Full wwPDB X-ray Structure Validation Report ⓘ

Jun 17, 2024 – 07:15 AM EDT

PDB ID	:	5OEV
Title	:	The structure of a glutathione synthetase like-effector (GSS22) from Globodera pallida in apoform.
Authors	:	Lilley, C.J.; Maqbool, A.; Wu, D.; Yusup, H.B.; Jones, L.M.; Birch, P.R.J.; Banfield, M.J.; Urwin, P.E.; Eves-van den Akker, S.
Deposited on	:	2017-07-10
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:

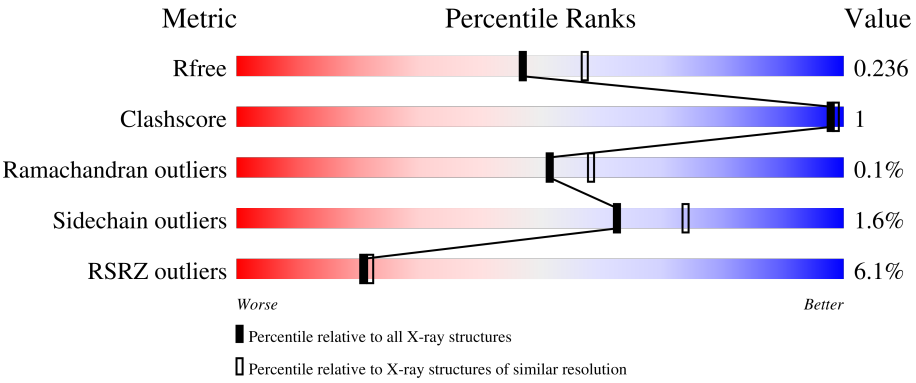
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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}	130704	6864 (2.20-2.16)
Clashscore	141614	7689 (2.20-2.16)
Ramachandran outliers	138981	7564 (2.20-2.16)
Sidechain outliers	138945	7564 (2.20-2.16)
RSRZ outliers	127900	6738 (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 <=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	510	4% 86% · 12%
1	B	510	7% 75% · 22%
1	C	510	3% 75% · 22%
1	D	510	7% 84% · 12%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 13835 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 Glutathione synthetase-like effector 22 (Gpa-GSS22-apo).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	451	Total	C	N	O	S	0	0	0
			3596	2280	631	670	15			
1	B	397	Total	C	N	O	S	0	0	0
			3150	1999	552	586	13			
1	C	397	Total	C	N	O	S	0	0	0
			3150	2000	553	584	13			
1	D	448	Total	C	N	O	S	0	0	0
			3574	2268	625	666	15			

- Molecule 2 is water.

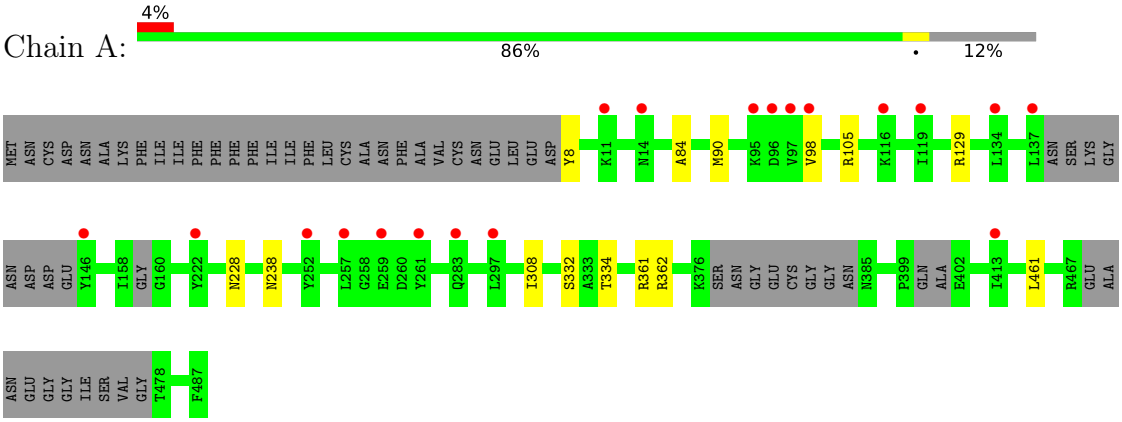
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	111	Total	O	0	0
			111	111		
2	B	58	Total	O	0	0
			58	58		
2	C	113	Total	O	0	0
			113	113		
2	D	83	Total	O	0	0
			83	83		

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.

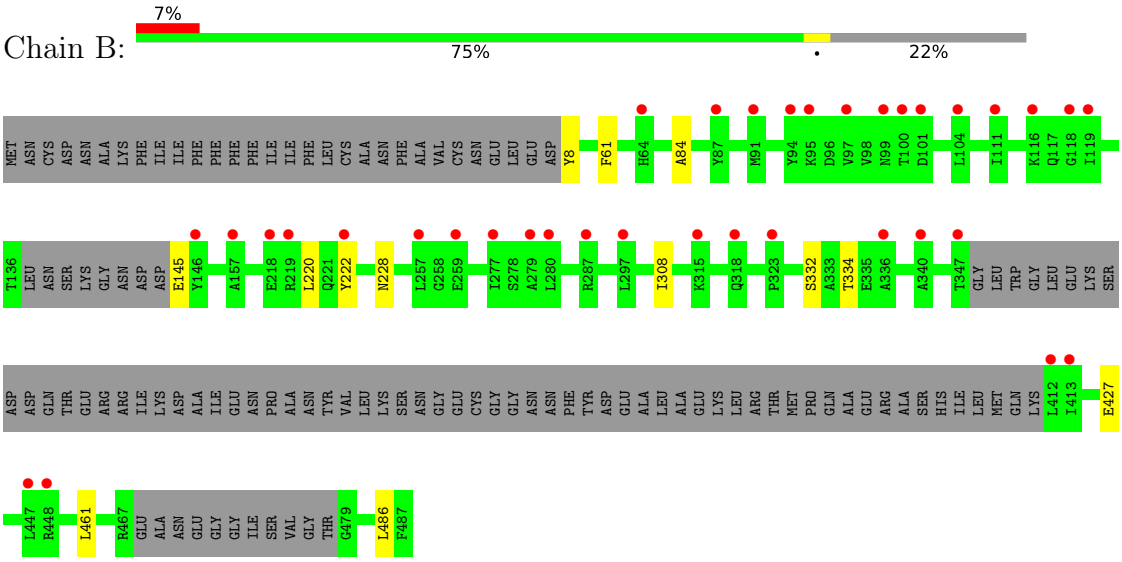
• Molecule 1: Glutathione synthetase-like effector 22 (Gpa-GSS22-apo)

Chain A:



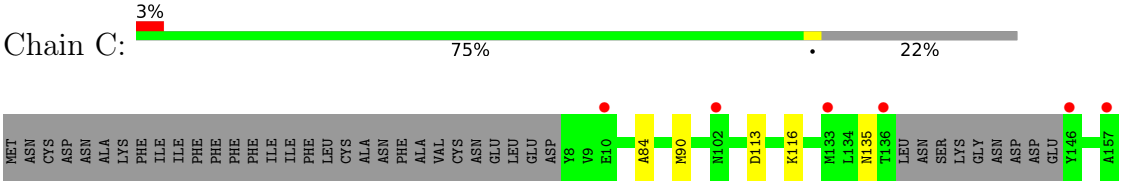
• Molecule 1: Glutathione synthetase-like effector 22 (Gpa-GSS22-apo)

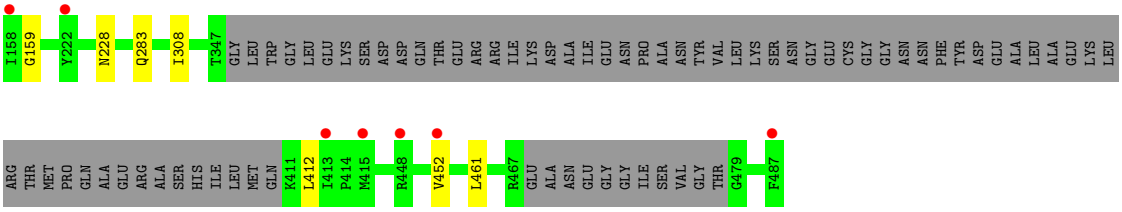
Chain B:



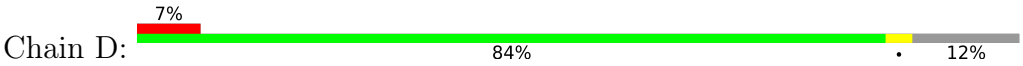
• Molecule 1: Glutathione synthetase-like effector 22 (Gpa-GSS22-apo)

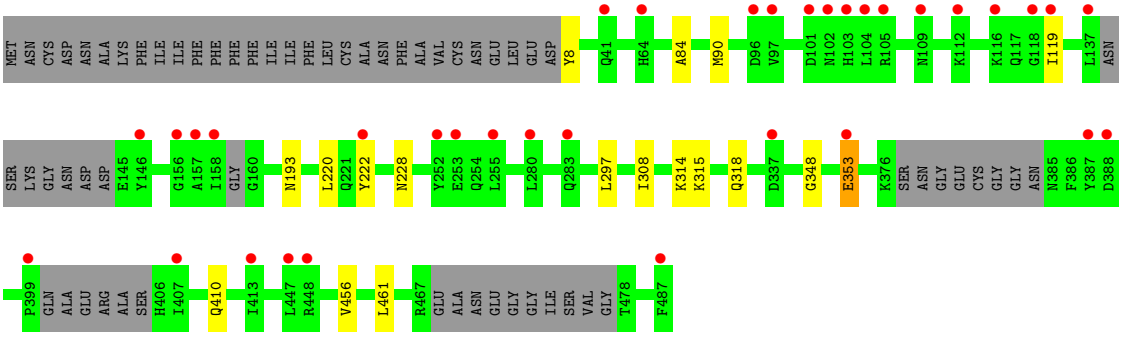
Chain C:





• Molecule 1: Glutathione synthetase-like effector 22 (Gpa-GSS22-apo)





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	62.26Å 122.39Å 132.77Å 90.00° 97.61° 90.00°	Depositor
Resolution (Å)	50.00 – 2.18 48.81 – 2.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (50.00-2.18) 100.0 (48.81-2.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.58 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.215 , 0.237 0.216 , 0.236	Depositor DCC
R_{free} test set	4973 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	39.6	Xtriage
Anisotropy	0.294	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 43.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	13835	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.49% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

5.1 Standard geometry

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	0.44	0/3658	0.67	2/4932 (0.0%)
1	B	0.46	0/3206	0.66	0/4326
1	C	0.43	0/3206	0.66	0/4325
1	D	0.45	0/3636	0.69	0/4903
All	All	0.44	0/13706	0.67	2/18486 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	362	ARG	NE-CZ-NH1	-6.62	116.99	120.30
1	A	129	ARG	NE-CZ-NH1	5.70	123.15	120.30

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	3596	0	3618	4	0
1	B	3150	0	3169	4	0
1	C	3150	0	3176	4	0
1	D	3574	0	3595	6	0
2	A	111	0	0	0	0
2	B	58	0	0	0	0
2	C	113	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	83	0	0	0	0
All	All	13835	0	13558	18	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 1.

All (18) 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:D:193:ASN:OD1	1:D:456:VAL:HG21	1.95	0.66
1:C:135:ASN:ND2	1:C:412:LEU:HA	2.19	0.57
1:D:220:LEU:HD12	1:D:222:TYR:CE2	2.41	0.56
1:D:315:LYS:NZ	1:D:353:GLU:OE2	2.37	0.56
1:B:220:LEU:HD12	1:B:222:TYR:CE2	2.42	0.55
1:B:332:SER:OG	1:B:334:THR:HG22	2.09	0.53
1:A:332:SER:OG	1:A:334:THR:HG22	2.09	0.52
1:D:348:GLY:H	1:D:410:GLN:HE21	1.61	0.49
1:A:98:VAL:HG13	1:A:105:ARG:HG3	1.94	0.47
1:D:84:ALA:CB	1:D:308:ILE:HD13	2.47	0.45
1:A:84:ALA:CB	1:A:308:ILE:HD13	2.46	0.45
1:B:84:ALA:CB	1:B:308:ILE:HD13	2.47	0.45
1:C:84:ALA:CB	1:C:308:ILE:HD13	2.47	0.45
1:C:135:ASN:HD22	1:C:412:LEU:HA	1.81	0.44
1:C:113:ASP:O	1:C:116:LYS:HG2	2.20	0.41
1:A:238:ASN:HD22	1:A:238:ASN:HA	1.74	0.41
1:D:456:VAL:O	1:D:456:VAL:HG23	2.20	0.41
1:B:61:PHE:O	1:B:486:LEU:HA	2.21	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	439/510 (86%)	435 (99%)	4 (1%)	0	100	100
1	B	389/510 (76%)	386 (99%)	3 (1%)	0	100	100
1	C	389/510 (76%)	383 (98%)	5 (1%)	1 (0%)	41	43
1	D	436/510 (86%)	432 (99%)	4 (1%)	0	100	100
All	All	1653/2040 (81%)	1636 (99%)	16 (1%)	1 (0%)	51	58

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	159	GLY

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	390/436 (89%)	385 (99%)	5 (1%)	69	79
1	B	342/436 (78%)	337 (98%)	5 (2%)	65	76
1	C	342/436 (78%)	337 (98%)	5 (2%)	65	76
1	D	388/436 (89%)	379 (98%)	9 (2%)	50	60
All	All	1462/1744 (84%)	1438 (98%)	24 (2%)	62	74

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	TYR
1	A	90	MET
1	A	228	ASN
1	A	361	ARG
1	A	461	LEU
1	B	8	TYR
1	B	145	GLU
1	B	228	ASN
1	B	427	GLU
1	B	461	LEU

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Mol	Chain	Res	Type
1	C	90	MET
1	C	228	ASN
1	C	283	GLN
1	C	452	VAL
1	C	461	LEU
1	D	8	TYR
1	D	90	MET
1	D	119	ILE
1	D	228	ASN
1	D	297	LEU
1	D	314	LYS
1	D	318	GLN
1	D	353	GLU
1	D	461	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	238	ASN
1	B	31	HIS
1	B	117	GLN
1	B	460	HIS
1	C	31	HIS
1	C	135	ASN
1	D	31	HIS
1	D	33	ASN
1	D	238	ASN
1	D	318	GLN
1	D	410	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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, 95^{th} 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	451/510 (88%)	0.48	19 (4%)	36	37	26, 45, 70, 82	0
1	B	397/510 (77%)	0.69	36 (9%)	9	9	30, 50, 78, 94	0
1	C	397/510 (77%)	0.45	13 (3%)	46	47	28, 41, 63, 82	0
1	D	448/510 (87%)	0.59	35 (7%)	13	13	29, 47, 72, 99	0
All	All	1693/2040 (82%)	0.55	103 (6%)	21	22	26, 46, 72, 99	0

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	146	TYR	6.2
1	B	413	ILE	6.0
1	B	119	ILE	5.8
1	D	222	TYR	5.2
1	B	100	THR	4.8
1	B	97	VAL	4.7
1	D	283	GLN	4.6
1	A	119	ILE	4.6
1	B	101	ASP	4.0
1	D	158	ILE	3.7
1	B	323	PRO	3.7
1	B	257	LEU	3.6
1	B	87	TYR	3.6
1	D	146	TYR	3.6
1	C	222	TYR	3.6
1	B	157	ALA	3.6
1	C	136	THR	3.6
1	C	413	ILE	3.5
1	D	104	LEU	3.5
1	A	283	GLN	3.4
1	D	137	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	447	LEU	3.3
1	D	252	TYR	3.3
1	D	280	LEU	3.3
1	D	118	GLY	3.2
1	D	413	ILE	3.2
1	B	347	THR	3.2
1	B	116	LYS	3.2
1	D	157	ALA	3.1
1	B	99	ASN	3.1
1	B	95	LYS	3.1
1	B	259	GLU	3.1
1	C	415	MET	3.1
1	A	222	TYR	3.0
1	B	222	TYR	3.0
1	B	315	LYS	3.0
1	C	102	ASN	3.0
1	D	102	ASN	3.0
1	A	146	TYR	2.9
1	D	447	LEU	2.9
1	A	297	LEU	2.9
1	B	336	ALA	2.9
1	D	387	TYR	2.9
1	B	448	ARG	2.8
1	D	103	HIS	2.8
1	D	119	ILE	2.8
1	B	340	ALA	2.7
1	B	318	GLN	2.7
1	B	219	ARG	2.7
1	B	279	ALA	2.7
1	D	399	PRO	2.7
1	A	116	LYS	2.7
1	B	146	TYR	2.7
1	B	111	ILE	2.7
1	A	259	GLU	2.6
1	D	109	ASN	2.6
1	A	137	LEU	2.6
1	A	96	ASP	2.6
1	A	14	ASN	2.6
1	B	104	LEU	2.6
1	C	487	PHE	2.5
1	D	253	GLU	2.5
1	C	157	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	287	ARG	2.5
1	A	261	TYR	2.4
1	B	412	LEU	2.4
1	D	353	GLU	2.4
1	D	487	PHE	2.4
1	C	452	VAL	2.4
1	B	118	GLY	2.3
1	D	101	ASP	2.3
1	D	407	ILE	2.3
1	B	94	TYR	2.3
1	B	297	LEU	2.3
1	B	91	MET	2.3
1	A	257	LEU	2.3
1	B	64	HIS	2.3
1	D	96	ASP	2.3
1	B	280	LEU	2.2
1	D	156	GLY	2.2
1	D	337	ASP	2.2
1	D	97	VAL	2.2
1	C	133	MET	2.2
1	C	158	ILE	2.2
1	D	105	ARG	2.2
1	A	98	VAL	2.2
1	D	116	LYS	2.2
1	A	134	LEU	2.2
1	C	448	ARG	2.2
1	A	413	ILE	2.1
1	D	255	LEU	2.1
1	C	10	GLU	2.1
1	D	64	HIS	2.1
1	D	112	LYS	2.1
1	D	448	ARG	2.1
1	D	41	GLN	2.1
1	A	252	TYR	2.1
1	A	11	LYS	2.1
1	A	97	VAL	2.0
1	B	218	GLU	2.0
1	B	277	ILE	2.0
1	A	95	LYS	2.0
1	D	388	ASP	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 monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.