



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:48 AM UTC

PDB ID : 7QPE / pdb_00007qpe
Title : Crystal structure of serine hydroxymethyltransferase, isoform 6 from *Arabidopsis thaliana* (SHM6)
Authors : Ruszkowski, M.; Grzechowiak, M.; Sekula, B.
Deposited on : 2022-01-04
Resolution : 2.18 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

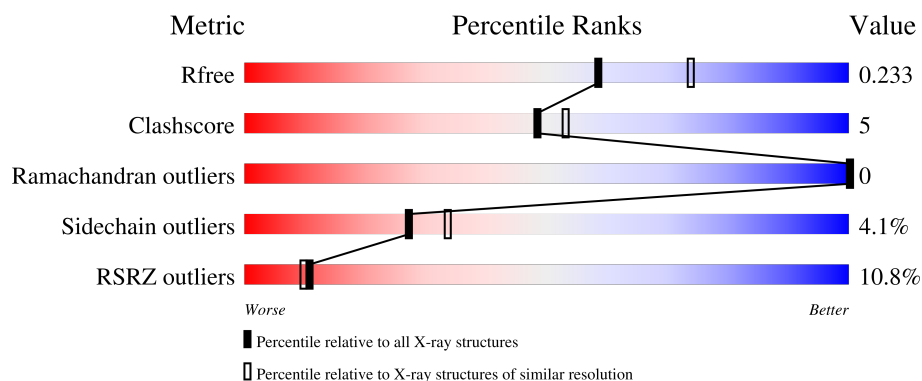
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.18 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	8975 (2.20-2.16)
Clashscore	190562	9786 (2.20-2.16)
Ramachandran outliers	187476	9664 (2.20-2.16)
Sidechain outliers	187428	9664 (2.20-2.16)
RSRZ outliers	180081	8979 (2.20-2.16)

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 $\leq 5\%$. 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	476	11% 76% 14% 10%
1	B	476	9% 77% 12% 10%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6851 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.

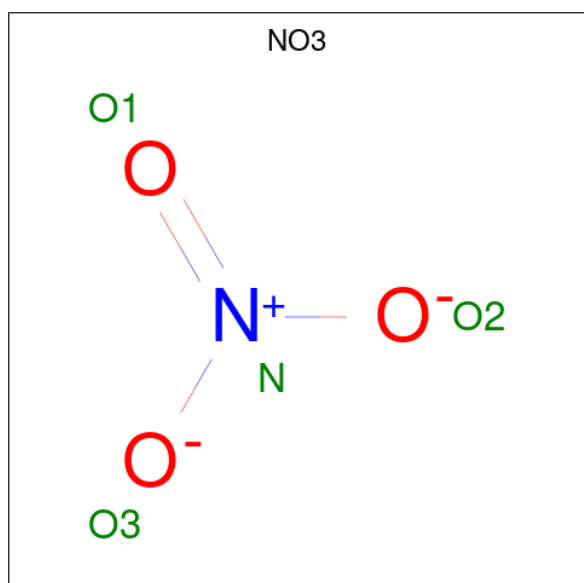
- Molecule 1 is a protein called Serine hydroxymethyltransferase 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	429	Total	C	N	O	S	0	0	0
			3360	2140	578	620	22			
1	B	429	Total	C	N	O	S	0	0	0
			3360	2140	578	620	22			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	124	SER	-	expression tag	UNP Q9LM59
A	125	ASN	-	expression tag	UNP Q9LM59
A	126	ALA	-	expression tag	UNP Q9LM59
B	124	SER	-	expression tag	UNP Q9LM59
B	125	ASN	-	expression tag	UNP Q9LM59
B	126	ALA	-	expression tag	UNP Q9LM59

- Molecule 2 is NITRATE ION (CCD ID: NO3) (formula: NO₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	N	O	0	0
			4	1	3		

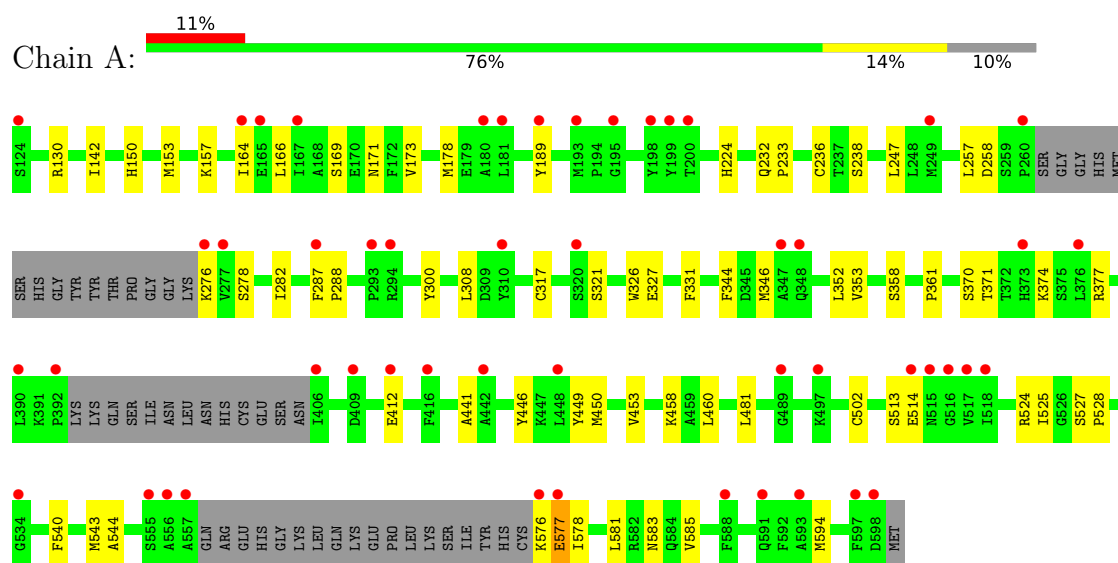
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	56	Total	O	0	0
			56	56		
3	B	71	Total	O	0	0
			71	71		

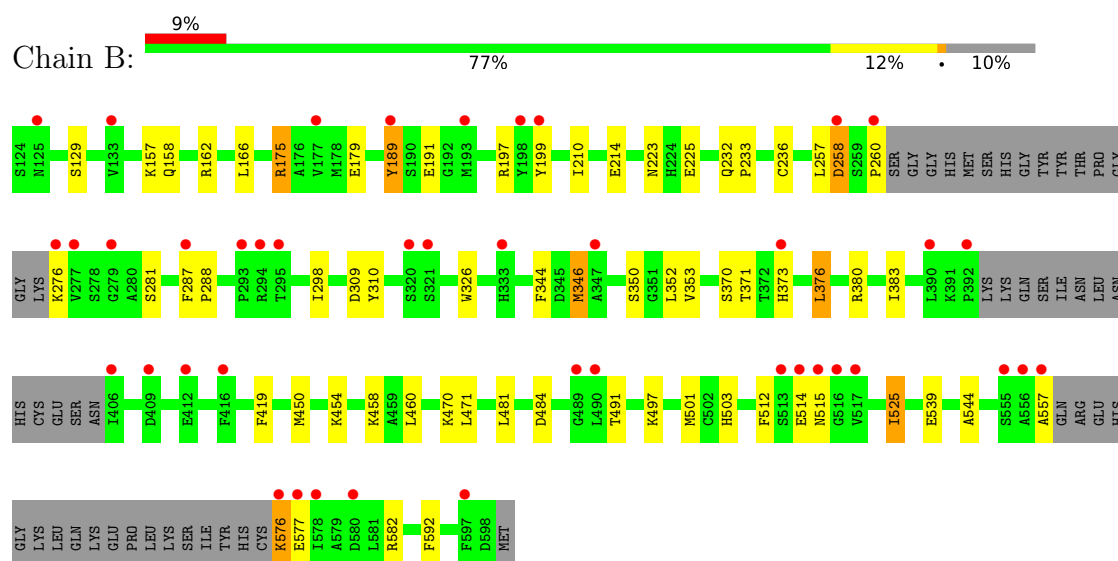
3 Residue-property plots [i](#)

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: Serine hydroxymethyltransferase 6



• Molecule 1: Serine hydroxymethyltransferase 6



4 Data and refinement statistics

Property	Value	Source
Space group	P 64 2 2	Depositor
Cell constants a, b, c, α , β , γ	129.68Å 129.68Å 302.31Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	63.40 – 2.18 63.40 – 2.18	Depositor EDS
% Data completeness (in resolution range)	62.0 (63.40-2.18) 62.1 (63.40-2.18)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 2.18Å)	Xtriage
Refinement program	PHENIX 1.19_4092	Depositor
R, R_{free}	0.208 , 0.230 0.209 , 0.233	Depositor DCC
R_{free} test set	983 reflections (1.24%)	wwPDB-VP
Wilson B-factor (Å ²)	56.9	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 50.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.54$, $\langle L^2 \rangle = 0.38$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6851	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 47.90 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.2845e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NO3

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.34	0/3435	0.52	0/4635
1	B	0.37	0/3435	0.55	0/4635
All	All	0.35	0/6870	0.54	0/9270

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

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	3360	0	3322	36	0
1	B	3360	0	3322	39	0
2	A	4	0	0	0	0
3	A	56	0	0	1	0
3	B	71	0	0	1	0
All	All	6851	0	6644	73	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 (73) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:ILE:HG22	1:A:150:HIS:HB2	1.73	0.69
1:A:236:CYS:HB2	1:A:371:THR:HG22	1.73	0.69
1:A:540:PHE:HA	1:A:543:MET:HE3	1.75	0.68
1:B:175:ARG:NH1	1:B:179:GLU:OE2	2.31	0.64
1:A:346:MET:HG3	1:A:370:SER:HB2	1.81	0.63
1:A:344:PHE:CE2	1:A:346:MET:HB3	2.35	0.62
1:A:258:ASP:HB2	1:A:288:PRO:HB2	1.82	0.62
1:A:257:LEU:HD22	1:A:326:TRP:HH2	1.68	0.58
1:B:191:GLU:HB3	1:B:419:PHE:CZ	2.38	0.58
1:B:344:PHE:CE2	1:B:346:MET:HB3	2.40	0.57
1:A:346:MET:HE1	1:A:353:VAL:HG11	1.87	0.55
1:A:481:LEU:HD11	1:A:525:ILE:HD11	1.89	0.54
1:B:481:LEU:HD11	1:B:525:ILE:HD11	1.89	0.53
1:B:346:MET:HE1	1:B:353:VAL:HG21	1.91	0.53
1:B:503:HIS:CE1	1:B:582:ARG:HD2	2.46	0.51
1:B:346:MET:HG3	1:B:370:SER:HB2	1.93	0.51
1:B:223:ASN:OD1	1:B:225:GLU:HG2	2.11	0.51
1:B:460:LEU:HD12	1:B:544:ALA:HB2	1.94	0.49
1:A:460:LEU:HD12	1:A:544:ALA:HB2	1.94	0.49
1:B:210:ILE:O	1:B:214:GLU:HG3	2.12	0.49
1:A:276:LYS:HD3	1:A:282:ILE:HA	1.94	0.49
1:A:346:MET:HE3	1:A:361:PRO:HG3	1.94	0.49
1:A:287:PHE:HE2	1:B:287:PHE:CE2	2.30	0.49
1:B:344:PHE:HE2	1:B:346:MET:HE3	1.77	0.49
1:A:502:CYS:SG	1:A:578:ILE:HG23	2.53	0.49
1:A:583:ASN:HB3	3:A:710:HOH:O	2.11	0.48
1:B:260:PRO:HB3	1:B:512:PHE:CE1	2.48	0.48
1:B:497:LYS:O	1:B:501:MET:HG3	2.13	0.48
1:A:169:SER:HB2	1:A:374:LYS:HE2	1.95	0.48
1:A:352:LEU:HG	1:A:450:MET:HE2	1.95	0.48
1:A:321:SER:HB3	1:A:524:ARG:HD2	1.96	0.47
1:B:287:PHE:HB2	1:B:310:TYR:CZ	2.50	0.47
1:B:514:GLU:H	1:B:514:GLU:CD	2.23	0.47
1:B:232:GLN:N	1:B:233:PRO:CD	2.78	0.46
1:A:441:ALA:HA	1:A:446:TYR:CD2	2.51	0.46
1:B:576:LYS:HB3	1:B:577:GLU:H	1.49	0.46
1:A:514:GLU:H	1:A:514:GLU:CD	2.24	0.46
1:B:257:LEU:HD22	1:B:326:TRP:HH2	1.81	0.46
1:A:577:GLU:H	1:A:577:GLU:HG3	1.61	0.45
1:A:287:PHE:HE1	1:B:309:ASP:OD1	2.00	0.45
1:B:276:LYS:HD3	1:B:281:SER:O	2.17	0.45
1:B:373:HIS:CG	1:B:380:ARG:HD3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:470:LYS:HD3	1:B:484:ASP:HB3	1.99	0.44
1:B:236:CYS:HB2	1:B:371:THR:HG23	1.99	0.44
1:B:352:LEU:HG	1:B:450:MET:HE2	2.00	0.44
1:A:164:ILE:HG13	1:A:585:VAL:HG13	2.00	0.44
1:A:164:ILE:HD13	1:A:543:MET:HG2	2.00	0.44
1:B:471:LEU:HD22	1:B:481:LEU:HD13	2.00	0.43
1:A:258:ASP:HB2	1:A:288:PRO:CB	2.46	0.43
1:B:344:PHE:CE2	1:B:346:MET:HE3	2.54	0.43
1:A:300:TYR:CZ	1:A:327:GLU:HB2	2.54	0.42
1:B:557:ALA:HB3	3:B:627:HOH:O	2.19	0.42
1:B:158:GLN:O	1:B:162:ARG:HG3	2.18	0.42
1:A:527:SER:N	1:A:528:PRO:HD3	2.35	0.42
1:B:258:ASP:HB2	1:B:288:PRO:HB2	2.01	0.42
1:B:189:TYR:HB3	1:B:199:TYR:CE2	2.54	0.42
1:B:576:LYS:HB3	1:B:576:LYS:HE2	1.71	0.42
1:B:166:LEU:HD23	1:B:166:LEU:HA	1.86	0.42
1:B:298:ILE:HD11	1:B:326:TRP:CZ3	2.55	0.41
1:A:232:GLN:N	1:A:233:PRO:CD	2.84	0.41
1:A:171:ASN:ND2	1:A:377:ARG:HG2	2.35	0.41
1:A:449:TYR:O	1:A:453:VAL:HG23	2.20	0.41
1:B:350:SER:OG	1:B:376:LEU:HD13	2.21	0.41
1:A:166:LEU:HD23	1:A:166:LEU:HA	1.86	0.41
1:A:308:LEU:HA	1:A:308:LEU:HD23	1.88	0.41
1:B:383:ILE:HD13	1:B:383:ILE:HG21	1.88	0.41
1:A:153:MET:HE2	1:A:153:MET:HB3	1.95	0.40
1:A:527:SER:N	1:A:528:PRO:CD	2.84	0.40
1:B:539:GLU:HG2	1:B:592:PHE:CZ	2.56	0.40
1:B:346:MET:HE2	1:B:346:MET:HB2	1.76	0.40
1:A:317:CYS:HB3	1:A:331:PHE:CZ	2.57	0.40
1:A:173:VAL:HG23	1:A:178:MET:HE3	2.03	0.40
1:B:346:MET:HE1	1:B:353:VAL:CG2	2.52	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	421/476 (88%)	407 (97%)	14 (3%)	0	100	100
1	B	421/476 (88%)	405 (96%)	16 (4%)	0	100	100
All	All	842/952 (88%)	812 (96%)	30 (4%)	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	354/395 (90%)	339 (96%)	15 (4%)	26	32
1	B	354/395 (90%)	340 (96%)	14 (4%)	28	35
All	All	708/790 (90%)	679 (96%)	29 (4%)	27	33

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	130	ARG
1	A	157	LYS
1	A	189	TYR
1	A	224	HIS
1	A	238	SER
1	A	247	LEU
1	A	278	SER
1	A	358	SER
1	A	412	GLU
1	A	458	LYS
1	A	513	SER
1	A	576	LYS
1	A	577	GLU
1	A	581	LEU
1	A	594	MET

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Mol	Chain	Res	Type
1	B	129	SER
1	B	157	LYS
1	B	175	ARG
1	B	189	TYR
1	B	197	ARG
1	B	258	ASP
1	B	346	MET
1	B	376	LEU
1	B	454	LYS
1	B	458	LYS
1	B	491	THR
1	B	515	ASN
1	B	525	ILE
1	B	576	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	140	GLN
1	B	452	GLN
1	B	456	ASN
1	B	503	HIS
1	B	552	GLN

5.3.3 RNA [i](#)

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](#)

1 ligand is 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	$\# Z > 2$
2	NO3	A	601	-	1,3,3	0.84	0	0,3,3	-	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	429/476 (90%)	0.90	51 (11%) 9 8	48, 64, 91, 126	0
1	B	429/476 (90%)	0.72	42 (9%) 13 12	42, 60, 88, 140	0
All	All	858/952 (90%)	0.81	93 (10%) 11 10	42, 62, 91, 140	0

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	406	ILE	7.8
1	A	557	ALA	7.3
1	B	406	ILE	7.1
1	B	576	LYS	6.6
1	B	557	ALA	6.3
1	B	199	TYR	6.2
1	A	392	PRO	5.9
1	A	277	VAL	5.8
1	A	576	LYS	5.4
1	B	277	VAL	5.3
1	B	390	LEU	5.1
1	A	199	TYR	5.0
1	A	556	ALA	4.6
1	A	320	SER	4.5
1	B	320	SER	4.4
1	A	390	LEU	4.2
1	A	198	TYR	4.2
1	A	189	TYR	4.0
1	A	294	ARG	4.0
1	A	534	GLY	3.9
1	B	556	ALA	3.7
1	B	392	PRO	3.6
1	A	164	ILE	3.4
1	B	597	PHE	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	513	SER	3.4
1	B	198	TYR	3.3
1	A	124	SER	3.3
1	B	577	GLU	3.2
1	A	515	ASN	3.2
1	A	597	PHE	3.2
1	A	181	LEU	3.1
1	B	260	PRO	3.0
1	A	276	LYS	3.0
1	A	416	PHE	3.0
1	A	287	PHE	2.9
1	A	200	THR	2.9
1	A	514	GLU	2.8
1	A	591	GLN	2.8
1	B	189	TYR	2.8
1	B	514	GLU	2.8
1	B	258	ASP	2.7
1	A	260	PRO	2.7
1	A	409	ASP	2.7
1	A	598	ASP	2.7
1	B	287	PHE	2.6
1	B	193	MET	2.5
1	B	373	HIS	2.5
1	A	517	VAL	2.5
1	A	165	GLU	2.5
1	B	555	SER	2.5
1	A	577	GLU	2.4
1	A	310	TYR	2.4
1	B	578	ILE	2.4
1	A	249	MET	2.3
1	B	321	SER	2.3
1	B	517	VAL	2.3
1	B	293	PRO	2.3
1	A	593	ALA	2.3
1	B	279	GLY	2.3
1	B	177	VAL	2.2
1	A	518	ILE	2.2
1	A	195	GLY	2.2
1	A	489	GLY	2.2
1	A	348	GLN	2.2
1	A	555	SER	2.2
1	B	276	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	416	PHE	2.2
1	A	180	ALA	2.2
1	B	333	HIS	2.2
1	A	376	LEU	2.2
1	B	490	LEU	2.2
1	B	125	ASN	2.2
1	A	293	PRO	2.1
1	A	412	GLU	2.1
1	B	489	GLY	2.1
1	A	373	HIS	2.1
1	B	347	ALA	2.1
1	A	448	LEU	2.1
1	B	515	ASN	2.1
1	A	497	LYS	2.1
1	A	193	MET	2.1
1	A	347	ALA	2.1
1	B	409	ASP	2.1
1	B	294	ARG	2.1
1	B	295	THR	2.1
1	A	516	GLY	2.1
1	A	167	ILE	2.1
1	B	133	VAL	2.1
1	A	442	ALA	2.1
1	B	412	GLU	2.0
1	A	588	PHE	2.0
1	B	580	ASP	2.0
1	B	516	GLY	2.0

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

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(Å ²)	Q<0.9
2	NO3	A	601	4/4	0.81	0.17	80,80,83,87	0

6.5 Other polymers [i](#)

There are no such residues in this entry.