
Sidechain outliers		0.8%
RSRZ outliers		13.0%

Worse *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
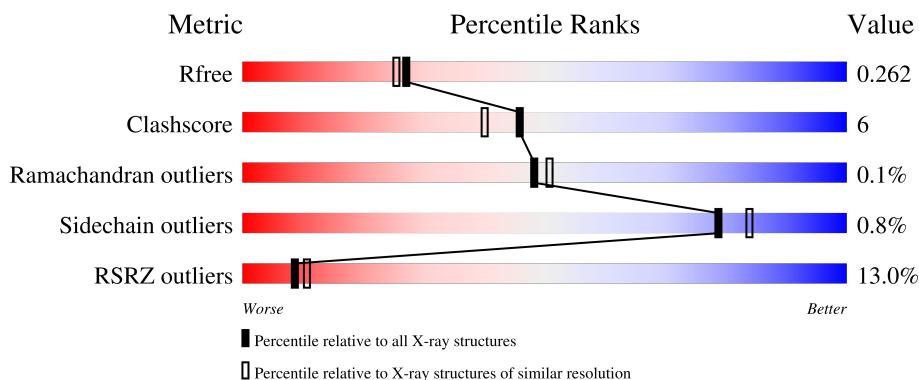
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	1881 (2.16-2.16)
Clashscore	180529	2047 (2.16-2.16)
Ramachandran outliers	177936	2027 (2.16-2.16)
Sidechain outliers	177891	2026 (2.16-2.16)
RSRZ outliers	164620	1882 (2.16-2.16)

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	12% / 84% / 15% / •
2	B	428	14% / 83% / 14% / •
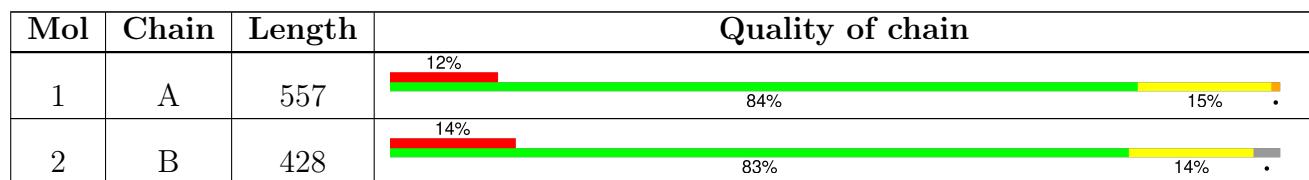
2 Entry composition ⓘ

There are 8 unique types of molecules in this entry. The entry contains 8910 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/ribonuclease H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	556	4538	2936	753	841	8	0	3	0

There are 8 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	101	PRO	LYS	engineered mutation	UNP P03366
A	103	ASN	LYS	engineered mutation	UNP P03366
A	108	ILE	VAL	engineered mutation	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 p51 RT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	414	3490	2276	575	632	7	0	7	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	280	SER	CYS	engineered mutation	UNP P03366

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).

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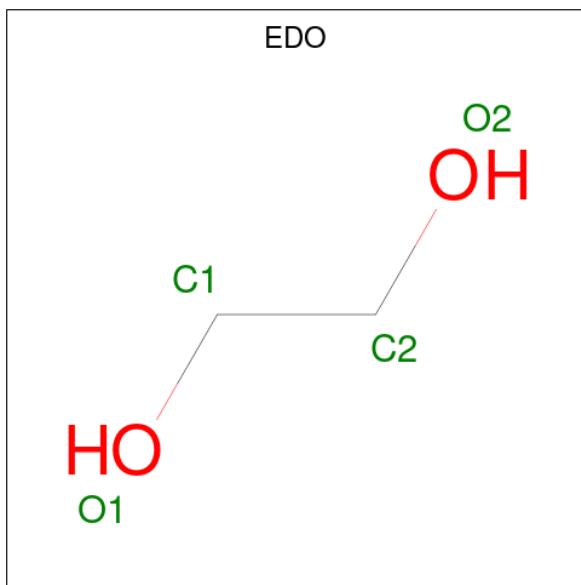
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 4	C 2	O 2	0	0
3	A	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O_4S).

SO4
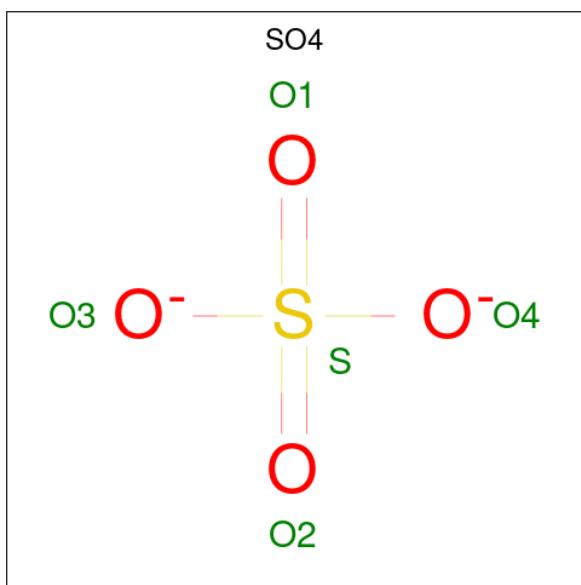
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 5	O 4	S 1	0	0
4	A	1	Total 5	O 4	S 1	0	0
4	A	1	Total 5	O 4	S 1	0	0
4	A	1	Total 5	O 4	S 1	0	0
4	B	1	Total 5	O 4	S 1	0	0
4	B	1	Total 5	O 4	S 1	0	0
4	B	1	Total 5	O 4	S 1	0	0

- Molecule 5 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C_2H_6OS).

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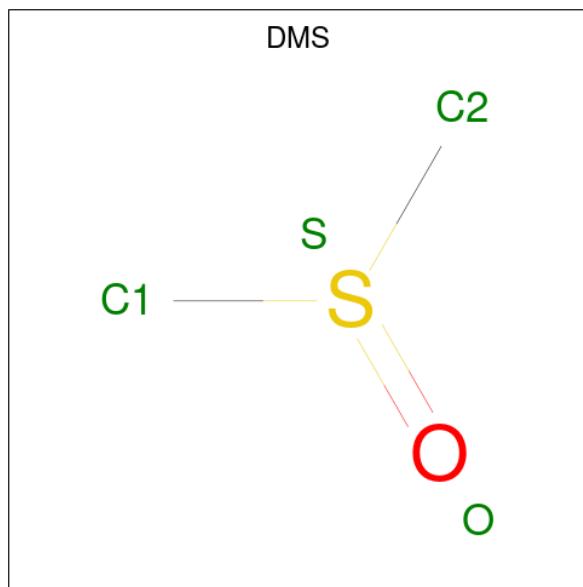
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total 4	C 2	O 1	S 1	0	0

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total 1	Mg 1	0	0

- Molecule 7 is 4-[(4-{[4-(4-cyano-2,6-dimethylphenoxy)-6,7-dimethoxyquinazolin-2-yl]amino}piperidin-1-yl)methyl]benzamide (CCD ID: PKX) (formula: $C_{32}H_{34}N_6O_4$) (labeled as "Ligand of Interest" by depositor).
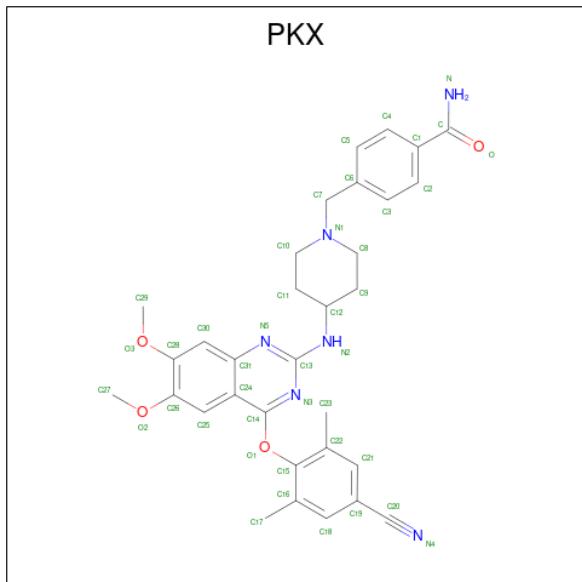
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
7	B	1	42	32	6	4	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	445	Total	O	0	0
			445	445		
8	B	335	Total	O	0	0
			335	335		

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/ribonuclease H
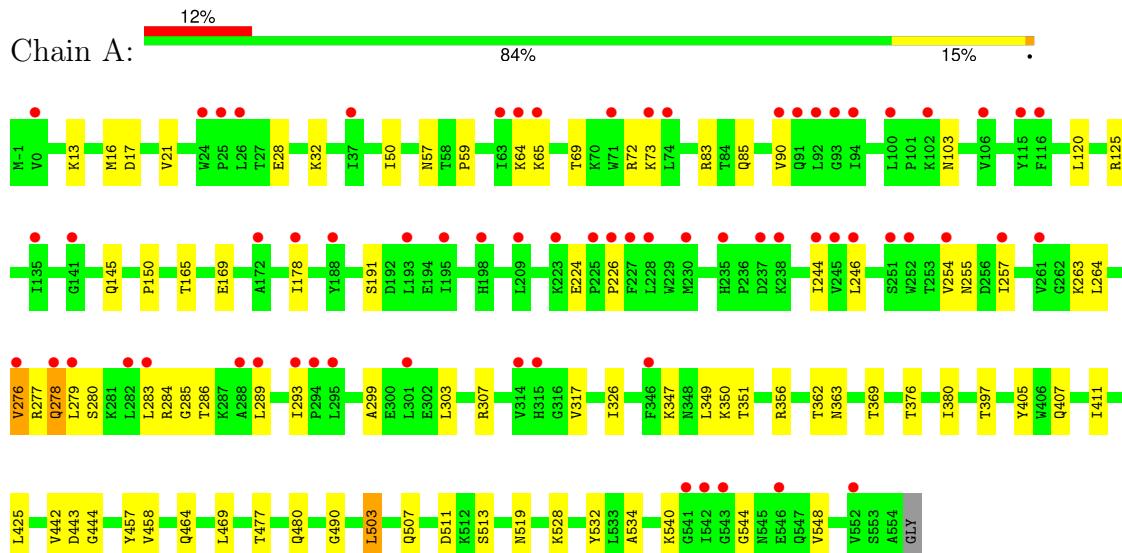
- Molecule 2: p51 RT
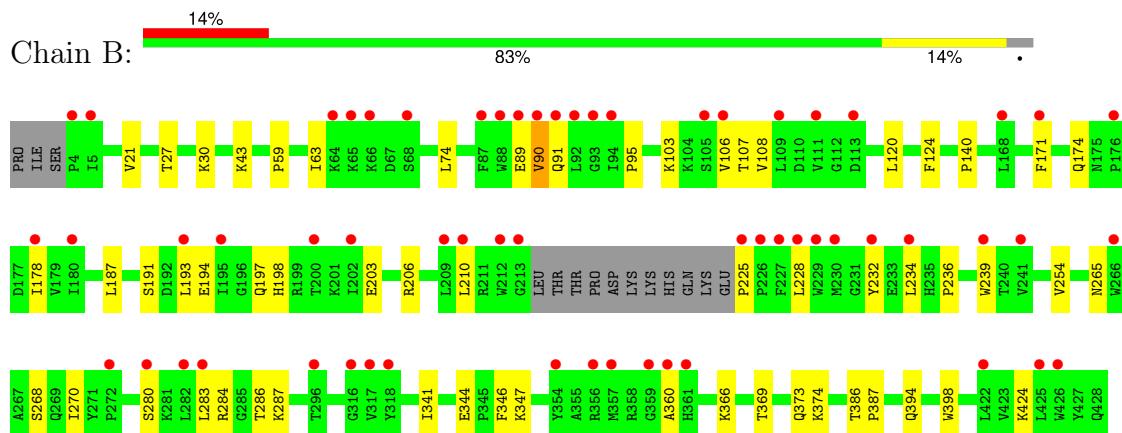
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	162.22Å 72.78Å 108.80Å 90.00° 99.73° 90.00°	Depositor
Resolution (Å)	48.48 – 2.15 48.48 – 2.15	Depositor EDS
% Data completeness (in resolution range)	96.5 (48.48-2.15) 96.8 (48.48-2.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.89 (at 2.14Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.233 , 0.265 0.236 , 0.262	Depositor DCC
R_{free} test set	66212 reflections (3.03%)	wwPDB-VP
Wilson B-factor (Å^2)	51.1	Xtriage
Anisotropy	0.105	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 54.2	EDS
L-test for twinning[2]	$< |L| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8910	wwPDB-VP
Average B, all atoms (Å^2)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.24% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: MG, SO4, EDO, DMS, PKX

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	0.23	0/4657	0.43	0/6334
2	B	0.23	0/3594	0.44	0/4884
All	All	0.23	0/8251	0.43	0/11218

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	4538	0	4584	56	0
2	B	3490	0	3503	40	1
3	A	8	0	12	0	0
3	B	12	0	18	0	0
4	A	20	0	0	0	0
4	B	15	0	0	2	0
5	A	4	0	6	0	0
6	A	1	0	0	0	0
7	B	42	0	0	0	1
8	A	445	0	0	14	0
8	B	335	0	0	10	0
All	All	8910	0	8123	92	1

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 6.

All (92) 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:107:THR:HG1	2:B:198:HIS:HE2	1.44	0.64
1:A:286:THR:HG21	1:A:293:ILE:HD11	1.81	0.60
2:B:284:ARG:O	2:B:287:LYS:NZ	2.35	0.60
2:B:30:LYS:NZ	8:B:705:HOH:O	2.31	0.60
1:A:356:ARG:HD2	1:A:362:THR:HG21	1.85	0.59
1:A:178:ILE:HD13	1:A:191:SER:HB3	1.85	0.58
2:B:108:VAL:HB	2:B:232:TYR:HB3	1.85	0.57
2:B:107:THR:OG1	2:B:198:HIS:NE2	2.37	0.56
1:A:13:LYS:HB2	1:A:16:MET:HG3	1.89	0.54
1:A:254:VAL:HB	1:A:289:LEU:HA	1.88	0.54
1:A:513:SER:O	1:A:519:ASN:ND2	2.35	0.54
1:A:317:VAL:HG23	1:A:349:LEU:HD23	1.89	0.54
1:A:469:LEU:HD12	1:A:477:THR:HG22	1.90	0.54
2:B:341:ILE:N	8:B:703:HOH:O	2.37	0.53
1:A:443:ASP:OD1	1:A:444:GLY:N	2.42	0.53
1:A:480:GLN:NE2	8:A:835:HOH:O	2.40	0.53
1:A:279:LEU:HD23	1:A:299:ALA:HB1	1.89	0.53
1:A:246:LEU:HD11	1:A:264:LEU:HD21	1.90	0.53
1:A:284:ARG:NH1	8:A:844:HOH:O	2.41	0.52
2:B:239:TRP:NE1	4:B:603:SO4:O3	2.36	0.52
1:A:280:SER:HA	1:A:283:LEU:HD13	1.92	0.52
1:A:90:VAL:HB	2:B:140:PRO:HB3	1.92	0.52
1:A:540:LYS:NZ	2:B:265:ASN:OD1	2.34	0.52
1:A:544:GLY:HA2	2:B:286[B]:THR:HG22	1.92	0.51
1:A:85:GLN:NE2	8:A:810:HOH:O	2.41	0.51
2:B:424:LYS:NZ	4:B:607:SO4:O1	2.40	0.51
2:B:210:LEU:HG	2:B:225:PRO:HG2	1.92	0.51
1:A:65:LYS:NZ	8:A:845:HOH:O	2.42	0.50
2:B:21:VAL:HB	2:B:59:PRO:HD3	1.92	0.50
1:A:442:VAL:HG12	1:A:457:TYR:HB3	1.93	0.50
2:B:394[A]:GLN:NE2	8:B:729:HOH:O	2.39	0.49
1:A:405:TYR:CE2	1:A:407:GLN:HB2	2.47	0.49
1:A:21:VAL:HB	1:A:59:PRO:HD3	1.94	0.49
2:B:103:LYS:HB3	8:B:704:HOH:O	2.13	0.49
1:A:224:GLU:HB3	1:A:226:PRO:HD2	1.94	0.49
1:A:326:ILE:N	8:A:803:HOH:O	2.38	0.49
1:A:21:VAL:O	1:A:57:ASN:ND2	2.35	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:397:THR:HG23	1:A:425:LEU:HG	1.96	0.48
1:A:254:VAL:HG13	1:A:257:ILE:HD12	1.95	0.48
2:B:265:ASN:O	2:B:268:SER:OG	2.31	0.48
2:B:270:ILE:HG12	2:B:346:PHE:HB3	1.96	0.48
1:A:277:ARG:NH2	1:A:278:GLN:OE1	2.47	0.47
2:B:63:ILE:HD13	2:B:74:LEU:HD22	1.96	0.47
2:B:369:THR:O	2:B:373:GLN:HG3	2.14	0.47
1:A:72:ARG:NH2	8:A:828:HOH:O	2.38	0.47
1:A:458:VAL:HG12	1:A:464:GLN:HG2	1.97	0.47
2:B:194:GLU:O	2:B:197:GLN:NE2	2.43	0.47
1:A:255:ASN:ND2	8:A:863:HOH:O	2.47	0.47
1:A:458:VAL:HG22	1:A:548:VAL:HB	1.97	0.47
1:A:145:GLN:HB3	8:A:854:HOH:O	2.14	0.47
1:A:380[B]:ILE:HD12	2:B:27:THR:HG22	1.95	0.46
2:B:89:GLU:HG2	2:B:90:VAL:HG22	1.97	0.46
2:B:344:GLU:HB2	2:B:347:LYS:HD2	1.96	0.46
1:A:244:ILE:HG23	1:A:263:LYS:HD3	1.96	0.46
1:A:264:LEU:HD12	1:A:276:VAL:HG23	1.98	0.46
2:B:203:GLU:OE1	2:B:206:ARG:NE	2.43	0.46
2:B:398:TRP:HA	8:B:998:HOH:O	2.16	0.46
2:B:171:PHE:HE2	2:B:178:ILE:HD13	1.81	0.46
2:B:106:VAL:O	2:B:234:LEU:N	2.42	0.45
1:A:528:LYS:HE2	8:A:802:HOH:O	2.16	0.45
2:B:191:SER:N	8:B:704:HOH:O	2.49	0.45
1:A:369:THR:HG23	1:A:411:ILE:HD11	1.99	0.45
2:B:236:PRO:HA	2:B:239:TRP:CD2	2.52	0.45
2:B:374:LYS:NZ	8:B:737:HOH:O	2.43	0.45
2:B:360:ALA:HB2	2:B:366:LYS:HD3	1.98	0.45
2:B:225:PRO:HB3	2:B:228:LEU:HD12	1.99	0.44
1:A:72:ARG:NH1	1:A:73:LYS:HG2	2.33	0.44
1:A:347:LYS:NZ	8:A:871:HOH:O	2.51	0.44
1:A:363:ASN:HA	1:A:511:ASP:OD1	2.17	0.44
1:A:503:LEU:HD22	1:A:507:GLN:HG3	2.00	0.44
1:A:303:LEU:HD21	1:A:307:ARG:HH21	1.83	0.44
1:A:17:ASP:O	1:A:83:ARG:HD3	2.18	0.43
1:A:350:LYS:NZ	1:A:351:THR:O	2.44	0.43
2:B:120:LEU:HD11	2:B:124:PHE:HB3	2.01	0.43
1:A:103:ASN:ND2	8:A:874:HOH:O	2.52	0.42
1:A:490:GLY:O	1:A:528:LYS:NZ	2.42	0.42
2:B:187:LEU:N	8:B:762:HOH:O	2.52	0.42
1:A:376:THR:O	1:A:380[B]:ILE:HG12	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:193:LEU:HD12	2:B:193:LEU:HA	1.87	0.42
1:A:64:LYS:HE3	1:A:69:THR:HA	2.01	0.41
2:B:386:THR:HA	2:B:387:PRO:HD3	1.92	0.41
1:A:254:VAL:O	1:A:257:ILE:HB	2.20	0.41
1:A:532:TYR:CE2	1:A:534:ALA:HB2	2.56	0.41
1:A:285:GLY:N	8:A:851:HOH:O	2.44	0.41
2:B:43:LYS:NZ	8:B:760:HOH:O	2.52	0.41
1:A:28:GLU:HG2	1:A:32:LYS:HE3	2.01	0.41
1:A:244:ILE:HD12	8:A:1097:HOH:O	2.19	0.41
2:B:120:LEU:HD13	8:B:994:HOH:O	2.20	0.41
1:A:120:LEU:HD23	1:A:125:ARG:HG2	2.03	0.41
2:B:254:VAL:HG13	2:B:283:LEU:HD22	2.03	0.40
8:A:938:HOH:O	2:B:280:SER:HB3	2.20	0.40
1:A:165:THR:O	1:A:169:GLU:HG3	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:95:PRO:CG	7:B:601:PKX:N[1_565]	1.43	0.77

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	557/557 (100%)	534 (96%)	22 (4%)	1 (0%)	44	44
2	B	417/428 (97%)	399 (96%)	18 (4%)	0	100	100
All	All	974/985 (99%)	933 (96%)	40 (4%)	1 (0%)	48	51

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	276	VAL

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	498/495 (101%)	494 (99%)	4 (1%)	79	84
2	B	383/390 (98%)	380 (99%)	3 (1%)	79	84
All	All	881/885 (100%)	874 (99%)	7 (1%)	79	84

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	ILE
1	A	150	PRO
1	A	278	GLN
1	A	503	LEU
2	B	90	VAL
2	B	91	GLN
2	B	174	GLN

Sometimes 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 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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 15 ligands modelled in this entry, 1 is monoatomic - leaving 14 for Mogul analysis.

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	SO4	B	607	-	4,4,4	0.24	0	6,6,6	0.07	0
4	SO4	A	706	-	4,4,4	0.24	0	6,6,6	0.07	0
4	SO4	A	703	-	4,4,4	0.23	0	6,6,6	0.07	0
4	SO4	A	704	-	4,4,4	0.24	0	6,6,6	0.08	0
3	EDO	A	701	-	3,3,3	0.42	0	2,2,2	0.38	0
3	EDO	A	707	-	3,3,3	0.42	0	2,2,2	0.37	0
4	SO4	A	702	-	4,4,4	0.23	0	6,6,6	0.08	0
3	EDO	B	604	-	3,3,3	0.42	0	2,2,2	0.39	0
4	SO4	B	605	-	4,4,4	0.23	0	6,6,6	0.07	0
5	DMS	A	705	-	3,3,3	0.67	0	3,3,3	0.54	0
7	PKX	B	601	-	46,46,46	0.18	0	64,65,65	0.51	1 (1%)
3	EDO	B	602	-	3,3,3	0.42	0	2,2,2	0.38	0
3	EDO	B	606	-	3,3,3	0.42	0	2,2,2	0.39	0
4	SO4	B	603	-	4,4,4	0.24	0	6,6,6	0.07	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
3	EDO	A	701	-	-	0/1/1/1	-
3	EDO	A	707	-	-	0/1/1/1	-
3	EDO	B	604	-	-	0/1/1/1	-
7	PKX	B	601	-	-	0/22/32/32	0/5/5/5
3	EDO	B	602	-	-	0/1/1/1	-
3	EDO	B	606	-	-	0/1/1/1	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	B	601	PKX	C25-C24-C14	2.52	127.67	123.97

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	607	SO4	1	0
7	B	601	PKX	0	1
4	B	603	SO4	1	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 PKX B 601
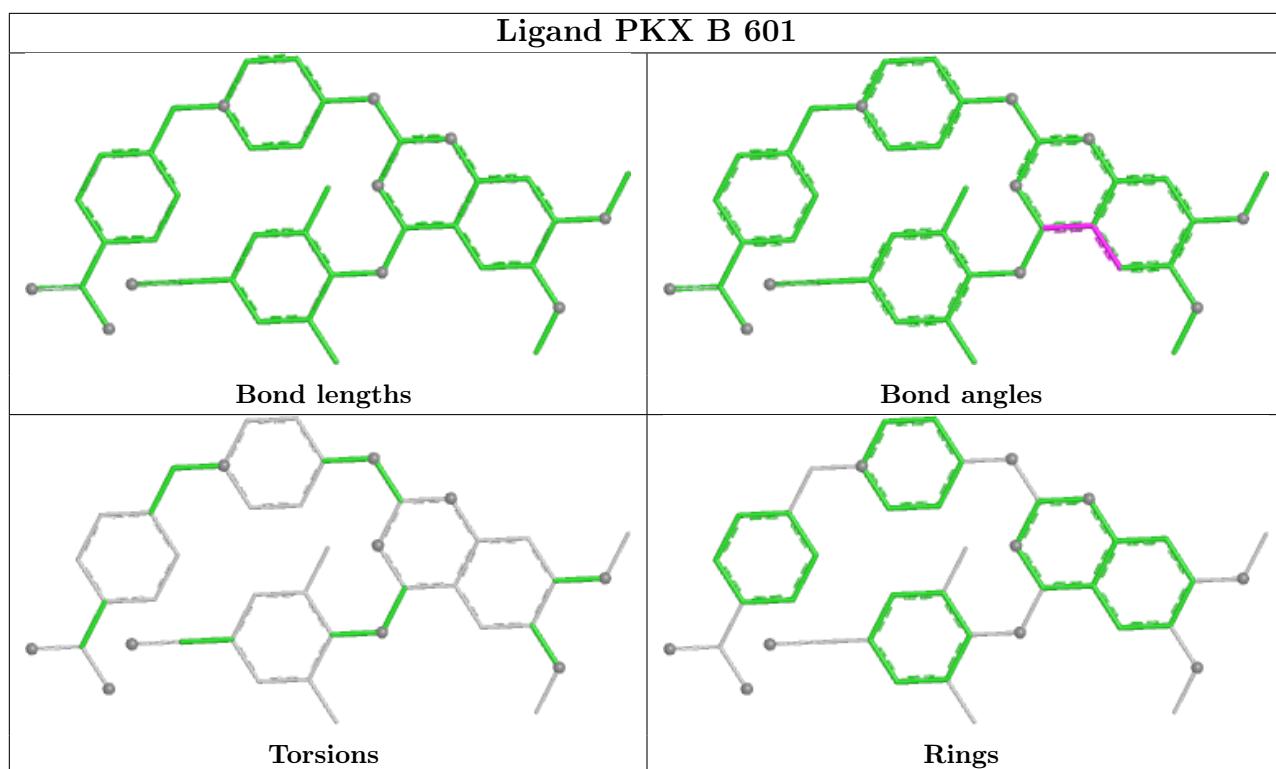
5.7 Other polymers ⓘ

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	556/557 (99%)	0.87	66 (11%)	10	12	20, 64, 144, 249	3 (0%)
2	B	414/428 (96%)	0.94	60 (14%)	7	9	19, 60, 151, 223	7 (1%)
All	All	970/985 (98%)	0.90	126 (12%)	9	11	19, 62, 148, 249	10 (1%)

All (126) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	246	LEU	7.6
1	A	225	PRO	5.5
2	B	92	LEU	5.3
2	B	193	LEU	4.9
1	A	90	VAL	4.7
2	B	209	LEU	4.7
2	B	228	LEU	4.6
2	B	93	GLY	4.4
1	A	92	LEU	4.3
2	B	210	LEU	4.2
2	B	425	LEU	4.1
2	B	282	LEU	4.0
2	B	227	PHE	4.0
1	A	289	LEU	3.9
2	B	5	ILE	3.9
2	B	241	VAL	3.9
2	B	316	GLY	3.7
2	B	94	ILE	3.7
1	A	91	GLN	3.7
2	B	212	TRP	3.6
2	B	426[A]	TRP	3.5
2	B	87	PHE	3.5
1	A	541	GLY	3.5
2	B	195	ILE	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	106	VAL	3.3
1	A	195	ILE	3.3
2	B	360	ALA	3.3
2	B	317	VAL	3.2
1	A	37	ILE	3.2
1	A	254	VAL	3.2
1	A	227	PHE	3.2
2	B	213	GLY	3.2
1	A	276	VAL	3.1
2	B	171	PHE	3.1
1	A	25	PRO	3.1
2	B	91	GLN	3.1
1	A	346	PHE	3.0
2	B	225	PRO	3.0
1	A	24	TRP	3.0
2	B	88	TRP	3.0
1	A	244	ILE	2.9
1	A	257	ILE	2.9
1	A	116	PHE	2.9
2	B	65	LYS	2.9
1	A	100	LEU	2.8
1	A	115	TYR	2.8
1	A	226	PRO	2.8
1	A	252	TRP	2.8
2	B	234	LEU	2.8
2	B	357	MET	2.8
1	A	94	ILE	2.8
2	B	232	TYR	2.7
1	A	74	LEU	2.7
1	A	282	LEU	2.7
1	A	546	GLU	2.7
1	A	237	ASP	2.7
2	B	176	PRO	2.7
1	A	26	LEU	2.7
1	A	295	LEU	2.7
2	B	229	TRP	2.7
2	B	266	TRP	2.7
1	A	223	LYS	2.6
2	B	90	VAL	2.6
1	A	198	HIS	2.6
2	B	200	THR	2.6
1	A	543	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	293	ILE	2.6
1	A	294	PRO	2.6
1	A	283	LEU	2.6
1	A	261	VAL	2.6
1	A	65	LYS	2.6
2	B	239	TRP	2.6
1	A	301	LEU	2.6
2	B	359	GLY	2.5
1	A	63	ILE	2.5
2	B	89	GLU	2.5
2	B	109	LEU	2.5
1	A	315	HIS	2.5
2	B	361	HIS	2.5
1	A	71	TRP	2.5
1	A	209	LEU	2.5
2	B	356	ARG	2.5
1	A	188	TYR	2.5
1	A	228	LEU	2.5
2	B	283	LEU	2.5
1	A	279	LEU	2.4
1	A	245	VAL	2.4
2	B	272	PRO	2.4
1	A	178	ILE	2.4
2	B	354	TYR	2.4
1	A	135	ILE	2.4
1	A	193	LEU	2.4
1	A	172	ALA	2.4
2	B	106	VAL	2.4
2	B	111	VAL	2.4
2	B	226	PRO	2.4
1	A	93	GLY	2.3
2	B	230	MET	2.3
1	A	73	LYS	2.3
2	B	180	ILE	2.3
2	B	202	ILE	2.3
1	A	542	ILE	2.2
2	B	68	SER	2.2
1	A	238	LYS	2.2
2	B	105	SER	2.2
1	A	64	LYS	2.2
2	B	66	LYS	2.2
1	A	0	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	314	VAL	2.2
1	A	102	LYS	2.2
1	A	235	HIS	2.2
1	A	278	GLN	2.2
2	B	296	THR	2.1
2	B	318	TYR	2.1
2	B	178	ILE	2.1
2	B	422	LEU	2.1
2	B	280	SER	2.1
1	A	141	GLY	2.1
1	A	552	VAL	2.1
2	B	4	PRO	2.1
1	A	251	SER	2.1
1	A	230	MET	2.1
2	B	64	LYS	2.0
2	B	168	LEU	2.0
1	A	288	ALA	2.0
2	B	113	ASP	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
4	SO4	A	706	5/5	0.52	0.13	88,99,118,136	0
4	SO4	A	702	5/5	0.72	0.11	71,77,90,96	0
6	MG	A	708	1/1	0.74	0.14	70,70,70,70	0
3	EDO	B	602	4/4	0.75	0.21	45,46,47,49	0
4	SO4	A	703	5/5	0.77	0.11	81,81,94,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	DMS	A	705	4/4	0.78	0.23	61,67,80,89	0
3	EDO	B	604	4/4	0.81	0.21	44,50,62,71	0
4	SO4	B	603	5/5	0.85	0.10	73,74,79,80	0
3	EDO	A	701	4/4	0.86	0.17	44,47,50,59	0
4	SO4	B	607	5/5	0.87	0.11	54,56,82,89	0
3	EDO	A	707	4/4	0.88	0.13	58,58,60,61	0
7	PKX	B	601	42/42	0.90	0.12	40,62,96,104	0
3	EDO	B	606	4/4	0.93	0.11	47,61,63,66	0
4	SO4	B	605	5/5	0.94	0.23	44,56,64,67	0
4	SO4	A	704	5/5	0.95	0.21	46,47,49,80	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 PKX B 601:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.