Full wwPDB X-ray Structure Validation Report (i)

May 30, 2023 – 04:04 pm BST

PDB ID	:	8AS3
Title	:	Structure of arrestin2 in complex with 6P CCR5 phosphopeptide and Fab30
Authors	:	Isaikina, P.; Jakob, R.P.; Maier, T.; Grzesiek, S.
Deposited on	:	2022-08-18
Resolution	:	3.50 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 (i) 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 (1)) were used in the production of this report:

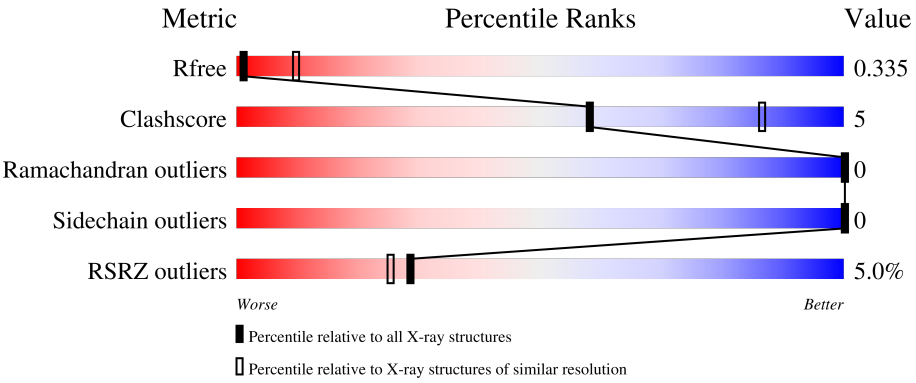
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.33
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.33

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 3.50 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	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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	359	5% 88% 8% .
2	B	21	5% 24% 10% 5% 62%
3	H	233	5% 81% 13% 6%
4	L	220	4% 81% 15% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12110 atoms, of which 6043 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 Beta-arrestin-1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	343	5508	1743	2793	465	501	6	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	150	LEU	CYS	engineered mutation	UNP P49407
A	242	VAL	CYS	engineered mutation	UNP P49407
A	251	VAL	CYS	engineered mutation	UNP P49407
A	269	SER	CYS	engineered mutation	UNP P49407

- Molecule 2 is a protein called C-C chemokine receptor type 5.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	P			
2	B	8	128	38	53	11	23	3	0	0	0

- Molecule 3 is a protein called Fab30 heavy chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
3	H	220	3254	1046	1604	275	324	5	0	0	0

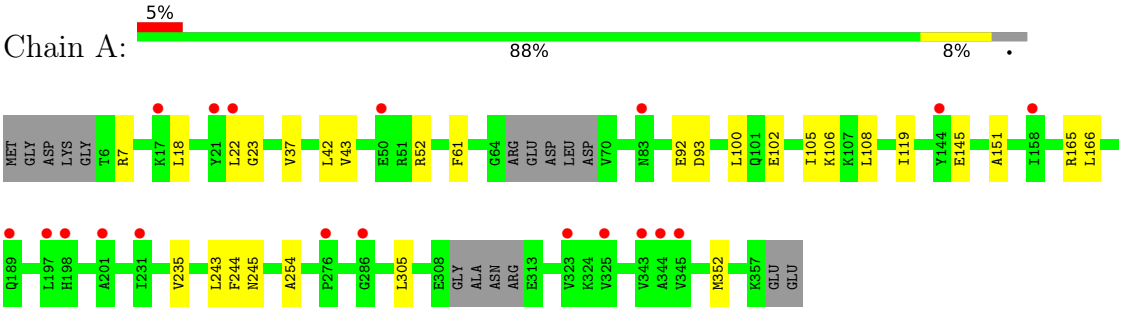
- Molecule 4 is a protein called Fab30 light chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
4	L	212	3220	1020	1593	273	329	5	0	0	0

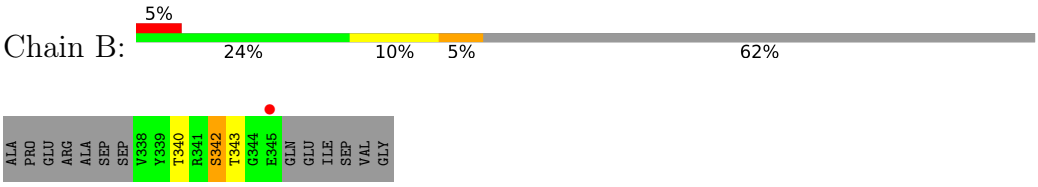
3 Residue-property plots (i)

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.

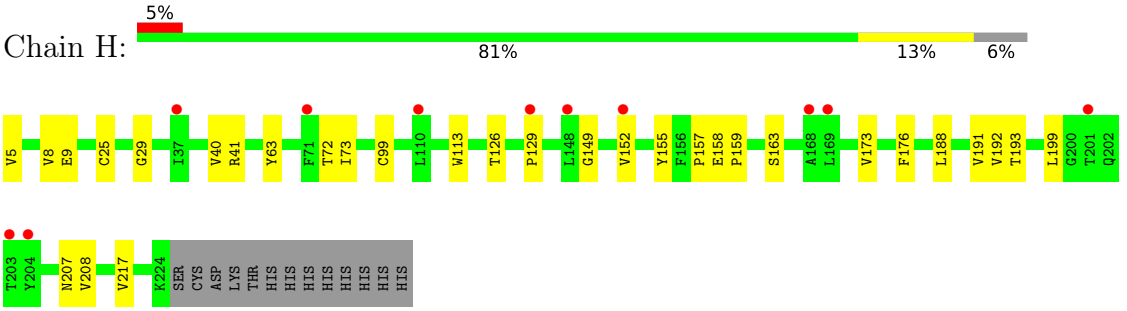
• Molecule 1: Beta-arrestin-1



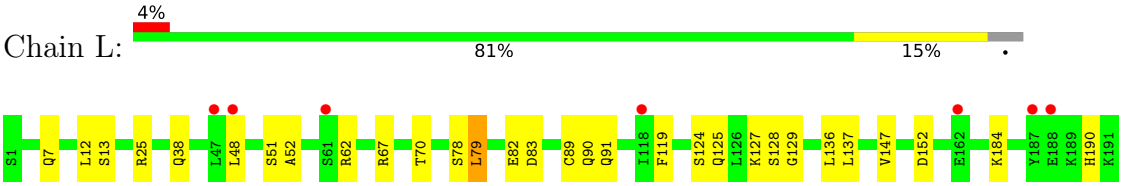
• Molecule 2: C-C chemokine receptor type 5

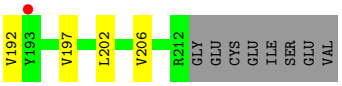


• Molecule 3: Fab30 heavy chain



• Molecule 4: Fab30 light chain




V192
V193
V197
L202
V206
R212
GLY
GLU
CYS
GLU
ILE
SER
GLU
VAL

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	116.31Å 121.06Å 145.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.31 – 3.50 49.31 – 3.50	Depositor EDS
% Data completeness (in resolution range)	98.3 (49.31-3.50) 98.3 (49.31-3.50)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.01 (at 3.48Å)	Xtriage
Refinement program	PHENIX 1.18.1_3865	Depositor
R, R_{free}	0.284 , 0.333 0.284 , 0.335	Depositor DCC
R_{free} test set	659 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	171.8	Xtriage
Anisotropy	0.281	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 137.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.036 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	12110	wwPDB-VP
Average B, all atoms (Å^2)	220.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.01% 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

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

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	0.25	0/2772	0.46	0/3759
2	B	0.23	0/41	0.35	0/50
3	H	0.33	0/1693	0.51	0/2309
4	L	0.29	0/1662	0.58	1/2257 (0.0%)
All	All	0.29	0/6168	0.51	1/8375 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	L	79	LEU	CB-CG-CD1	-9.55	94.76	111.00

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	2715	2793	2793	19	0
2	B	75	53	52	1	0
3	H	1650	1604	1604	18	0
4	L	1627	1593	1596	22	0
All	All	6067	6043	6045	58	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 5.

All (58) 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:H:63:TYR:OH	3:H:73:ILE:N	2.18	0.76
3:H:5:VAL:HG12	3:H:29:GLY:HA3	1.68	0.75
3:H:8:VAL:O	3:H:25:CYS:HA	1.88	0.74
3:H:63:TYR:OH	3:H:72:THR:HA	1.98	0.63
1:A:305:LEU:HD13	1:A:352:MET:HE1	1.82	0.61
1:A:42:LEU:HD22	1:A:108:LEU:HD12	1.83	0.60
1:A:18:LEU:HD12	1:A:43:VAL:HG22	1.85	0.58
1:A:23:GLY:HA3	1:A:100:LEU:HD11	1.87	0.56
4:L:202:LEU:HD13	4:L:206:VAL:HG22	1.86	0.56
1:A:18:LEU:CD1	1:A:43:VAL:HG22	2.36	0.56
1:A:22:LEU:HD12	1:A:166:LEU:HD23	1.89	0.55
3:H:199:LEU:C	3:H:199:LEU:HD23	2.29	0.52
1:A:61:PHE:CE2	1:A:243:LEU:HD11	2.45	0.52
4:L:137:LEU:HD12	4:L:137:LEU:N	2.25	0.52
1:A:37:VAL:HG23	1:A:119:ILE:HD11	1.90	0.52
1:A:305:LEU:HD13	1:A:352:MET:CE	2.40	0.52
4:L:25:ARG:HG3	4:L:70:THR:OG1	2.11	0.50
1:A:105:ILE:HG13	1:A:106:LYS:N	2.27	0.49
1:A:93:ASP:O	1:A:93:ASP:OD1	2.31	0.49
3:H:126:THR:HG23	3:H:157:PRO:HG2	1.95	0.48
3:H:9:GLU:OE2	3:H:99:CYS:HB3	2.14	0.48
3:H:208:VAL:HB	3:H:217:VAL:HB	1.95	0.47
4:L:152:ASP:HA	4:L:192:VAL:HB	1.97	0.47
4:L:119:PHE:CE1	4:L:136:LEU:HD12	2.49	0.47
3:H:176:PHE:O	3:H:188:LEU:HG	2.15	0.46
1:A:235:VAL:HB	1:A:254:ALA:HB3	1.97	0.46
4:L:129:GLY:HA2	4:L:184:LYS:HD3	1.98	0.46
1:A:102:GLU:HA	1:A:105:ILE:HG12	1.98	0.46
4:L:82:GLU:HA	4:L:82:GLU:OE1	2.15	0.46
1:A:52:ARG:HB2	1:A:151:ALA:O	2.17	0.45
3:H:192:VAL:HG12	3:H:193:THR:N	2.31	0.45
4:L:62:ARG:HD2	4:L:78:SER:O	2.17	0.45
4:L:12:LEU:HD23	4:L:13:SER:N	2.32	0.45
1:A:145:GLU:OE2	1:A:165:ARG:HD3	2.18	0.44
4:L:125:GLN:O	4:L:128:SER:OG	2.25	0.44
3:H:149:GLY:HA3	3:H:191:VAL:HG12	2.00	0.44
4:L:206:VAL:HG23	4:L:206:VAL:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:124:SER:HA	4:L:127:LYS:HE2	2.00	0.44
3:H:163:SER:O	3:H:207:ASN:HB3	2.18	0.43
3:H:173:VAL:HG23	3:H:192:VAL:HG22	2.00	0.43
1:A:92:GLU:O	1:A:92:GLU:HG3	2.18	0.43
4:L:192:VAL:O	4:L:192:VAL:HG12	2.18	0.43
3:H:152:VAL:HG12	3:H:155:TYR:CD1	2.53	0.42
4:L:90:GLN:HG2	4:L:91:GLN:N	2.34	0.42
3:H:40:VAL:HG12	3:H:41:ARG:N	2.34	0.42
1:A:7:ARG:NH2	2:B:342:SEP:C	2.82	0.42
4:L:147:VAL:HG12	4:L:197:VAL:HG12	2.01	0.42
1:A:7:ARG:HD3	4:L:67:ARG:NH2	2.34	0.42
4:L:38:GLN:HB2	4:L:48:LEU:HD11	2.02	0.42
4:L:62:ARG:NH1	4:L:83:ASP:OD2	2.48	0.42
4:L:79:LEU:HD12	4:L:79:LEU:HA	1.76	0.42
3:H:158:GLU:N	3:H:159:PRO:CD	2.83	0.42
1:A:244:PHE:O	1:A:245:ASN:HB2	2.20	0.41
3:H:40:VAL:HG21	3:H:113:TRP:CZ3	2.55	0.41
4:L:51:SER:O	4:L:52:ALA:HB3	2.20	0.41
3:H:129:PRO:HB2	3:H:152:VAL:HG13	2.03	0.41
4:L:7:GLN:HG3	4:L:89:CYS:SG	2.61	0.41
4:L:152:ASP:HB2	4:L:190:HIS:HB2	2.01	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	337/359 (94%)	325 (96%)	12 (4%)	0	100	100
2	B	3/21 (14%)	3 (100%)	0	0	100	100
3	H	218/233 (94%)	212 (97%)	6 (3%)	0	100	100
4	L	210/220 (96%)	197 (94%)	13 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	768/833 (92%)	737 (96%)	31 (4%)	0	100 100

There are no Ramachandran outliers to report.

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	305/317 (96%)	305 (100%)	0	100 100
2	B	4/11 (36%)	4 (100%)	0	100 100
3	H	183/196 (93%)	183 (100%)	0	100 100
4	L	188/195 (96%)	188 (100%)	0	100 100
All	All	680/719 (95%)	680 (100%)	0	100 100

There are no protein residues with a non-rotameric sidechain to report.

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues 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	SEP	B	342	2	8,9,10	1.56	1 (12%)	8,12,14	1.21	1 (12%)
2	TPO	B	340	2	8,10,11	1.67	1 (12%)	10,14,16	1.96	1 (10%)
2	TPO	B	343	2	8,10,11	1.58	1 (12%)	10,14,16	1.82	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	SEP	B	342	2	-	0/5/8/10	-
2	TPO	B	340	2	-	0/9/11/13	-
2	TPO	B	343	2	-	2/9/11/13	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	340	TPO	P-O1P	3.54	1.62	1.50
2	B	342	SEP	P-O1P	3.38	1.61	1.50
2	B	343	TPO	P-O1P	3.35	1.61	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	340	TPO	P-OG1-CB	-5.70	105.98	123.21
2	B	343	TPO	P-OG1-CB	-5.10	107.79	123.21
2	B	342	SEP	P-OG-CB	-2.13	112.42	118.30

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	343	TPO	N-CA-CB-OG1
2	B	343	TPO	O-C-CA-CB

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	342	SEP	1	0

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	343/359 (95%)	0.48	19 (5%)	25	22	144, 204, 265, 310	0
2	B	5/21 (23%)	1.26	1 (20%)	1	1	199, 206, 250, 294	0
3	H	220/233 (94%)	0.34	11 (5%)	28	25	138, 181, 250, 312	0
4	L	212/220 (96%)	0.31	8 (3%)	40	36	151, 192, 254, 348	0
All	All	780/833 (93%)	0.40	39 (5%)	28	25	138, 196, 258, 348	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	L	187	TYR	4.3
2	B	345	GLU	3.5
1	A	325	VAL	3.5
3	H	148	LEU	3.3
3	H	204	TYR	3.3
1	A	344	ALA	3.2
4	L	47	LEU	3.2
1	A	158	ILE	3.1
1	A	197	LEU	3.0
3	H	169	LEU	2.9
1	A	83	ASN	2.9
3	H	168	ALA	2.9
3	H	201	THR	2.9
1	A	189	GLN	2.9
1	A	144	TYR	2.7
1	A	286	GLY	2.6
1	A	17	LYS	2.5
1	A	345	VAL	2.5
3	H	203	THR	2.4
3	H	110	LEU	2.4
4	L	118	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	198	HIS	2.4
1	A	276	PRO	2.4
1	A	231	ILE	2.3
4	L	193	TYR	2.3
1	A	21	TYR	2.3
3	H	129	PRO	2.3
3	H	152	VAL	2.3
4	L	48	LEU	2.2
3	H	71	PHE	2.2
1	A	22	LEU	2.2
4	L	61	SER	2.2
1	A	343	VAL	2.2
1	A	323	VAL	2.1
3	H	37	ILE	2.1
4	L	162	GLU	2.1
4	L	188	GLU	2.1
1	A	201	ALA	2.1
1	A	50	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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, 95^{th} 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	TPO	B	343	11/12	0.79	0.38	198,220,259,265	0
2	TPO	B	340	11/12	0.84	0.24	200,211,252,254	0
2	SEP	B	342	10/11	0.91	0.32	205,230,278,280	0

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.