



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:51 AM UTC

PDB ID : 5HHJ / pdb_00005hhj
Title : Reverse transcriptase domain of group II intron maturase from *Roseburia intestinalis* in P21 space group
Authors : Zhao, C.; Pyle, A.M.
Deposited on : 2016-01-11
Resolution : 1.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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

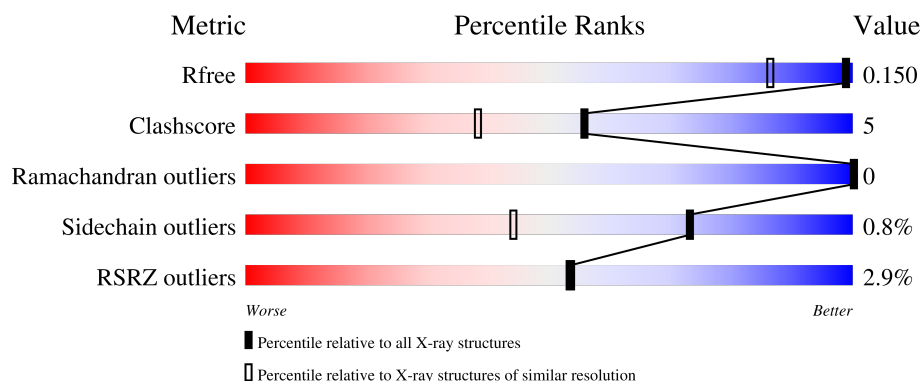
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.20 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	1216 (1.20-1.20)
Clashscore	190562	1265 (1.20-1.20)
Ramachandran outliers	187476	1226 (1.20-1.20)
Sidechain outliers	187428	1226 (1.20-1.20)
RSRZ outliers	180081	1214 (1.20-1.20)

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 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	305	
1	B	305	

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
4	GLY	A	403	-	X	-	-
4	GLY	B	404	-	X	-	-

2 Entry composition [i](#)

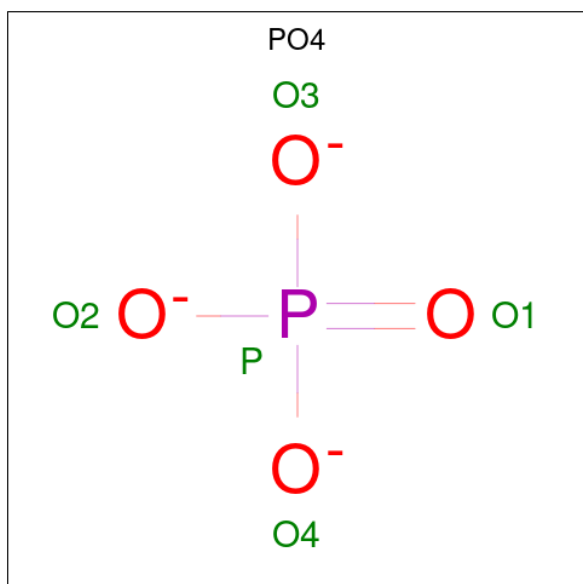
There are 7 unique types of molecules in this entry. The entry contains 11015 atoms, of which 5193 are hydrogens and 0 are deuteriums.

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 Retron-type reverse transcriptase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	294	Total	C	H	N	O	S	0	29	0
			5142	1600	2625	440	459	18			
1	B	292	Total	C	H	N	O	S	0	24	0
			5006	1565	2544	424	455	18			

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).

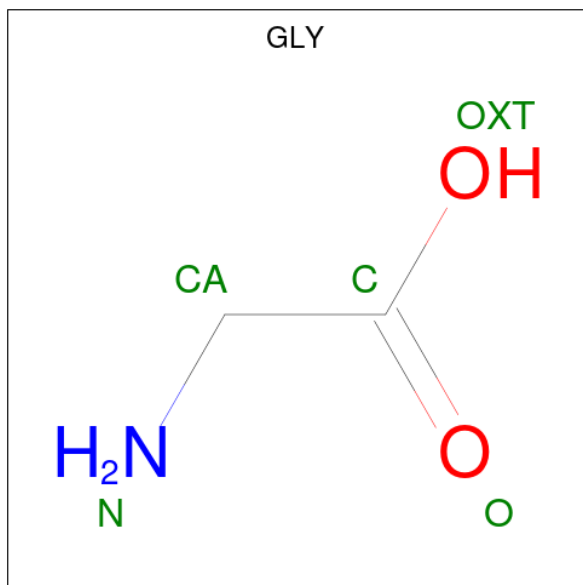


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is POTASSIUM ION (CCD ID: K) (formula: K).

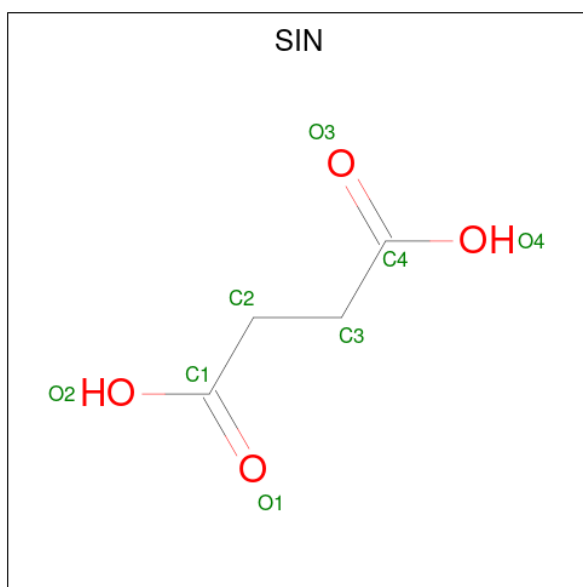
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total K 1 1	0	0
3	B	1	Total K 1 1	0	0

- Molecule 4 is GLYCINE (CCD ID: GLY) (formula: $C_2H_5NO_2$).



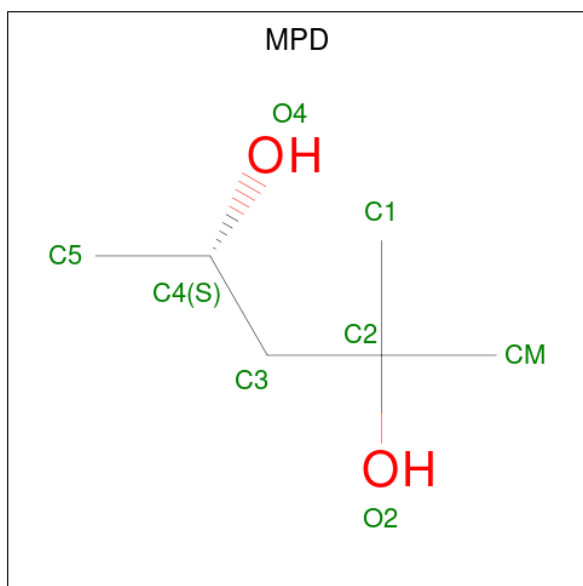
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C H N O 7 2 2 1 2	0	0
4	A	1	Total C H N O 7 2 2 1 2	0	0
4	B	1	Total C H N O 7 2 2 1 2	0	0

- Molecule 5 is SUCCINIC ACID (CCD ID: SIN) (formula: $C_4H_6O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			12	4	4	4		

- Molecule 6 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: $C_6H_{14}O_2$).

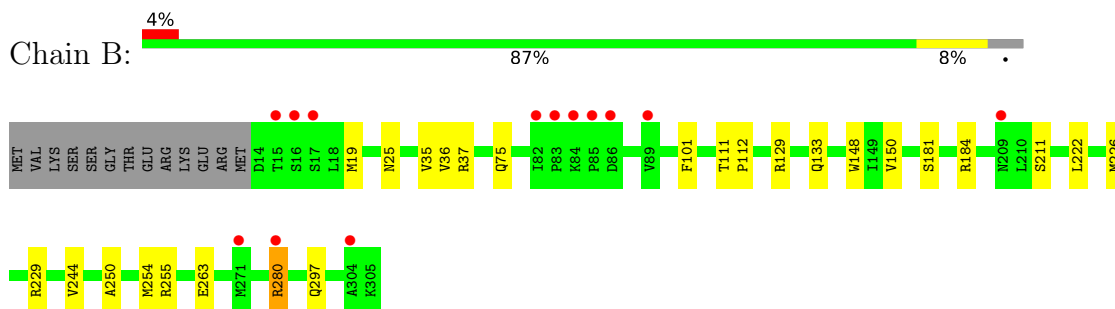


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	H	O	0	0
			22	6	14	2		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	462	Total 470	O 470	0	8
7	B	325	Total 330	O 330	0	5

- Molecule 1: Retron-type reverse transcriptase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	42.08Å 88.06Å 79.76Å 90.00° 95.44° 90.00°	Depositor
Resolution (Å)	44.03 – 1.20 44.03 – 1.20	Depositor EDS
% Data completeness (in resolution range)	98.8 (44.03-1.20) 98.8 (44.03-1.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.18 (at 1.20Å)	Xtriage
Refinement program	PHENIX (dev_2254: ???)	Depositor
R, R_{free}	0.123 , 0.147 0.126 , 0.150	Depositor DCC
R_{free} test set	8915 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	13.1	Xtriage
Anisotropy	0.420	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 41.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	11015	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.05% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: K, MPD, PO4, SIN

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	0.48	0/2642	0.61	0/3547
1	B	0.43	0/2572	0.60	1/3458 (0.0%)
All	All	0.45	0/5214	0.60	1/7005 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	19	MET	CG-SD-CE	-5.64	88.50	100.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	100	ARG	Sidechain

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	2517	2625	2645	29	0
1	B	2462	2544	2561	18	0
2	A	5	0	0	0	0
2	B	5	0	0	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	10	4	4	0	0
4	B	5	2	2	0	0
5	A	8	4	4	2	0
6	B	8	14	14	2	0
7	A	470	0	0	15	0
7	B	330	0	0	9	0
All	All	5822	5193	5230	48	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 5.

All (48) 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:B:25[B]:ASN:OD1	7:B:501:HOH:O	1.95	0.84
1:B:184[A]:ARG:NH2	7:B:502:HOH:O	2.08	0.83
1:A:78:ARG:NH2	7:A:505:HOH:O	2.17	0.76
1:A:75[B]:GLN:OE1	7:A:501:HOH:O	2.08	0.71
1:A:140:ASP:OD1	7:A:502:HOH:O	2.14	0.65
6:B:401:MPD:O4	6:B:401:MPD:H11	1.97	0.65
1:A:29:ASN:OD1	7:A:504:HOH:O	2.16	0.64
1:A:81[A]:GLU:HG2	1:A:89[A]:VAL:CG2	2.29	0.63
1:B:181:SER:OG	2:B:402:PO4:O4	2.11	0.60
1:A:90[A]:ARG:NE	7:A:507:HOH:O	2.23	0.59
1:A:78:ARG:NH2	7:A:515:HOH:O	2.37	0.57
1:A:204[A]:THR:OG1	7:A:503:HOH:O	2.15	0.57
1:A:79:ARG:NH2	1:A:91:ASN:HB3	2.21	0.56
1:A:81[A]:GLU:HG2	1:A:89[A]:VAL:HG21	1.87	0.56
1:B:75[B]:GLN:OE1	7:B:503:HOH:O	2.18	0.56
1:A:259[A]:ARG:NH2	7:A:517:HOH:O	2.37	0.55
1:A:26:ASP:OD1	7:A:506:HOH:O	2.18	0.54
1:B:229:ARG:O	7:B:504:HOH:O	2.18	0.52
1:A:26:ASP:OD2	1:A:30[B]:ARG:NH2	2.33	0.52
1:B:148:TRP:O	1:B:244[B]:VAL:HG23	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:ARG:HH12	5:A:405:SIN:C3	2.24	0.51
1:A:70:ARG:HH12	5:A:405:SIN:H31	1.75	0.51
1:A:81[A]:GLU:CG	1:A:89[A]:VAL:HG21	2.40	0.51
1:B:35:VAL:HG21	1:B:101:PHE:HA	1.94	0.49
1:A:79:ARG:NH1	7:A:523:HOH:O	2.45	0.49
1:A:58:LYS:NZ	7:A:522:HOH:O	2.45	0.48
1:A:222:LEU:HG	1:A:226:MET:HE2	1.95	0.48
1:A:90[A]:ARG:NH2	7:A:507:HOH:O	2.44	0.48
1:A:297[A]:GLN:NE2	7:A:525[A]:HOH:O	2.48	0.47
1:B:255:ARG:NH1	7:B:513:HOH:O	2.47	0.47
1:A:136[B]:LEU:CD1	7:A:502:HOH:O	2.62	0.47
1:B:263[B]:GLU:OE1	7:B:505:HOH:O	2.20	0.47
1:A:81[A]:GLU:CG	1:A:89[A]:VAL:CG2	2.94	0.45
1:B:36[B]:VAL:CG2	7:B:547:HOH:O	2.65	0.45
1:B:150:VAL:HG13	1:B:254[B]:MET:HE3	2.00	0.44
1:A:244[B]:VAL:HG11	1:A:250:ALA:CA	2.48	0.44
1:B:111:THR:HB	1:B:112:PRO:HD3	1.99	0.44
1:B:280:ARG:HD3	7:B:750:HOH:O	2.18	0.43
1:A:244[B]:VAL:HG21	1:A:249[B]:SER:OG	2.18	0.43
1:A:244[B]:VAL:CG1	1:A:250:ALA:HB2	2.48	0.43
1:B:244[B]:VAL:HG21	1:B:250:ALA:HA	2.00	0.43
1:A:204[B]:THR:OG1	1:B:297[B]:GLN:OE1	2.22	0.42
1:B:129:ARG:HA	1:B:133:GLN:OE1	2.19	0.42
1:B:222:LEU:HG	1:B:226:MET:HE2	2.01	0.42
1:A:65[B]:GLU:HG2	7:A:512:HOH:O	2.19	0.42
1:B:36[B]:VAL:HG23	7:B:547:HOH:O	2.21	0.41
1:A:244[B]:VAL:HG22	1:A:245:GLY:H	1.86	0.41
6:B:401:MPD:O4	6:B:401:MPD:C1	2.66	0.41

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	321/305 (105%)	317 (99%)	4 (1%)	0	100	100
1	B	314/305 (103%)	311 (99%)	3 (1%)	0	100	100
All	All	635/610 (104%)	628 (99%)	7 (1%)	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	288/269 (107%)	287 (100%)	1 (0%)	86	67
1	B	281/269 (104%)	278 (99%)	3 (1%)	65	31
All	All	569/538 (106%)	565 (99%)	4 (1%)	73	47

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	211	SER
1	B	37	ARG
1	B	211	SER
1	B	280	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	34	GLN
1	B	91	ASN
1	B	104	GLN
1	B	108	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 2 are monoatomic - leaving 7 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	$\# Z > 2$
5	SIN	A	405	-	7,7,7	0.93	0	8,8,8	1.57	2 (25%)
6	MPD	B	401	-	7,7,7	0.45	0	9,10,10	0.35	0
4	GLY	A	404	-	4,4,4	1.00	0	3,4,4	1.49	0
4	GLY	B	404	-	4,4,4	1.13	1 (25%)	3,4,4	1.97	2 (66%)
2	PO4	B	402	-	4,4,4	1.03	0	6,6,6	0.68	0
2	PO4	A	401	-	4,4,4	0.83	0	6,6,6	0.86	0
4	GLY	A	403	-	4,4,4	1.14	1 (25%)	3,4,4	1.73	1 (33%)

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	MPD	B	401	-	-	1/5/5/5	-
4	GLY	A	404	-	-	2/2/2/2	-
4	GLY	B	404	-	-	2/2/2/2	-
5	SIN	A	405	-	-	2/5/5/5	-
4	GLY	A	403	-	-	2/2/2/2	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	404	GLY	OXT-C	-2.18	1.23	1.30
4	A	403	GLY	OXT-C	-2.16	1.23	1.30

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	404	GLY	OXT-C-O	-2.71	116.36	123.33
5	A	405	SIN	C3-C2-C1	-2.60	106.77	113.67
4	A	403	GLY	OXT-C-O	-2.30	117.41	123.33
4	B	404	GLY	OXT-C-CA	2.06	121.57	113.38
5	A	405	SIN	O2-C1-C2	2.00	120.33	114.00

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	403	GLY	O-C-CA-N
4	A	403	GLY	OXT-C-CA-N
4	A	404	GLY	O-C-CA-N
4	A	404	GLY	OXT-C-CA-N
4	B	404	GLY	O-C-CA-N
4	B	404	GLY	OXT-C-CA-N
6	B	401	MPD	O2-C2-C3-C4
5	A	405	SIN	O2-C1-C2-C3
5	A	405	SIN	O1-C1-C2-C3

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	405	SIN	2	0
6	B	401	MPD	2	0
2	B	402	PO4	1	0

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	294/305 (96%)	-0.51	4 (1%) 73 75	7, 15, 26, 38	29 (9%)
1	B	292/305 (95%)	-0.17	13 (4%) 38 39	8, 19, 38, 71	24 (8%)
All	All	586/610 (96%)	-0.34	17 (2%) 53 53	7, 16, 33, 71	53 (9%)

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	86	ASP	4.6
1	B	15	THR	3.6
1	B	85	PRO	3.3
1	B	17	SER	2.9
1	B	16	SER	2.9
1	B	280	ARG	2.4
1	A	291	TYR	2.3
1	A	15	THR	2.3
1	A	13	MET	2.3
1	B	304	ALA	2.2
1	B	82	ILE	2.2
1	B	271	MET	2.2
1	B	84	LYS	2.1
1	B	83	PRO	2.1
1	A	12	ARG	2.0
1	B	209	ASN	2.0
1	B	89	VAL	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 [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [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($\text{\AA}^2$)	Q<0.9
4	GLY	B	404	5/5	0.70	0.20	42,45,53,53	7
5	SIN	A	405	8/8	0.71	0.21	30,34,39,39	12
4	GLY	A	404	5/5	0.74	0.20	17,21,29,30	7
4	GLY	A	403	5/5	0.82	0.16	29,30,36,36	7
2	PO4	B	402	5/5	0.87	0.10	36,40,41,41	0
6	MPD	B	401	8/8	0.90	0.10	14,23,29,30	0
2	PO4	A	401	5/5	0.94	0.10	28,31,37,40	5
3	K	B	403	1/1	1.00	0.11	27,27,27,27	0
3	K	A	402	1/1	1.00	0.06	21,21,21,21	0

6.5 Other polymers [i](#)

There are no such residues in this entry.