WORLDWIDE PDB
PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 23, 2023 – 03:18 AM EDT

PDB ID	:	3DFS
Title	:	Dihydroxyacetone phosphate Schiff base intermediate in D33S mutant fructose-1,6-bisphosphate aldolase from rabbit muscle
Authors	:	St-Jean, M.; Sygusch, J.
Deposited on	:	2008-06-12
Resolution	:	2.03 Å(reported)

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

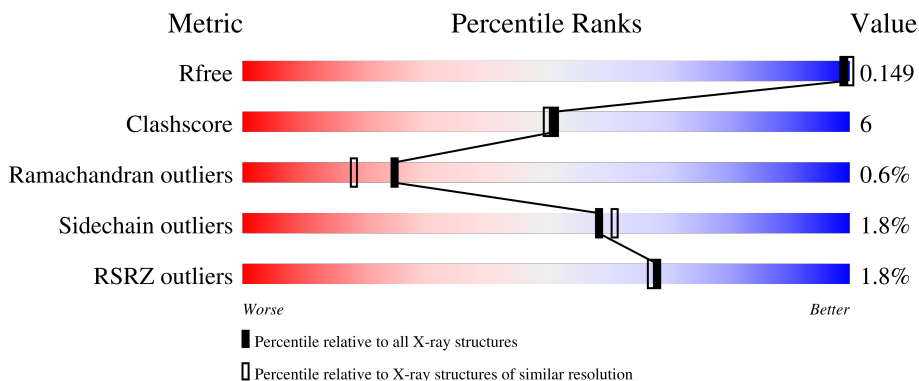|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
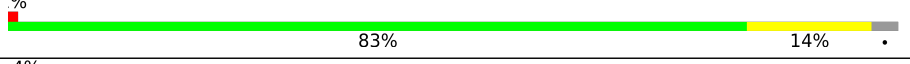*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.03 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		0.149
Clashscore		6
Ramachandran outliers		0.6%
Sidechain outliers		1.8%
RSRZ outliers		1.8%

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}	130704	10434 (2.04-2.00)
Clashscore	141614	11643 (2.04-2.00)
Ramachandran outliers	138981	11493 (2.04-2.00)
Sidechain outliers	138945	11492 (2.04-2.00)
RSRZ outliers	127900	10220 (2.04-2.00)

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	363	% — 85% / 11% • •
1	B	363	% — 83% / 13% • •
1	C	363	% — 83% / 14% •
1	D	363	4% — 85% / 14% •

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 12915 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.
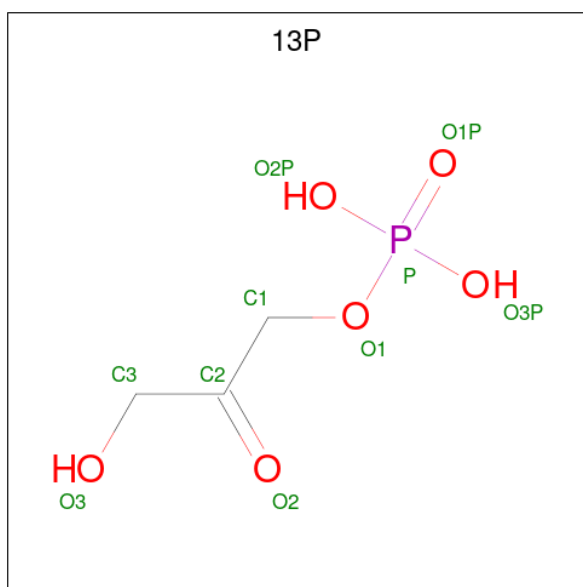
- Molecule 1 is a protein called Fructose-bisphosphate aldolase A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	350	Total	C	N	O	S	0	0	0
			2671	1679	475	506	11			
1	B	350	Total	C	N	O	S	0	0	0
			2671	1679	475	506	11			
1	C	353	Total	C	N	O	S	0	0	0
			2689	1689	479	510	11			
1	D	360	Total	C	N	O	S	0	0	0
			2728	1714	484	519	11			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	33	SER	ASP	engineered mutation	UNP P00883
B	33	SER	ASP	engineered mutation	UNP P00883
C	33	SER	ASP	engineered mutation	UNP P00883
D	33	SER	ASP	engineered mutation	UNP P00883

- Molecule 2 is 1,3-DIHYDROXYACETONEPHOSPHATE (three-letter code: 13P) (formula: $C_3H_7O_6P$).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 9	C 3	O 5	P 1	0	0
2	B	1	Total 9	C 3	O 5	P 1	0	0
2	C	1	Total 9	C 3	O 5	P 1	0	0
2	D	1	Total 9	C 3	O 5	P 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	544	Total 544	O 544	0	0
3	B	549	Total 549	O 549	0	0
3	C	518	Total 518	O 518	0	0
3	D	509	Total 509	O 509	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 co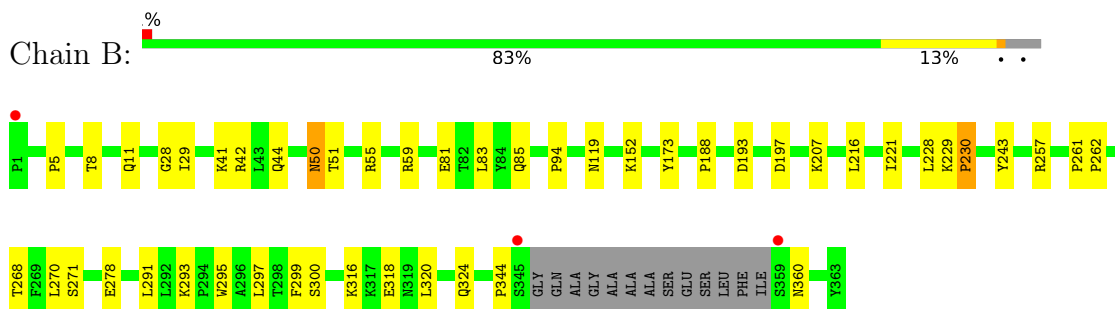ntain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Fructose-bisphosphate aldolase A
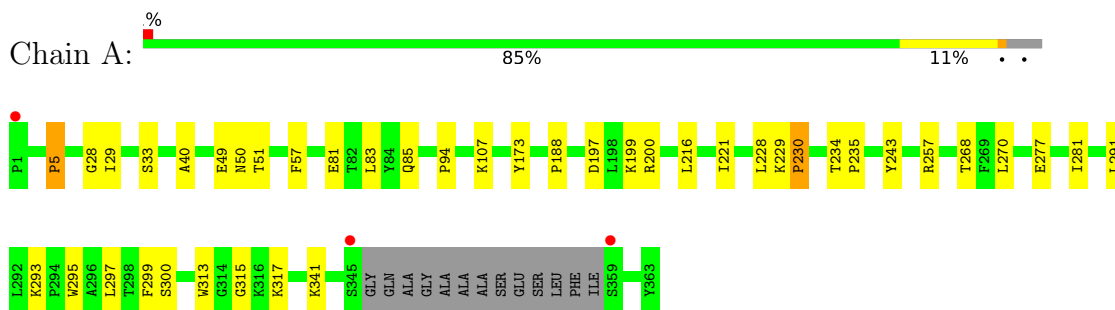
Chain A:

• Molecule 1: Fructose-bisphosphate aldolase A

Chain B:

• Molecule 1: Fructose-bisphosphate aldolase A

Chain C:

• Molecule 1: Fructose-bisphosphate aldolase A

Chain D:

P1 H4 P5 G28 I29 T36 A40 K41 R42 L43 N50 R59 Q60 L61 P92 K98 N119 Y173 P188 D193 D197 R200 K207 Y213 L228 K229 P230 T234 P235 Q241 K242 Y243 M250 P261 P262 T268 F269 L270

E276 N284 L291 L292 K293 P294 W295 T298 F299 S300 Y301 L305 Q306 A307 A312 K316 N319 L320 K321 A322 A323 Q324 E325 K329 G340 K341 Y342 S345 G346 Q347 A348 G349 A350 S353 E354 S355 I358 S359 N360 HIS ALA TYR
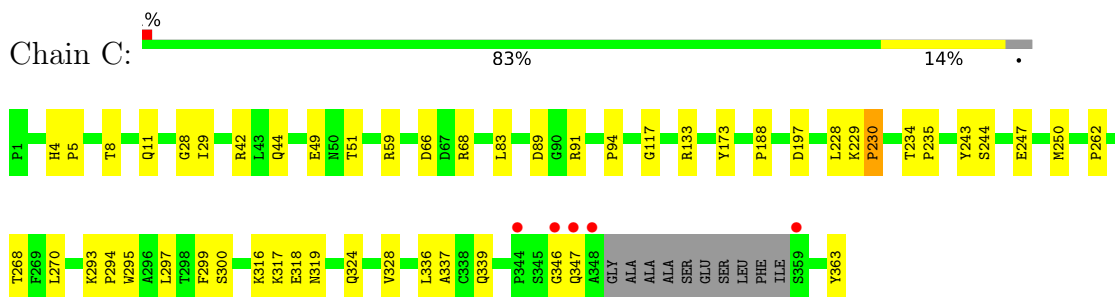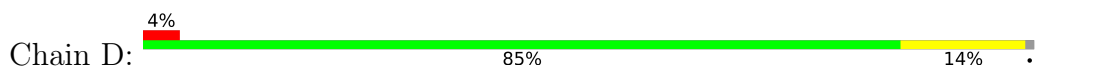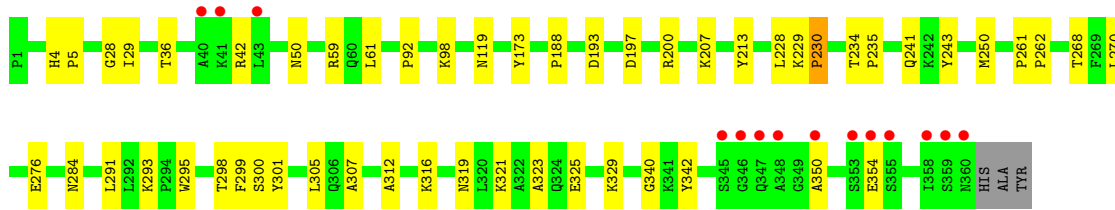
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	83.88Å 103.80Å 84.81Å 90.00° 98.91° 90.00°	Depositor
Resolution (Å)	44.11 – 2.03 44.12 – 1.80	Depositor EDS
% Data completeness (in resolution range)	91.9 (44.11-2.03) 79.2 (44.12-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.10 (at 1.79Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.141 , 0.187 0.148 , 0.149	Depositor DCC
R_{free} test set	9008 reflections (8.19%)	wwPDB-VP
Wilson B-factor (Å^2)	13.4	Xtriage
Anisotropy	0.483	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 62.1	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.017 for l,-k,h	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	12915	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 5.59% 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: 13P

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	0.28	0/2723	0.57	0/3688
1	B	0.29	0/2723	0.57	0/3688
1	C	0.28	0/2741	0.56	0/3712
1	D	0.28	0/2780	0.56	0/3767
All	All	0.28	0/10967	0.57	0/14855

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	D	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	213	TYR	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	2671	0	2692	24	0
1	B	2671	0	2692	35	0
1	C	2689	0	2708	32	0
1	D	2728	0	2753	36	0
2	A	9	0	5	1	0
2	B	9	0	5	1	0
2	C	9	0	5	0	0
2	D	9	0	5	1	0
3	A	544	0	0	3	0
3	B	549	0	0	5	0
3	C	518	0	0	3	0
3	D	509	0	0	7	0
All	All	12915	0	10865	122	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 6.

The worst 5 of 122 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:C:8:THR:H	1:C:11:GLN:HE21	1.31	0.79
1:B:8:THR:H	1:B:11:GLN:HE21	1.37	0.72
1:D:284:ASN:ND2	1:D:342:TYR:H	1.87	0.72
1:B:41:LYS:HA	1:B:44:GLN:HG2	1.71	0.70
1:D:316:LYS:HB2	1:D:319:ASN:ND2	2.06	0.70

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	346/363 (95%)	334 (96%)	10 (3%)	2 (1%)	25	18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	346/363 (95%)	334 (96%)	10 (3%)	2 (1%)	25	18
1	C	349/363 (96%)	336 (96%)	11 (3%)	2 (1%)	25	18
1	D	358/363 (99%)	341 (95%)	15 (4%)	2 (1%)	25	18
All	All	1399/1452 (96%)	1345 (96%)	46 (3%)	8 (1%)	25	18

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	PRO
1	B	5	PRO
1	C	5	PRO
1	A	188	PRO
1	D	5	PRO

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	284/291 (98%)	280 (99%)	4 (1%)	67	70
1	B	284/291 (98%)	277 (98%)	7 (2%)	47	48
1	C	285/291 (98%)	280 (98%)	5 (2%)	59	61
1	D	289/291 (99%)	284 (98%)	5 (2%)	60	63
All	All	1142/1164 (98%)	1121 (98%)	21 (2%)	59	61

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	230	PRO
1	D	173	TYR
1	D	295	TRP
1	D	193	ASP
1	D	59	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	54	ASN
1	D	319	ASN
1	D	284	ASN
1	B	136	GLN
1	C	347	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 ⓘ

4 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	$\#|Z| > 2$
2	13P	C	3003	1	8,8,9	0.71	0	10,10,12	0.99	1 (10%)
2	13P	B	3002	1	8,8,9	0.67	0	10,10,12	0.98	1 (10%)
2	13P	A	3001	1	8,8,9	0.65	0	10,10,12	0.91	1 (10%)
2	13P	D	3004	1	8,8,9	0.72	0	10,10,12	0.99	1 (10%)

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
2	13P	C	3003	1	-	2/6/6/8	-
2	13P	B	3002	1	-	1/6/6/8	-
2	13P	A	3001	1	-	1/6/6/8	-
2	13P	D	3004	1	-	1/6/6/8	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	3004	13P	C1-C2-C3	2.94	120.36	113.95
2	C	3003	13P	C1-C2-C3	2.92	120.31	113.95
2	B	3002	13P	C1-C2-C3	2.90	120.26	113.95
2	A	3001	13P	C1-C2-C3	2.63	119.69	113.95

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	3003	13P	O1-C1-C2-C3
2	D	3004	13P	O1-C1-C2-C3
2	B	3002	13P	O1-C1-C2-C3
2	A	3001	13P	O1-C1-C2-C3
2	C	3003	13P	C1-C2-C3-O3

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	3002	13P	1	0
2	A	3001	13P	1	0
2	D	3004	13P	1	0

5.7   Other polymers (i)

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	350/363 (96%)	-0.76	3 (0%)	84	83	6, 13, 36, 53	2 (0%)
1	B	350/363 (96%)	-0.68	3 (0%)	84	83	5, 13, 37, 58	2 (0%)
1	C	353/363 (97%)	-0.55	5 (1%)	75	74	6, 14, 40, 66	4 (1%)
1	D	360/363 (99%)	-0.46	14 (3%)	39	39	6, 16, 47, 85	0
All	All	1413/1452 (97%)	-0.61	25 (1%)	68	67	5, 14, 41, 85	8 (0%)

The worst 5 of 25 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	348	ALA	8.4
1	D	345	SER	6.4
1	A	345	SER	6.4
1	C	359	SER	5.2
1	C	346	GLY	4.8

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
2	13P	A	3001	9/10	0.97	0.07	14,20,26,30	0
2	13P	B	3002	9/10	0.97	0.07	14,20,23,26	0
2	13P	C	3003	9/10	0.97	0.08	17,18,28,42	0
2	13P	D	3004	9/10	0.98	0.07	17,21,36,41	0

6.5 Other polymers ⓘ

There are no such residues in this entry.