Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:06 AM GMT

PDB ID	:	2VXQ
Title	:	CRYSTAL STRUCTURE OF THE MAJOR GRASS POLLEN ALLERGEN PHL P 2 IN COMPLEX WITH ITS SPECIFIC IGE-FAB
Authors	:	Padavattan, S.; Flicker, S.; Schirmer, T.; Madritsch, C.; Randow, S.; Reese, G.; Vieths, S.; Lupinek, C.; Ebner, C.; Valenta, R.; Markovic-Housley, Z.
Deposited on	:	2008-07-08
Resolution	:	1.90 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

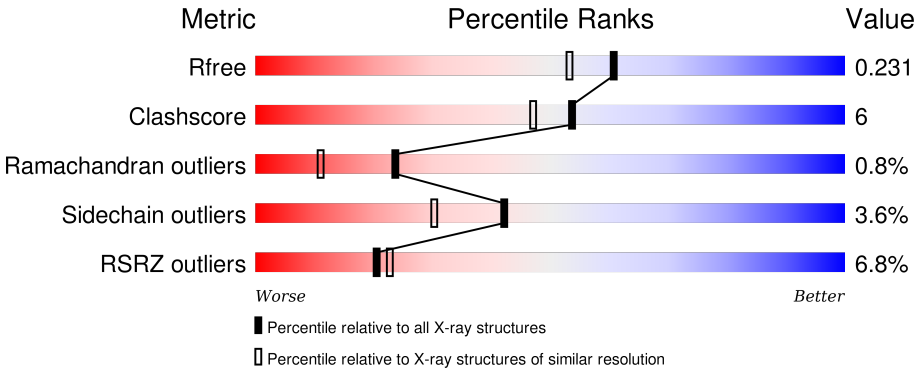
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 1.90 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}	91344	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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. 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	96	7%, 85%, 7%
2	H	216	6%, 82%, 12%
3	L	214	7%, 89%, 9%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4491 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 POLLEN ALLERGEN PHL P 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	92	Total	C	N	O	S	29	0	0
			730	467	116	144	3			

- Molecule 2 is a protein called FAB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	213	Total	C	N	O	S	39	0	0
			1596	1013	267	311	5			

- Molecule 3 is a protein called FAB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	213	Total	C	N	O	S	32	0	0
			1641	1026	275	335	5			

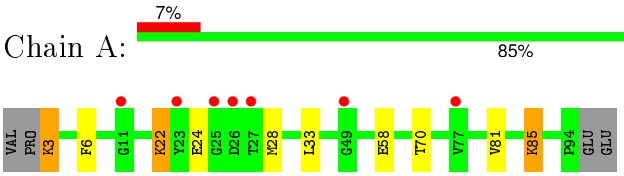
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	62	Total	O	0	0
			62	62		
4	H	211	Total	O	0	0
			211	211		
4	L	251	Total	O	0	0
			251	251		

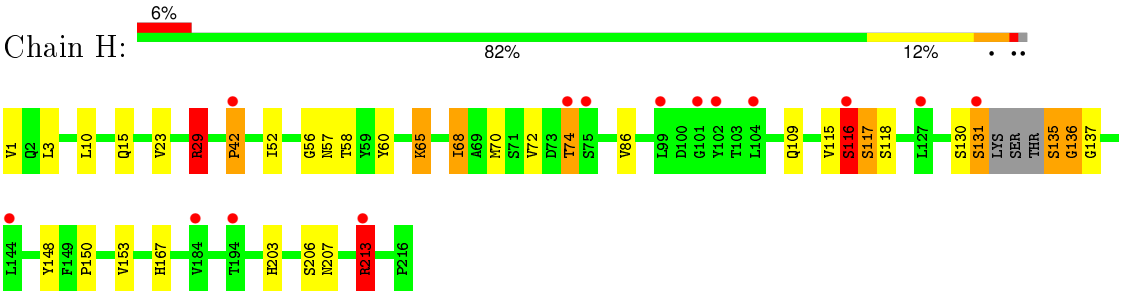
3 Residue-property plots (i)

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.

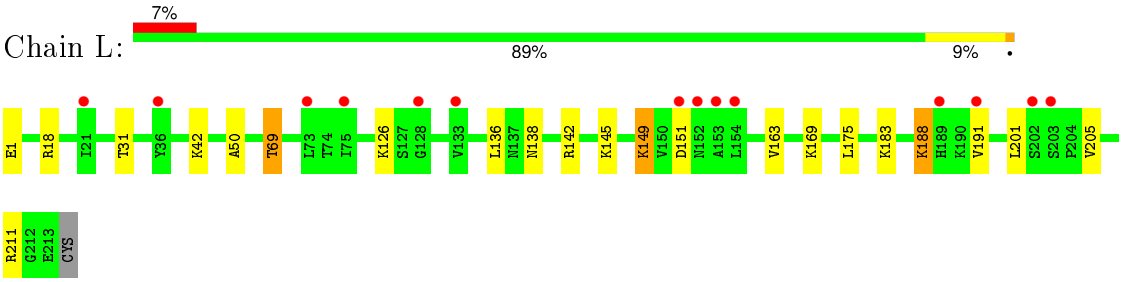
- Molecule 1: POLLEN ALLERGEN PHL P 2



- Molecule 2: FAB



- Molecule 3: FAB



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α, β, γ	105.44Å 105.44Å 110.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.90 27.56 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.3 (30.00-1.90) 98.3 (27.56-1.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.45 (at 1.91Å)	Xtriage
Refinement program	REFMAC 5.2.0019 24/04/2001	Depositor
R, R_{free}	0.177 , 0.226 0.182 , 0.231	Depositor DCC
R_{free} test set	2466 reflections (5.34%)	DCC
Wilson B-factor (Å^2)	25.0	Xtriage
Anisotropy	0.379	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 42.1	EDS
Estimated twinning fraction	0.015 for -h,l,k 0.014 for -l,-k,-h	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 48678 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	4491	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.31% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.83	4/748 (0.5%)	0.84	5/1011 (0.5%)
2	H	2.39	10/1637 (0.6%)	3.89	8/2236 (0.4%)
3	L	1.66	11/1676 (0.7%)	1.64	10/2273 (0.4%)
All	All	1.89	25/4061 (0.6%)	2.71	23/5520 (0.4%)

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
2	H	0	4

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	213	ARG	CZ-NH2	-62.05	0.52	1.33
2	H	213	ARG	CD-NE	50.53	2.32	1.46
3	L	211	ARG	NE-CZ	-40.67	0.80	1.33
2	H	213	ARG	CZ-NH1	36.15	1.80	1.33
3	L	149	LYS	CD-CE	33.23	2.34	1.51
2	H	116	SER	CB-OG	26.97	1.77	1.42
3	L	1	GLU	CG-CD	-25.92	1.13	1.51
2	H	213	ARG	CG-CD	-17.49	1.08	1.51
3	L	145	LYS	CD-CE	-16.36	1.10	1.51
1	A	85	LYS	CG-CD	-15.75	0.98	1.52
3	L	145	LYS	CE-NZ	11.37	1.77	1.49
3	L	149	LYS	CG-CD	11.17	1.90	1.52
3	L	126	LYS	CG-CD	10.34	1.87	1.52
2	H	130	SER	CA-CB	-9.01	1.39	1.52
3	L	183	LYS	CD-CE	-8.73	1.29	1.51
3	L	126	LYS	CD-CE	-8.59	1.29	1.51
3	L	188	LYS	CA-CB	-8.59	1.35	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	131	SER	CB-OG	8.28	1.53	1.42
1	A	58	GLU	CG-CD	7.27	1.62	1.51
2	H	136	GLY	C-N	-6.95	1.20	1.33
1	A	24	GLU	CB-CG	6.43	1.64	1.52
3	L	145	LYS	CB-CG	6.37	1.69	1.52
2	H	57	ASN	CB-CG	-6.22	1.36	1.51
1	A	22	LYS	CB-CG	5.84	1.68	1.52
2	H	109	GLN	CB-CG	-5.38	1.38	1.52

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	213	ARG	NE-CZ-NH1	-170.40	35.10	120.30
2	H	213	ARG	NE-CZ-NH2	43.84	142.22	120.30
2	H	213	ARG	NH1-CZ-NH2	37.75	160.93	119.40
3	L	211	ARG	NE-CZ-NH1	-37.53	101.53	120.30
3	L	211	ARG	NE-CZ-NH2	36.84	138.72	120.30
3	L	149	LYS	CD-CE-NZ	-35.76	29.45	111.70
3	L	211	ARG	CD-NE-CZ	28.86	164.01	123.60
2	H	29	ARG	CA-CB-CG	-13.76	83.14	113.40
1	A	85	LYS	CB-CG-CD	13.75	147.36	111.60
3	L	42	LYS	CD-CE-NZ	10.50	135.86	111.70
3	L	42	LYS	CG-CD-CE	10.24	142.62	111.90
1	A	3	LYS	CA-CB-CG	9.58	134.47	113.40
2	H	213	ARG	CB-CG-CD	8.38	133.38	111.60
3	L	126	LYS	CB-CG-CD	-8.35	89.89	111.60
1	A	22	LYS	CA-CB-CG	-7.39	97.13	113.40
2	H	57	ASN	CA-CB-CG	6.92	128.61	113.40
3	L	145	LYS	CA-CB-CG	-6.43	99.25	113.40
1	A	22	LYS	CB-CG-CD	6.38	128.20	111.60
2	H	65	LYS	CG-CD-CE	-5.97	93.99	111.90
2	H	116	SER	N-CA-C	5.48	125.80	111.00
1	A	85	LYS	CG-CD-CE	5.47	128.32	111.90
3	L	183	LYS	CG-CD-CE	5.37	128.02	111.90
3	L	169	LYS	CD-CE-NZ	5.11	123.45	111.70

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	115	VAL	Peptide
2	H	116	SER	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
2	H	135	SER	Peptide
2	H	213	ARG	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	730	0	696	5	0
2	H	1596	0	1567	33	0
3	L	1641	0	1589	13	0
4	A	62	0	0	0	0
4	H	211	0	0	4	0
4	L	251	0	0	4	1
All	All	4491	0	3852	49	1

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.

All (49) 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)
3:L:149:LYS:CG	3:L:149:LYS:CD	1.90	1.45
2:H:10:LEU:CD1	2:H:116:SER:HB2	1.53	1.38
2:H:213:ARG:NE	2:H:213:ARG:NH2	1.78	1.28
2:H:10:LEU:HD11	2:H:116:SER:HB2	1.14	1.10
2:H:10:LEU:HD12	2:H:116:SER:HB2	1.37	1.05
2:H:10:LEU:CD1	2:H:116:SER:CB	2.36	1.03
2:H:10:LEU:HD11	2:H:116:SER:CB	1.89	1.03
2:H:213:ARG:CD	2:H:213:ARG:NE	2.32	0.92
1:A:28:MET:CE	1:A:70:THR:HG22	2.09	0.83
2:H:213:ARG:NH1	2:H:213:ARG:NH2	2.29	0.80
2:H:10:LEU:HD12	2:H:116:SER:CB	2.09	0.79
2:H:68:ILE:HD11	2:H:70:MET:HG3	1.66	0.78
1:A:28:MET:HE2	1:A:70:THR:HG22	1.66	0.77
3:L:149:LYS:CD	3:L:149:LYS:CB	2.63	0.75
2:H:117:SER:N	4:H:2129:HOH:O	2.24	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:65:LYS:HA	2:H:68:ILE:HG22	1.74	0.69
3:L:201:LEU:HD13	3:L:205:VAL:HG23	1.75	0.68
2:H:213:ARG:NH2	2:H:213:ARG:CZ	0.52	0.66
3:L:18:ARG:NH2	4:L:2044:HOH:O	2.18	0.64
2:H:150:PRO:O	2:H:203:HIS:HE1	1.81	0.64
1:A:28:MET:HE1	1:A:70:THR:HG22	1.80	0.61
2:H:117:SER:HA	4:H:2126:HOH:O	1.99	0.60
2:H:1:VAL:N	4:H:2003:HOH:O	2.29	0.57
2:H:68:ILE:CD1	2:H:70:MET:HG3	2.33	0.56
2:H:213:ARG:CZ	2:H:213:ARG:HH21	1.21	0.55
3:L:163:VAL:HG22	3:L:175:LEU:HD12	1.89	0.55
2:H:213:ARG:CZ	2:H:213:ARG:HH22	1.21	0.54
2:H:167:HIS:HE1	3:L:138:ASN:HD21	1.56	0.54
2:H:15:GLN:O	2:H:86:VAL:HG22	2.08	0.54
2:H:167:HIS:CE1	3:L:138:ASN:HD21	2.25	0.53
3:L:151:ASP:HA	3:L:191:VAL:CG1	2.39	0.52
1:A:33:LEU:HD12	1:A:33:LEU:C	2.30	0.51
2:H:167:HIS:HD2	4:H:2078:HOH:O	1.95	0.50
2:H:60:TYR:CD1	2:H:68:ILE:HD12	2.47	0.49
3:L:142:ARG:CZ	3:L:163:VAL:HG21	2.43	0.49
3:L:69:THR:HB	4:L:2061:HOH:O	2.12	0.49
2:H:203:HIS:HD2	2:H:206:SER:OG	1.95	0.49
2:H:65:LYS:HA	2:H:68:ILE:CG2	2.42	0.49
2:H:60:TYR:CE1	2:H:68:ILE:HD12	2.49	0.47
3:L:31:THR:O	3:L:50:ALA:HA	2.15	0.46
2:H:148:TYR:CE1	2:H:153:VAL:HG13	2.52	0.45
3:L:69:THR:CG2	4:L:2061:HOH:O	2.65	0.45
2:H:52:ILE:HD13	2:H:72:VAL:HG23	1.99	0.44
1:A:6:PHE:CD1	1:A:81:VAL:HG11	2.54	0.43
3:L:69:THR:HG22	4:L:2061:HOH:O	2.18	0.43
2:H:213:ARG:CD	2:H:213:ARG:HH11	2.32	0.41
2:H:56:GLY:O	2:H:58:THR:HG23	2.21	0.41
2:H:29:ARG:HB2	2:H:74:THR:HG23	2.04	0.40
2:H:3:LEU:HD22	2:H:23:VAL:HG22	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:2128:HOH:O	4:L:2128:HOH:O[7_555]	1.28	0.92

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	90/96 (94%)	90 (100%)	0	0	100 100
2	H	209/216 (97%)	201 (96%)	4 (2%)	4 (2%)	10 2
3	L	211/214 (99%)	203 (96%)	8 (4%)	0	100 100
All	All	510/526 (97%)	494 (97%)	12 (2%)	4 (1%)	24 11

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	42	PRO
2	H	136	GLY
2	H	118	SER
2	H	137	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	78/82 (95%)	75 (96%)	3 (4%)	40 28
2	H	180/183 (98%)	170 (94%)	10 (6%)	26 14
3	L	187/188 (100%)	184 (98%)	3 (2%)	70 66
All	All	445/453 (98%)	429 (96%)	16 (4%)	42 30

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	22	LYS
1	A	85	LYS
2	H	29	ARG
2	H	42	PRO
2	H	68	ILE
2	H	74	THR
2	H	116	SER
2	H	117	SER
2	H	131	SER
2	H	135	SER
2	H	207	ASN
2	H	213	ARG
3	L	69	THR
3	L	136	LEU
3	L	188	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
2	H	84	ASN
2	H	167	HIS
2	H	203	HIS
2	H	207	ASN
3	L	79	GLN
3	L	137	ASN
3	L	138	ASN
3	L	155	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 carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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, 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	92/96 (95%)	0.61	7 (7%)	17	18	21, 29, 43, 54	8 (8%)
2	H	211/216 (97%)	0.62	14 (6%)	22	24	19, 27, 39, 50	10 (4%)
3	L	213/214 (99%)	0.63	14 (6%)	22	24	20, 27, 40, 69	10 (4%)
All	All	516/526 (98%)	0.63	35 (6%)	20	23	19, 27, 41, 69	28 (5%)

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	116	SER	4.4
2	H	104	LEU	4.4
2	H	99	LEU	3.8
3	L	191	VAL	3.8
3	L	153	ALA	3.4
3	L	154	LEU	3.2
1	A	11	GLY	3.1
2	H	75	SER	3.1
1	A	49	GLY	3.1
1	A	27	THR	3.1
2	H	144	LEU	3.0
3	L	133	VAL	3.0
2	H	127	LEU	2.9
3	L	152	ASN	2.8
1	A	77	VAL	2.8
2	H	74	THR	2.6
2	H	102	TYR	2.5
2	H	42	PRO	2.3
2	H	131	SER	2.3
1	A	23	TYR	2.3
3	L	189	HIS	2.3
3	L	151	ASP	2.3
2	H	184	VAL	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	L	75	ILE	2.2
3	L	128	GLY	2.2
1	A	26	ASP	2.2
3	L	36	TYR	2.2
3	L	202	SER	2.2
3	L	21	ILE	2.1
2	H	101	GLY	2.1
3	L	73	LEU	2.1
2	H	194	THR	2.1
1	A	25	GLY	2.1
2	H	213	ARG	2.0
3	L	203	SER	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 carbohydrates 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.