



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 07:47 PM EDT

PDB ID : 5A11 / pdb_00005a11
Title : The crystal structure of Ta-TFP, a thiocyanate-forming protein involved in glucosinolate breakdown (space group P21)
Authors : Krausze, J.; Gumz, F.; Wittstock, U.
Deposited on : 2015-04-27
Resolution : 2.47 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
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

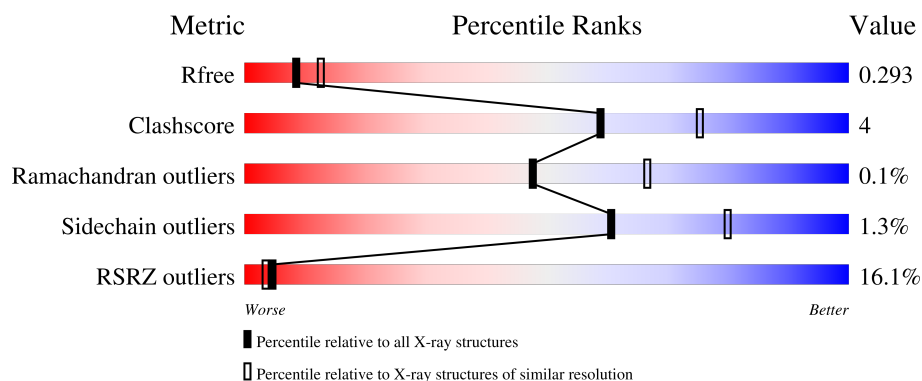
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.47 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	7589 (2.50-2.46)
Clashscore	190562	8295 (2.50-2.46)
Ramachandran outliers	187476	8164 (2.50-2.46)
Sidechain outliers	187428	8166 (2.50-2.46)
RSRZ outliers	180081	7593 (2.50-2.46)

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	356	13% 85% 11% ••
1	B	356	18% 86% 11% •

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5448 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 THIOCYANATE FORMING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	345	Total	C	N	O	S	0	0	0
			2712	1728	457	518	9			
1	B	345	Total	C	N	O	S	0	0	0
			2699	1719	455	516	9			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	GLY	-	expression tag	UNP G1FNI6
A	-6	PRO	-	expression tag	UNP G1FNI6
A	-5	LEU	-	expression tag	UNP G1FNI6
A	-4	GLY	-	expression tag	UNP G1FNI6
A	-3	SER	-	expression tag	UNP G1FNI6
A	-2	PRO	-	expression tag	UNP G1FNI6
A	-1	GLU	-	expression tag	UNP G1FNI6
A	0	PHE	-	expression tag	UNP G1FNI6
B	-7	GLY	-	expression tag	UNP G1FNI6
B	-6	PRO	-	expression tag	UNP G1FNI6
B	-5	LEU	-	expression tag	UNP G1FNI6
B	-4	GLY	-	expression tag	UNP G1FNI6
B	-3	SER	-	expression tag	UNP G1FNI6
B	-2	PRO	-	expression tag	UNP G1FNI6
B	-1	GLU	-	expression tag	UNP G1FNI6
B	0	PHE	-	expression tag	UNP G1FNI6

- Molecule 2 is IODIDE ION (CCD ID: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	I	0	0
			3	3		
2	B	4	Total	I	0	0
			4	4		

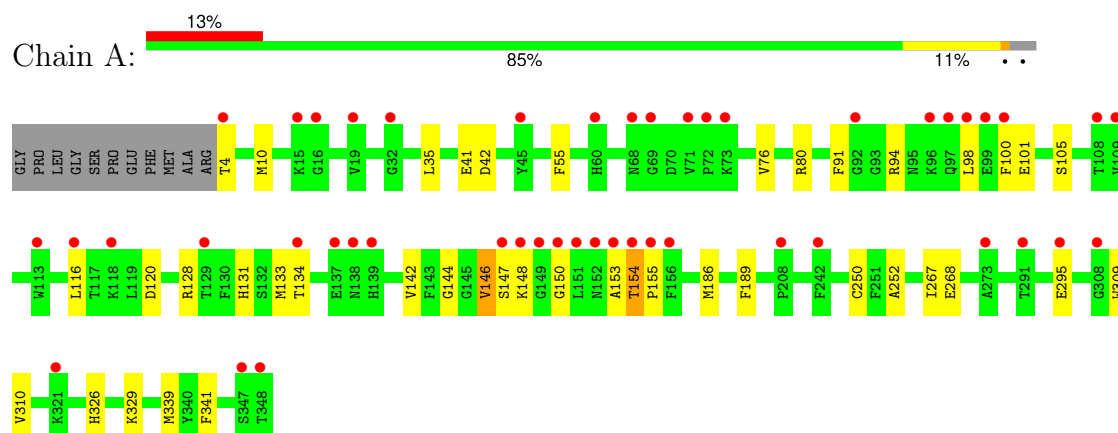
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	23	Total 23	O 23	0	0
3	B	7	Total 7	O 7	0	0

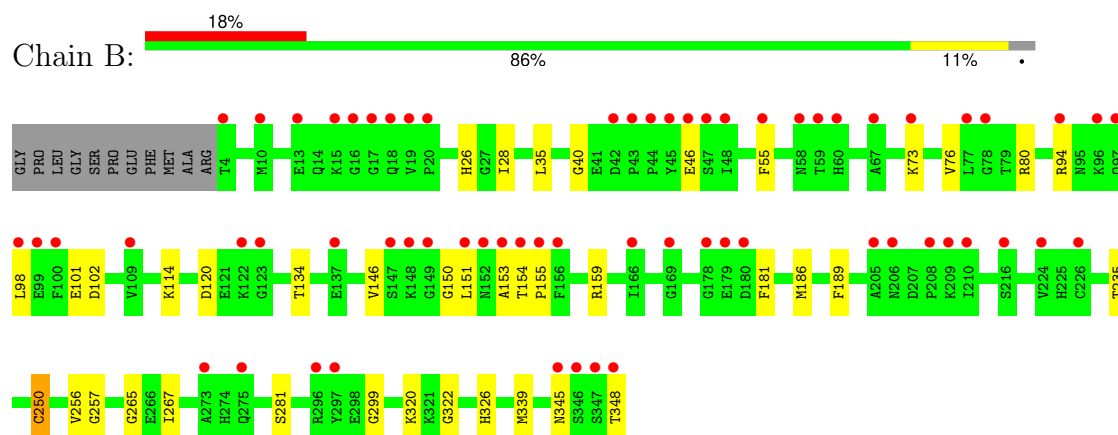
3 Residue-property plots [i](#)

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: THIOCYANATE FORMING PROTEIN



• Molecule 1: THIOCYANATE FORMING PROTEIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	48.37Å 89.61Å 83.84Å 90.00° 101.08° 90.00°	Depositor
Resolution (Å)	45.03 – 2.47 45.03 – 2.47	Depositor EDS
% Data completeness (in resolution range)	98.5 (45.03-2.47) 98.5 (45.03-2.47)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 2.48Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.260 , 0.288 0.280 , 0.293	Depositor DCC
R_{free} test set	1246 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	24.6	Xtriage
Anisotropy	0.323	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 36.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	5448	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.97% 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: IOD

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	0.30	0/2789	0.79	3/3782 (0.1%)
1	B	0.30	0/2776	0.82	5/3768 (0.1%)
All	All	0.30	0/5565	0.80	8/7550 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	154	THR	CA-C-N	9.29	129.35	119.78
1	A	154	THR	C-N-CA	9.29	129.35	119.78
1	B	154	THR	N-CA-C	-7.86	99.83	110.36
1	B	154	THR	CA-C-N	7.39	129.08	119.84
1	B	154	THR	C-N-CA	7.39	129.08	119.84
1	A	146	VAL	N-CA-C	5.70	116.09	108.11
1	B	322	GLY	N-CA-C	5.58	118.67	110.80
1	B	146	VAL	N-CA-C	5.22	115.42	108.11

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	2712	0	2562	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2699	0	2534	21	0
2	A	3	0	0	2	0
2	B	4	0	0	1	0
3	A	23	0	0	0	0
3	B	7	0	0	1	0
All	All	5448	0	5096	46	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 4.

All (46) 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:80:ARG:NH2	1:A:186:MET:SD	2.57	0.77
1:A:35:LEU:HB3	1:A:55:PHE:HB3	1.73	0.70
1:B:73:LYS:NZ	1:B:102:ASP:OD2	2.25	0.68
1:A:326:HIS:HD2	1:A:339:MET:HE2	1.63	0.63
1:B:150:GLY:H	1:B:153:ALA:HB2	1.64	0.61
1:A:80:ARG:HD2	2:A:1350:IOD:I	2.74	0.58
1:B:80:ARG:NH2	1:B:186:MET:SD	2.78	0.57
1:B:150:GLY:H	1:B:153:ALA:CB	2.18	0.55
1:B:80:ARG:HD2	2:B:1350:IOD:I	2.78	0.54
1:B:76:VAL:HG11	1:B:101:GLU:HB2	1.90	0.54
1:B:35:LEU:HB3	1:B:55:PHE:HB3	1.91	0.53
1:A:10:MET:HE2	1:A:341:PHE:HD2	1.76	0.51
1:B:159:ARG:HB2	1:B:181:PHE:CD1	2.47	0.50
1:A:133:MET:HG2	1:A:142:VAL:HG22	1.94	0.49
1:B:28:ILE:HB	1:B:35:LEU:HD11	1.94	0.49
1:A:98:LEU:HD22	1:A:148:LYS:HD2	1.96	0.48
1:A:150:GLY:H	1:A:153:ALA:HB2	1.78	0.48
1:B:299:GLY:O	3:B:2001:HOH:O	2.20	0.47
1:A:309:TRP:CD1	1:A:329:LYS:HE3	2.50	0.46
1:A:326:HIS:CD2	1:A:339:MET:HE2	2.48	0.45
1:A:76:VAL:HG11	1:A:101:GLU:HB2	1.98	0.45
1:B:320:LYS:HE2	1:B:345:ASN:OD1	2.17	0.44
1:A:134:THR:HG22	1:A:189:PHE:CE2	2.53	0.44
1:A:94:ARG:CZ	1:A:148:LYS:HE3	2.47	0.43
1:A:153:ALA:O	1:A:155:PRO:HD3	2.19	0.43
1:B:114:LYS:HE3	1:B:114:LYS:HB2	1.65	0.43
1:A:94:ARG:HD3	1:A:100:PHE:CZ	2.53	0.43
1:B:26:HIS:HB3	1:B:40:GLY:HA2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:256:VAL:HG12	1:B:348:THR:OG1	2.18	0.43
1:A:128:ARG:HD3	1:A:144:GLY:O	2.19	0.43
1:A:80:ARG:HB2	1:A:133:MET:SD	2.58	0.42
1:A:4:THR:OG1	1:A:295:GLU:OE2	2.37	0.42
1:A:146:VAL:HG22	1:A:147:SER:O	2.19	0.42
1:B:98:LEU:HD11	1:B:151:LEU:HA	2.02	0.42
1:B:257:GLY:HA3	1:B:348:THR:O	2.20	0.41
1:A:91:PHE:O	1:A:131:HIS:NE2	2.52	0.41
1:A:154:THR:HA	1:A:155:PRO:HD2	1.84	0.41
1:A:41:GLU:O	1:A:42:ASP:HB2	2.21	0.41
1:A:252:ALA:HB2	1:A:310:VAL:HG21	2.02	0.41
1:A:268:GLU:OE2	1:B:281:SER:OG	2.38	0.41
1:B:326:HIS:HD2	1:B:339:MET:HE2	1.86	0.41
1:A:267:ILE:HD12	1:B:267:ILE:HD12	2.03	0.40
1:B:250:CYS:O	1:B:265:GLY:HA2	2.21	0.40
1:A:10:MET:HE3	2:A:1351:IOD:I	2.91	0.40
1:A:105:SER:HB3	1:A:116:LEU:HD11	2.02	0.40
1:B:134:THR:HG22	1:B:189:PHE:CE2	2.56	0.40

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	343/356 (96%)	332 (97%)	11 (3%)	0	100	100
1	B	343/356 (96%)	333 (97%)	9 (3%)	1 (0%)	36	53
All	All	686/712 (96%)	665 (97%)	20 (3%)	1 (0%)	48	66

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	155	PRO

5.3.2 Protein sidechains [i](#)

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	280/293 (96%)	278 (99%)	2 (1%)	76	88
1	B	277/293 (94%)	272 (98%)	5 (2%)	51	74
All	All	557/586 (95%)	550 (99%)	7 (1%)	61	80

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

Mol	Chain	Res	Type
1	A	120	ASP
1	A	250	CYS
1	B	46	GLU
1	B	94	ARG
1	B	120	ASP
1	B	235	THR
1	B	250	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	68	ASN
1	B	275	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](#)

Of 7 ligands modelled in this entry, 7 are monoatomic - leaving 0 for Mogul analysis.

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	345/356 (96%)	1.06	47 (13%) 7 5	12, 25, 50, 76	0
1	B	345/356 (96%)	1.25	64 (18%) 3 2	12, 27, 55, 89	0
All	All	690/712 (96%)	1.16	111 (16%) 4 3	12, 26, 54, 89	0

All (111) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	19	VAL	7.5
1	B	347	SER	6.7
1	B	346	SER	5.9
1	B	348	THR	5.5
1	B	273	ALA	5.3
1	B	16	GLY	5.1
1	B	156	PHE	5.1
1	B	153	ALA	5.0
1	A	100	PHE	5.0
1	B	148	LYS	4.9
1	B	18	GLN	4.8
1	A	73	LYS	4.7
1	A	147	SER	4.7
1	A	148	LYS	4.7
1	B	152	ASN	4.6
1	B	17	GLY	4.6
1	B	209	LYS	4.4
1	A	149	GLY	4.4
1	B	147	SER	4.4
1	A	150	GLY	4.1
1	A	151	LEU	3.9
1	A	96	LYS	3.9
1	A	152	ASN	3.9
1	B	155	PRO	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	71	VAL	3.8
1	A	15	LYS	3.7
1	A	32	GLY	3.7
1	B	208	PRO	3.7
1	B	60	HIS	3.6
1	A	109	VAL	3.5
1	B	154	THR	3.5
1	A	156	PHE	3.5
1	B	45	TYR	3.5
1	B	123	GLY	3.4
1	A	153	ALA	3.4
1	A	97	GLN	3.3
1	B	151	LEU	3.3
1	B	179	GLU	3.2
1	B	59	THR	3.2
1	A	98	LEU	3.2
1	B	99	GLU	3.1
1	B	13	GLU	3.1
1	B	47	SER	3.0
1	A	108	THR	3.0
1	B	43	PRO	3.0
1	A	138	ASN	3.0
1	B	149	GLY	3.0
1	A	273	ALA	3.0
1	B	4	THR	2.9
1	A	72	PRO	2.9
1	A	16	GLY	2.9
1	A	208	PRO	2.9
1	B	73	LYS	2.9
1	A	137	GLU	2.9
1	B	178	GLY	2.9
1	B	67	ALA	2.8
1	A	68	ASN	2.8
1	B	44	PRO	2.8
1	B	169	GLY	2.8
1	B	297	TYR	2.8
1	B	46	GLU	2.7
1	B	206	ASN	2.7
1	B	180	ASP	2.6
1	B	58	ASN	2.6
1	A	99	GLU	2.6
1	A	69	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	113	TRP	2.6
1	B	109	VAL	2.6
1	A	60	HIS	2.6
1	B	10	MET	2.5
1	B	137	GLU	2.5
1	A	347	SER	2.5
1	B	77	LEU	2.5
1	B	226	CYS	2.4
1	A	92	GLY	2.4
1	B	94	ARG	2.4
1	B	42	ASP	2.4
1	A	45	TYR	2.4
1	A	348	THR	2.4
1	A	242	PHE	2.4
1	A	321	LYS	2.3
1	B	78	GLY	2.3
1	B	97	GLN	2.3
1	B	275	GLN	2.3
1	A	116	LEU	2.3
1	B	55	PHE	2.3
1	B	20	PRO	2.3
1	A	134	THR	2.2
1	B	98	LEU	2.2
1	A	155	PRO	2.2
1	B	100	PHE	2.2
1	B	15	LYS	2.2
1	B	122	LYS	2.2
1	B	296	ARG	2.2
1	B	48	ILE	2.2
1	A	19	VAL	2.1
1	A	154	THR	2.1
1	A	308	GLY	2.1
1	B	205	ALA	2.1
1	A	291	THR	2.1
1	A	139	HIS	2.1
1	A	4	THR	2.1
1	B	224	VAL	2.1
1	B	166	ILE	2.1
1	B	210	ILE	2.1
1	B	345	ASN	2.0
1	A	118	LYS	2.0
1	A	129	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	216	SER	2.0
1	A	295	GLU	2.0
1	B	96	LYS	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($\text{\AA}^2$)	Q<0.9
2	IOD	B	1351	1/1	0.93	0.13	91,91,91,91	0
2	IOD	B	1350	1/1	0.94	0.19	88,88,88,88	0
2	IOD	A	1350	1/1	0.95	0.14	80,80,80,80	0
2	IOD	A	1351	1/1	0.97	0.10	73,73,73,73	0
2	IOD	B	1352	1/1	0.97	0.08	70,70,70,70	0
2	IOD	A	1349	1/1	0.98	0.03	46,46,46,46	0
2	IOD	B	1349	1/1	0.99	0.02	43,43,43,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.