Full wwPDB X-ray Structure Validation Report ⓘ

Sep 25, 2023 – 01:39 AM EDT

PDB ID	:	5VJO
Title	:	Complex between HyHEL10 Fab fragment heavy chain mutant I29F and Pekin duck egg lysozyme isoform I (DEL-I)
Authors	:	Langley, D.B.; Christ, D.
Deposited on	:	2017-04-19
Resolution	:	2.43 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:

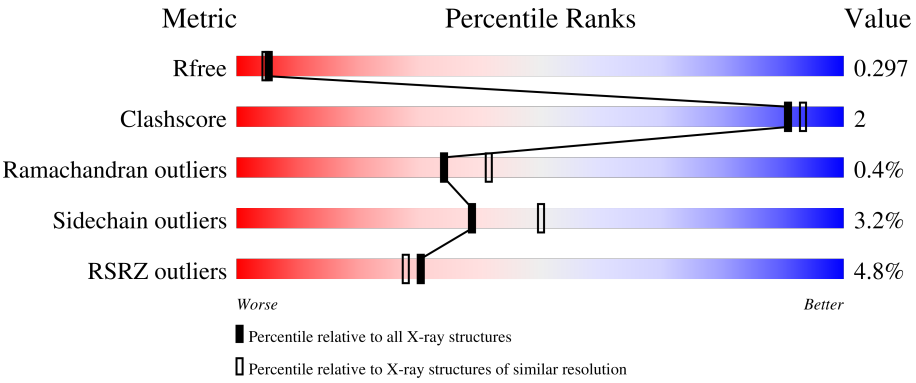
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.43 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	1564 (2.46-2.42)
Clashscore	141614	1631 (2.46-2.42)
Ramachandran outliers	138981	1617 (2.46-2.42)
Sidechain outliers	138945	1617 (2.46-2.42)
RSRZ outliers	127900	1547 (2.46-2.42)

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	213	8% 91% 6%
1	C	213	2% 91% 6%
2	B	211	9% 90% 9%
2	D	211	3% 91% 9%
3	E	129	97%

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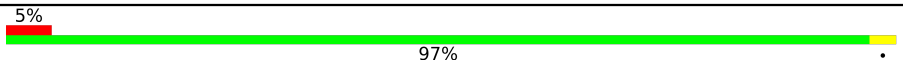
Mol	Chain	Length	Quality of chain
3	F	129	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 8226 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 HyHEL10 heavy chain Fab fragment carrying I29F mutation..

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	206	Total	C	N	O	S	0	0	0
			1525	966	245	308	6			
1	C	208	Total	C	N	O	S	0	1	0
			1564	996	247	315	6			

- Molecule 2 is a protein called HyHEL10 light chain Fab fragment.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	211	Total	C	N	O	S	0	0	0
			1584	988	267	323	6			
2	D	211	Total	C	N	O	S	0	0	0
			1565	976	262	321	6			

- Molecule 3 is a protein called lysozyme isoform I (DEL-I).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	127	Total	C	N	O	S	0	0	0
			966	592	180	184	10			
3	F	129	Total	C	N	O	S	0	0	0
			972	597	180	185	10			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	37	SER	GLY	conflict	UNP U3J0P1
E	71	GLY	ARG	conflict	UNP U3J0P1
F	37	SER	GLY	conflict	UNP U3J0P1
F	71	GLY	ARG	conflict	UNP U3J0P1

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Cl 1 1	0	0
4	B	1	Total Cl 1 1	0	0
4	C	1	Total Cl 1 1	0	0
4	D	1	Total Cl 1 1	0	0

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	E	1	Total Na 1 1	0	0

- Molecule 6 is water.

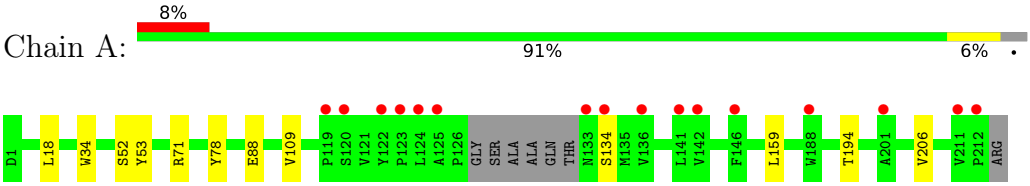
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	13	Total O 13 13	0	0
6	B	11	Total O 11 11	0	0
6	C	1	Total O 1 1	0	0
6	D	8	Total O 8 8	0	0
6	E	8	Total O 8 8	0	0
6	F	4	Total O 4 4	0	0

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.

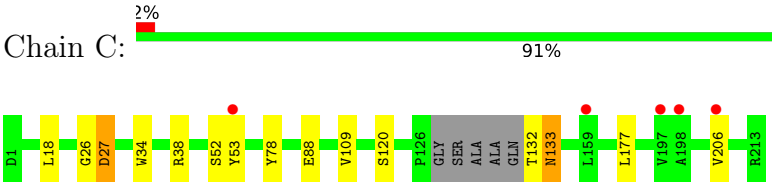
• Molecule 1: HyHEL10 heavy chain Fab fragment carrying I29F mutation.

Chain A:



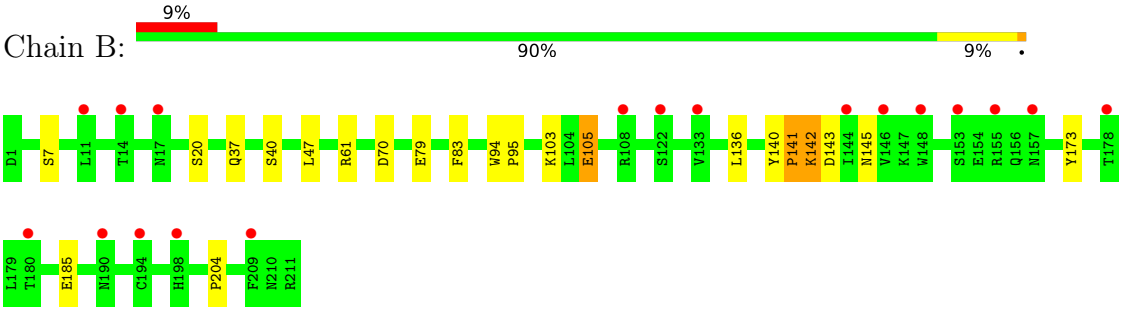
• Molecule 1: HyHEL10 heavy chain Fab fragment carrying I29F mutation.

Chain C:



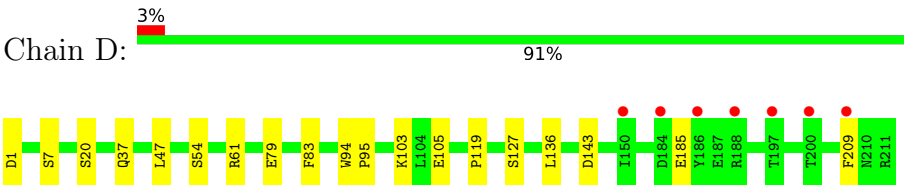
• Molecule 2: HyHEL10 light chain Fab fragment

Chain B:



• Molecule 2: HyHEL10 light chain Fab fragment

Chain D:

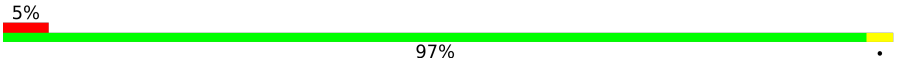


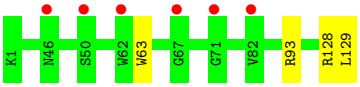
• Molecule 3: lysozyme isoform I (DEL-I)

Chain E:

• Molecule 3: lysozyme isoform I (DEL-I)

Chain F:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 2 21	Depositor
Cell constants a, b, c, α, β, γ	89.02Å 102.91Å 133.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.49 – 2.43 47.49 – 2.43	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.49-2.43) 99.8 (47.49-2.43)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.80 (at 2.42Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.262 , 0.296 0.264 , 0.297	Depositor DCC
R_{free} test set	2327 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	50.5	Xtriage
Anisotropy	0.353	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 29.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	8226	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.68% 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: NA, CL

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	0.58	0/1570	0.72	1/2164 (0.0%)
1	C	0.55	0/1609	0.73	1/2218 (0.0%)
2	B	0.58	0/1622	0.72	2/2209 (0.1%)
2	D	0.56	0/1603	0.70	0/2189
3	E	0.55	0/985	0.81	4/1337 (0.3%)
3	F	0.53	0/991	0.76	2/1347 (0.1%)
All	All	0.56	0/8380	0.74	10/11464 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	93	ARG	NE-CZ-NH1	-9.47	115.57	120.30
3	E	93	ARG	NE-CZ-NH1	-7.64	116.48	120.30
3	F	93	ARG	NE-CZ-NH2	6.05	123.33	120.30
3	E	93	ARG	NE-CZ-NH2	5.84	123.22	120.30
2	B	141	PRO	N-CA-C	5.71	126.95	112.10
3	E	116	ARG	NE-CZ-NH2	-5.62	117.49	120.30
2	B	70	ASP	CB-CG-OD1	5.48	123.23	118.30
3	E	116	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	A	71	ARG	NE-CZ-NH2	5.40	123.00	120.30
1	C	38	ARG	NE-CZ-NH1	5.22	122.91	120.30

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	1525	0	1379	5	0
1	C	1564	0	1451	8	0
2	B	1584	0	1453	9	0
2	D	1565	0	1413	6	0
3	E	966	0	899	0	0
3	F	972	0	898	2	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	E	1	0	0	0	0
6	A	13	0	0	0	0
6	B	11	0	0	0	0
6	C	1	0	0	0	0
6	D	8	0	0	0	0
6	E	8	0	0	0	0
6	F	4	0	0	0	0
All	All	8226	0	7493	27	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 2.

All (27) 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)
2:B:79:GLU:OE2	2:D:61:ARG:NH1	2.34	0.61
2:B:61:ARG:NH1	2:D:79:GLU:OE2	2.34	0.60
2:D:94:TRP:CD2	2:D:95:PRO:HA	2.38	0.59
2:B:94:TRP:CD2	2:B:95:PRO:HA	2.38	0.58
2:B:141:PRO:O	2:B:142:LYS:CB	2.55	0.54
1:A:18:LEU:CD1	1:A:109:VAL:HG11	2.37	0.54
1:C:18:LEU:CD1	1:C:109:VAL:HG11	2.37	0.54
2:B:105:GLU:OE2	2:B:173:TYR:OH	2.21	0.51
2:B:37:GLN:HB2	2:B:47:LEU:HD11	1.92	0.51
1:C:26:GLY:O	1:C:27:ASP:CB	2.58	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:LEU:HD12	1:A:109:VAL:HG11	1.94	0.49
1:A:34:TRP:HB3	1:A:78:TYR:CZ	2.48	0.48
2:D:37:GLN:HB2	2:D:47:LEU:HD11	1.95	0.48
1:C:18:LEU:HD11	1:C:109:VAL:HG11	1.95	0.48
1:C:34:TRP:HB3	1:C:78:TYR:CZ	2.48	0.47
1:C:53:TYR:OH	3:F:63:TRP:CH2	2.69	0.46
2:B:136:LEU:HD12	2:B:136:LEU:N	2.33	0.43
2:D:136:LEU:N	2:D:136:LEU:HD12	2.34	0.43
1:A:52:SER:OG	1:A:53:TYR:N	2.50	0.43
1:C:132:THR:O	1:C:133:ASN:CB	2.66	0.43
1:C:52[A]:SER:OG	1:C:53:TYR:N	2.51	0.43
2:B:141:PRO:O	2:B:142:LYS:HB3	2.19	0.42
1:A:18:LEU:HD11	1:A:109:VAL:HG11	2.03	0.41
2:B:140:TYR:CG	2:B:141:PRO:HA	2.56	0.41
1:C:18:LEU:HD12	1:C:109:VAL:HG11	2.02	0.40
2:D:119:PRO:HB3	2:D:209:PHE:CE2	2.55	0.40
3:F:128:ARG:O	3:F:129:LEU:C	2.59	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	202/213 (95%)	198 (98%)	3 (2%)	1 (0%)	29	34
1	C	205/213 (96%)	198 (97%)	5 (2%)	2 (1%)	15	16
2	B	209/211 (99%)	203 (97%)	5 (2%)	1 (0%)	29	34
2	D	209/211 (99%)	205 (98%)	4 (2%)	0	100	100
3	E	125/129 (97%)	124 (99%)	1 (1%)	0	100	100
3	F	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
All	All	1077/1106 (97%)	1053 (98%)	20 (2%)	4 (0%)	34	41

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	133	ASN
1	A	134	SER
2	B	142	LYS
1	C	27	ASP

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	164/190 (86%)	160 (98%)	4 (2%)	49	61
1	C	174/190 (92%)	170 (98%)	4 (2%)	50	63
2	B	173/189 (92%)	163 (94%)	10 (6%)	20	26
2	D	168/189 (89%)	158 (94%)	10 (6%)	19	25
3	E	99/106 (93%)	99 (100%)	0	100	100
3	F	98/106 (92%)	98 (100%)	0	100	100
All	All	876/970 (90%)	848 (97%)	28 (3%)	39	50

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	88	GLU
1	A	159	LEU
1	A	194	THR
1	A	206	VAL
2	B	7	SER
2	B	20	SER
2	B	40	SER
2	B	83	PHE
2	B	103	LYS
2	B	105	GLU
2	B	143	ASP
2	B	145	ASN
2	B	185	GLU

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Mol	Chain	Res	Type
2	B	204	PRO
1	C	88	GLU
1	C	120	SER
1	C	177	LEU
1	C	206	VAL
2	D	1	ASP
2	D	7	SER
2	D	20	SER
2	D	54	SER
2	D	83	PHE
2	D	103	LYS
2	D	105	GLU
2	D	127	SER
2	D	143	ASP
2	D	185	GLU

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)

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)

Of 5 ligands modelled in this entry, 5 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, 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	206/213 (96%)	0.44	16 (7%) 13 10	30, 64, 103, 110	0
1	C	208/213 (97%)	0.17	5 (2%) 59 54	37, 58, 88, 101	0
2	B	211/211 (100%)	0.53	18 (8%) 10 8	38, 68, 97, 112	0
2	D	211/211 (100%)	0.11	7 (3%) 46 43	37, 53, 91, 104	0
3	E	127/129 (98%)	-0.12	0 100 100	33, 54, 75, 90	0
3	F	129/129 (100%)	0.15	6 (4%) 31 29	45, 67, 95, 111	0
All	All	1092/1106 (98%)	0.24	52 (4%) 30 28	30, 60, 96, 112	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	194	CYS	4.4
2	B	11	LEU	4.1
2	B	146	VAL	4.0
3	F	50	SER	3.9
2	D	188	ARG	3.9
2	B	180	THR	3.7
2	B	144	ILE	3.7
2	B	122	SER	3.6
1	A	211	VAL	3.6
1	A	133	ASN	3.6
1	A	122	TYR	3.5
2	B	17	ASN	3.5
2	B	14	THR	3.4
2	B	108	ARG	3.3
3	F	67	GLY	3.3
1	A	120	SER	3.3
1	A	125	ALA	3.3
2	D	197	THR	3.2
2	B	148	TRP	3.2

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Mol	Chain	Res	Type	RSRZ
2	D	200	THR	3.1
2	B	155	ARG	2.8
2	B	157	ASN	2.8
1	A	188	TRP	2.8
2	D	150	ILE	2.8
1	C	53	TYR	2.8
1	A	124	LEU	2.8
2	B	190	ASN	2.8
1	A	119	PRO	2.7
1	C	206	VAL	2.6
2	B	133	VAL	2.6
3	F	62	TRP	2.6
2	D	184	ASP	2.6
1	A	212	PRO	2.5
2	B	209	PHE	2.5
1	A	201	ALA	2.4
2	D	186	TYR	2.3
2	B	178	THR	2.3
2	B	153	SER	2.3
3	F	82	VAL	2.3
1	A	123	PRO	2.3
1	C	197	VAL	2.3
1	A	146	PHE	2.3
3	F	46	ASN	2.2
1	A	142	VAL	2.2
1	C	198	ALA	2.2
1	A	134	SER	2.2
1	A	136	VAL	2.1
2	B	198	HIS	2.1
1	A	141	LEU	2.1
1	C	159	LEU	2.1
3	F	71	GLY	2.0
2	D	209	PHE	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

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
4	CL	C	301	1/1	0.75	0.12	91,91,91,91	0
5	NA	E	201	1/1	0.75	0.08	61,61,61,61	0
4	CL	B	301	1/1	0.91	0.09	43,43,43,43	0
4	CL	D	301	1/1	0.96	0.13	46,46,46,46	0
4	CL	A	301	1/1	0.96	0.07	68,68,68,68	0

6.5 Other polymers

There are no such residues in this entry.