



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 03:24 AM GMT

PDB ID : 1NJS
Title : human GAR Tfase in complex with hydrolyzed form of 10-trifluoroacetyl-5,10-dideaza-acyclic-5,6,7,8-tetrahydrofolicacid
Authors : Zhang, Y.; Desharnais, J.; Marsilje, T.H.; Li, C.; Hedrick, M.P.; Gooljarsingh, L.T.; Tavassoli, A.; Benkovic, S.J.; Olson, A.J.; Boger, D.L.; Wilson, I.A.
Deposited on : 2003-01-02
Resolution : 1.98 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

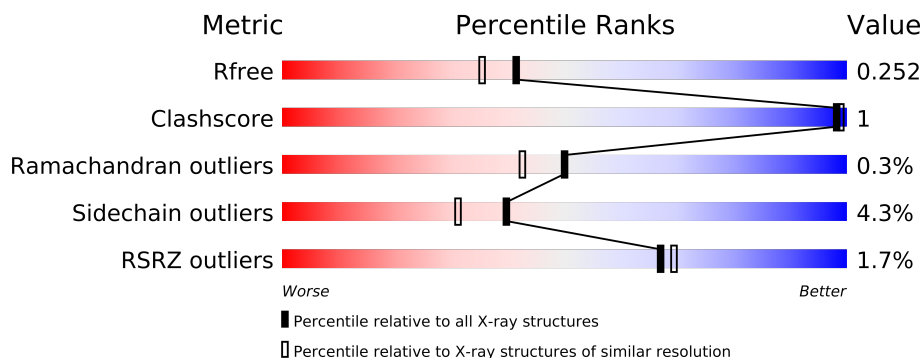
The following versions of software and data (see [references](#)) were used in the production of this report:

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

1 Overall quality at a glance


The reported resolution of this entry is 1.98 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	6577 (2.00-1.96)
Clashscore	79885	8091 (2.00-1.96)
Ramachandran outliers	78287	7989 (2.00-1.96)
Sidechain outliers	78261	7987 (2.00-1.96)
RSRZ outliers	66119	6578 (2.00-1.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	209	
1	B	209	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3356 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Phosphoribosylglycinamideformyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	200	Total	C	N	O	S	0	0	0
			1507	954	264	284	5			
1	B	200	Total	C	N	O	S	0	0	0
			1507	954	264	284	5			

There are 12 discrepancies between the modelled and reference sequences:

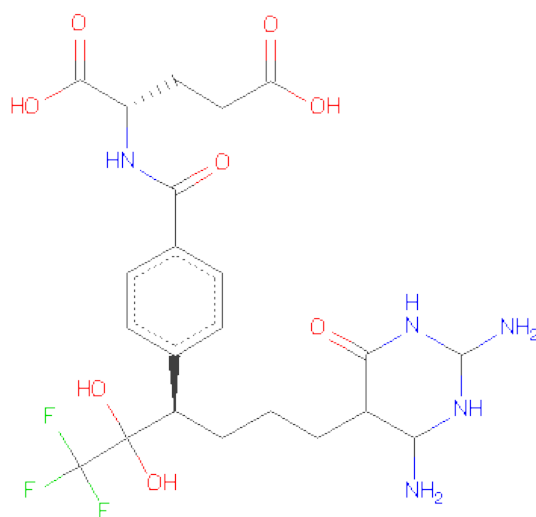
Chain	Residue	Modelled	Actual	Comment	Reference
A	204	HIS	-	EXPRESSION TAG	UNP P22102
A	205	HIS	-	EXPRESSION TAG	UNP P22102
A	206	HIS	-	EXPRESSION TAG	UNP P22102
A	207	HIS	-	EXPRESSION TAG	UNP P22102
A	208	HIS	-	EXPRESSION TAG	UNP P22102
A	209	HIS	-	EXPRESSION TAG	UNP P22102
B	204	HIS	-	EXPRESSION TAG	UNP P22102
B	205	HIS	-	EXPRESSION TAG	UNP P22102
B	206	HIS	-	EXPRESSION TAG	UNP P22102
B	207	HIS	-	EXPRESSION TAG	UNP P22102
B	208	HIS	-	EXPRESSION TAG	UNP P22102
B	209	HIS	-	EXPRESSION TAG	UNP P22102

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
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 N-{4-[(1R)-4-[(2R,4R,5S)-2,4-DIAMINO-6-OXOHEXAHYDROPYRIMIDIN-5-YL]-1-(2,2,2-TRIFLUORO-1,1-DIHYDROXYETHYL)BUTYL]BENZOYL}-D-GLUTAMIC ACID (three-letter code: KEU) (formula: C₂₂H₃₀F₃N₅O₈).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	0	0
			38	22	3	5	8		
3	B	1	Total	C	F	N	O	0	0
			38	22	3	5	8		

- Molecule 4 is water.

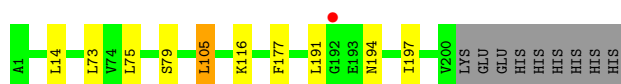
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	147	Total	O	0	0
			147	147		
4	B	104	Total	O	0	0
			104	104		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Phosphoribosylglycinamideformyltransferase

Chain A: 



- Molecule 1: Phosphoribosylglycinamideformyltransferase

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	126.23Å 126.23Å 94.42Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	41.32 – 1.98 43.34 – 1.98	Depositor EDS
% Data completeness (in resolution range)	96.0 (41.32-1.98) 95.6 (43.34-1.98)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.20 (at 1.98Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.227 , 0.247 0.229 , 0.252	Depositor DCC
R_{free} test set	2913 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	28.8	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 41.2	EDS
Estimated twinning fraction	0.027 for -h,-k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 60325 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	3356	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.83% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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

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	0.62	0/1530	0.71	1/2076 (0.0%)
1	B	0.58	0/1530	0.71	3/2076 (0.1%)
All	All	0.60	0/3060	0.71	4/4152 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	142	ASP	CB-CG-OD2	5.79	123.52	118.30
1	B	72	ASP	CB-CG-OD2	5.59	123.33	118.30
1	B	105	LEU	CA-CB-CG	5.38	127.68	115.30
1	A	105	LEU	CA-CB-CG	5.37	127.65	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1507	0	0	1	0
1	B	1507	0	0	1	0
2	A	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	5	0	0	0	0
3	A	38	0	0	0	0
3	B	38	0	0	0	0
4	A	147	0	0	1	0
4	B	104	0	0	1	0
All	All	3356	0	0	2	0

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

All (2) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:116:LYS:NZ	4:A:541:HOH:O	2.07	0.85
1:B:175:LYS:NZ	4:B:718:HOH:O	2.40	0.55

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	198/209 (95%)	194 (98%)	3 (2%)	1 (0%)	38	27
1	B	198/209 (95%)	195 (98%)	3 (2%)	0	100	100
All	All	396/418 (95%)	389 (98%)	6 (2%)	1 (0%)	50	42

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	194	ASN

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	164/173 (95%)	156 (95%)	8 (5%)	35	25
1	B	164/173 (95%)	158 (96%)	6 (4%)	45	38
All	All	328/346 (95%)	314 (96%)	14 (4%)	40	31

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	LEU
1	A	73	LEU
1	A	75	LEU
1	A	79	SER
1	A	105	LEU
1	A	177	PHE
1	A	191	LEU
1	A	197	ILE
1	B	73	LEU
1	B	77	GLU
1	B	105	LEU
1	B	125	LEU
1	B	177	PHE
1	B	197	ILE

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

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

5 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	$\# Z > 2$
3	KEU	A	510	-	39,39,39	6.59	21 (53%)	57,57,57	5.62	26 (45%)
2	PO4	A	521	-	4,4,4	0.44	0	6,6,6	0.30	0
2	PO4	A	522	-	4,4,4	0.14	0	6,6,6	0.31	0
3	KEU	B	610	-	39,39,39	7.00	19 (48%)	57,57,57	5.66	26 (45%)
2	PO4	B	621	-	4,4,4	0.47	0	6,6,6	0.32	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	KEU	A	510	-	3/3/11/14	1/42/58/58	0/1/2/2
2	PO4	A	521	-	-	0/0/0/0	0/0/0/0
2	PO4	A	522	-	-	0/0/0/0	0/0/0/0
3	KEU	B	610	-	3/3/11/14	1/42/58/58	0/1/2/2
2	PO4	B	621	-	-	0/0/0/0	0/0/0/0

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	610	KEU	OA2-C5	-24.17	1.15	1.40
3	A	510	KEU	OA2-C5	-22.31	1.16	1.40
3	B	610	KEU	OA1-C5	20.23	1.61	1.40
3	A	510	KEU	OA1-C5	19.27	1.60	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	610	KEU	C9-N3	17.65	1.63	1.33
3	A	510	KEU	C9-N3	16.82	1.61	1.33
3	B	610	KEU	C4-C9	-11.00	1.34	1.51
3	A	510	KEU	C4-C9	-10.96	1.34	1.51
3	B	610	KEU	C12-C11	9.43	1.55	1.39
3	B	610	KEU	O1-C9	9.05	1.41	1.23
3	A	510	KEU	C12-C11	9.03	1.54	1.39
3	B	610	KEU	C11-C10	8.95	1.65	1.51
3	A	510	KEU	O1-C9	8.71	1.40	1.23
3	A	510	KEU	C11-C10	7.57	1.63	1.51
3	B	610	KEU	C13-C14	7.09	1.51	1.39
3	A	510	KEU	C13-C14	6.14	1.50	1.39
3	B	610	KEU	C15-C14	6.02	1.49	1.39
3	A	510	KEU	C15-C14	5.91	1.49	1.39
3	B	610	KEU	C16-C11	5.12	1.47	1.39
3	A	510	KEU	C16-C11	5.07	1.47	1.39
3	B	610	KEU	C5-C10	4.54	1.60	1.53
3	B	610	KEU	C12-C13	4.48	1.47	1.38
3	A	510	KEU	C4-C7	-4.34	1.47	1.54
3	A	510	KEU	C2-C1	3.78	1.70	1.52
3	B	610	KEU	C2-C1	3.69	1.70	1.52
3	B	610	KEU	C4-C7	-3.45	1.49	1.54
3	B	610	KEU	C17-N	3.21	1.53	1.45
3	A	510	KEU	C5-C10	3.01	1.58	1.53
3	A	510	KEU	C12-C13	2.97	1.44	1.38
3	B	610	KEU	C17-C18	2.64	1.59	1.52
3	A	510	KEU	C14-C	-2.64	1.44	1.50
3	A	510	KEU	C17-C18	2.60	1.59	1.52
3	A	510	KEU	C17-N	2.52	1.51	1.45
3	A	510	KEU	O2-C18	2.32	1.38	1.30
3	B	610	KEU	O2-C18	2.30	1.38	1.30
3	A	510	KEU	C8-N1	-2.27	1.26	1.39
3	B	610	KEU	C15-C16	2.24	1.43	1.38
3	B	610	KEU	C-N	2.18	1.39	1.34
3	A	510	KEU	C3-C4	-2.18	1.50	1.54
3	A	510	KEU	C-N	2.18	1.39	1.34

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	610	KEU	C3-C4-C7	27.84	141.60	114.25
3	A	510	KEU	C3-C4-C7	27.09	140.86	114.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	510	KEU	O1-C9-N3	-16.10	100.62	122.71
3	B	610	KEU	O1-C9-N3	-15.51	101.44	122.71
3	A	510	KEU	C8-N1-C7	13.58	126.88	111.89
3	B	610	KEU	C4-C7-N1	12.66	122.19	110.70
3	B	610	KEU	C8-N1-C7	11.80	124.92	111.89
3	A	510	KEU	C4-C7-N1	10.58	120.31	110.70
3	B	610	KEU	F1-C6-C5	-9.38	98.50	111.74
3	A	510	KEU	F1-C6-C5	-8.34	99.97	111.74
3	A	510	KEU	C2-C3-C4	-7.70	98.89	114.41
3	B	610	KEU	C2-C3-C4	-7.69	98.90	114.41
3	B	610	KEU	C2-C1-C10	-7.29	99.92	114.03
3	A	510	KEU	C2-C1-C10	-6.94	100.59	114.03
3	A	510	KEU	O1-C9-C4	6.35	133.60	121.92
3	B	610	KEU	F2-C6-C5	6.26	120.57	111.74
3	B	610	KEU	O1-C9-C4	6.12	133.19	121.92
3	A	510	KEU	F2-C6-C5	5.96	120.15	111.74
3	A	510	KEU	C5-C10-C11	5.83	123.19	114.23
3	B	610	KEU	C5-C10-C11	4.52	121.18	114.23
3	B	610	KEU	OA1-C5-C6	-4.43	95.33	107.68
3	A	510	KEU	OA1-C5-C10	-4.30	97.58	108.80
3	A	510	KEU	OA1-C5-C6	-4.24	95.84	107.68
3	A	510	KEU	C6-C5-C10	4.18	118.19	110.86
3	A	510	KEU	C19-C17-N	-4.02	103.17	110.83
3	A	510	KEU	OA2-C5-C6	3.95	118.70	107.68
3	B	610	KEU	OA1-C5-C10	-3.92	98.57	108.80
3	B	610	KEU	C6-C5-C10	3.86	117.62	110.86
3	B	610	KEU	N1-C8-N3	3.85	120.53	110.73
3	B	610	KEU	OA2-C5-C6	3.81	118.31	107.68
3	B	610	KEU	OA2-C5-C10	3.71	118.48	108.80
3	A	510	KEU	C4-C9-N3	3.66	125.77	116.75
3	A	510	KEU	N1-C8-N3	3.59	119.87	110.73
3	B	610	KEU	C13-C12-C11	-3.57	117.42	121.20
3	B	610	KEU	C4-C9-N3	3.50	125.37	116.75
3	B	610	KEU	C19-C17-N	-3.46	104.24	110.83
3	A	510	KEU	C13-C12-C11	-3.43	117.57	121.20
3	A	510	KEU	OA2-C5-C10	3.37	117.58	108.80
3	B	610	KEU	OA1-C5-OA2	-3.28	99.79	110.27
3	B	610	KEU	C16-C11-C10	-3.21	114.44	121.09
3	A	510	KEU	C16-C11-C10	-3.19	114.47	121.09
3	A	510	KEU	OA1-C5-OA2	-3.16	100.16	110.27
3	A	510	KEU	C1-C10-C5	-2.96	107.61	112.15
3	A	510	KEU	C19-C17-C18	2.70	116.52	110.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	510	KEU	C8-N3-C9	-2.53	115.76	123.17
3	B	610	KEU	C8-N3-C9	-2.52	115.81	123.17
3	B	610	KEU	C12-C11-C10	2.36	125.99	121.09
3	B	610	KEU	C1-C10-C5	-2.30	108.62	112.15
3	A	510	KEU	C15-C14-C13	2.23	121.81	118.63
3	B	610	KEU	N2-C8-N3	2.21	121.04	116.58
3	A	510	KEU	N2-C8-N3	2.20	121.02	116.58
3	B	610	KEU	C19-C17-C18	2.12	115.28	110.71

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	B	610	KEU	C4
3	B	610	KEU	C8
3	B	610	KEU	C7
3	A	510	KEU	C4
3	A	510	KEU	C8
3	A	510	KEU	C7

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	610	KEU	OA1-C5-C10-C1
3	A	510	KEU	OA1-C5-C10-C1

There are no ring outliers.

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	200/209 (95%)	-0.17	1 (0%) 88 91	18, 28, 46, 66	0
1	B	200/209 (95%)	0.10	6 (3%) 48 49	20, 32, 58, 76	0
All	All	400/418 (95%)	-0.03	7 (1%) 67 68	18, 31, 53, 76	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	193	GLU	3.9
1	B	62	LYS	3.6
1	B	60	LEU	3.3
1	B	200	VAL	3.0
1	A	192	GLY	2.7
1	B	195	GLY	2.6
1	B	192	GLY	2.3

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 carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	PO4	A	522	5/5	0.14	1.67	44,46,50,50	0
3	KEU	A	510	38/38	0.12	1.05	20,25,30,33	0
3	KEU	B	610	38/38	0.13	0.67	30,36,53,56	0
2	PO4	A	521	5/5	0.10	0.57	30,30,31,33	0
2	PO4	B	621	5/5	0.13	0.51	26,27,28,28	0

6.5 Other polymers ⓘ

There are no such residues in this entry.