wwPDB X-ray Structure Validation Summary Report (i)

Feb 19, 2016 – 08:49 PM GMT

PDB ID	:	4YZF
Title	:	Crystal structure of the anion exchanger domain of human erythrocyte Band 3
Authors	:	Alguel, Y.; Arakawa, T.; Yugiri, T.K.; Iwanari, H.; Hatae, H.; Iwata, M.; Abe, Y.; Hino, T.; Suno, C.I.; Kuma, H.; Kang, D.; Murata, T.; Hamakubo, T.; Cameron, A.D.; Kobayashi, T.; Hamasaki, N.; Iwata, S.
Deposited on	:	2015-03-25
Resolution	:	3.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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:

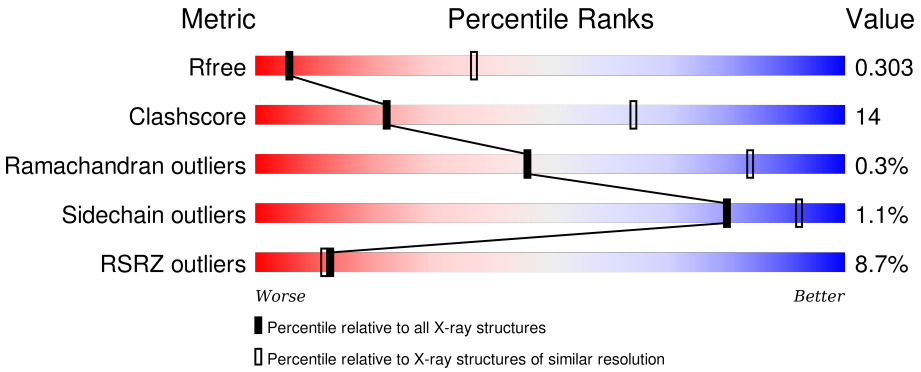
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

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}	91344	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (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 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	911	% 32% 19% • 48%
1	B	911	3% 32% 20% 48%
1	C	911	% 32% 20% 48%
1	D	911	3% 32% 20% 48%
2	E	223	10% 76% 22% •

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Mol	Chain	Length	Quality of chain
2	G	223	9% 84% 16%
2	I	223	18% 71% 27%
2	K	223	8% 80% 20%
3	F	218	9% 79% 21%
3	H	218	22% 83% 17%
3	J	218	20% 76% 23%
3	L	218	14% 85% 14%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 28724 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 Band 3 anion transport protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	475	Total	C	N	O	S	0	0	0
			3769	2535	598	619	17			
1	B	475	Total	C	N	O	S	0	0	0
			3769	2535	598	619	17			
1	C	475	Total	C	N	O	S	0	0	0
			3769	2535	598	619	17			
1	D	475	Total	C	N	O	S	0	0	0
			3769	2535	598	619	17			

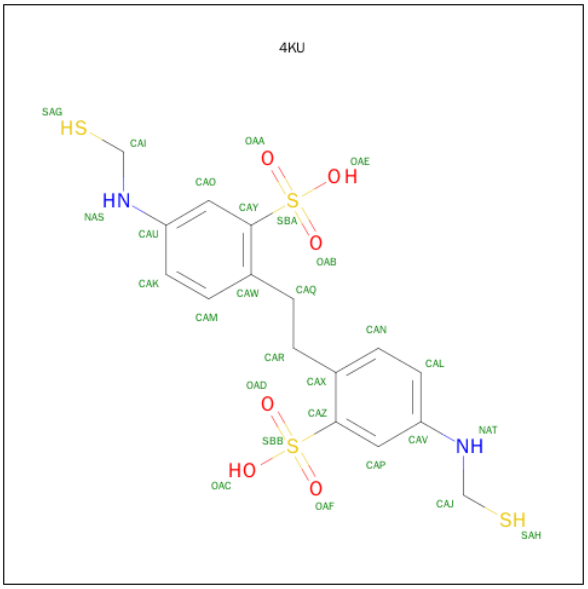
- Molecule 2 is a protein called FAB fragment of Immunoglobulin (IgG) molecule.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	223	Total	C	N	O	S	0	0	0
			1690	1077	274	334	5			
2	G	223	Total	C	N	O	S	0	0	0
			1690	1077	274	334	5			
2	I	223	Total	C	N	O	S	0	0	0
			1690	1077	274	334	5			
2	K	223	Total	C	N	O	S	0	0	0
			1690	1077	274	334	5			

- Molecule 3 is a protein called FAB fragment of Immunoglobulin (IgG) molecule.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	218	Total	C	N	O	S	0	0	0
			1694	1055	285	346	8			
3	H	218	Total	C	N	O	S	0	0	0
			1694	1055	285	346	8			
3	J	218	Total	C	N	O	S	0	0	0
			1694	1055	285	346	8			
3	L	218	Total	C	N	O	S	0	0	0
			1694	1055	285	346	8			

- Molecule 4 is 2,2'-ethane-1,2-diylbis{5-[(sulfanylmethyl)amino]benzenesulfonic acid} (three-letter code: 4KU) (formula: $C_{16}H_{20}N_2O_6S_4$).



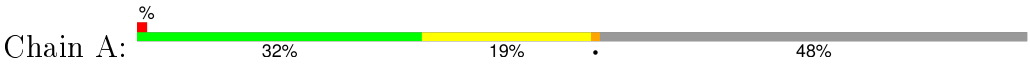
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			28	16	2	6	4		
4	B	1	Total	C	N	O	S	0	0
			28	16	2	6	4		
4	C	1	Total	C	N	O	S	0	0
			28	16	2	6	4		
4	D	1	Total	C	N	O	S	0	0
			28	16	2	6	4		

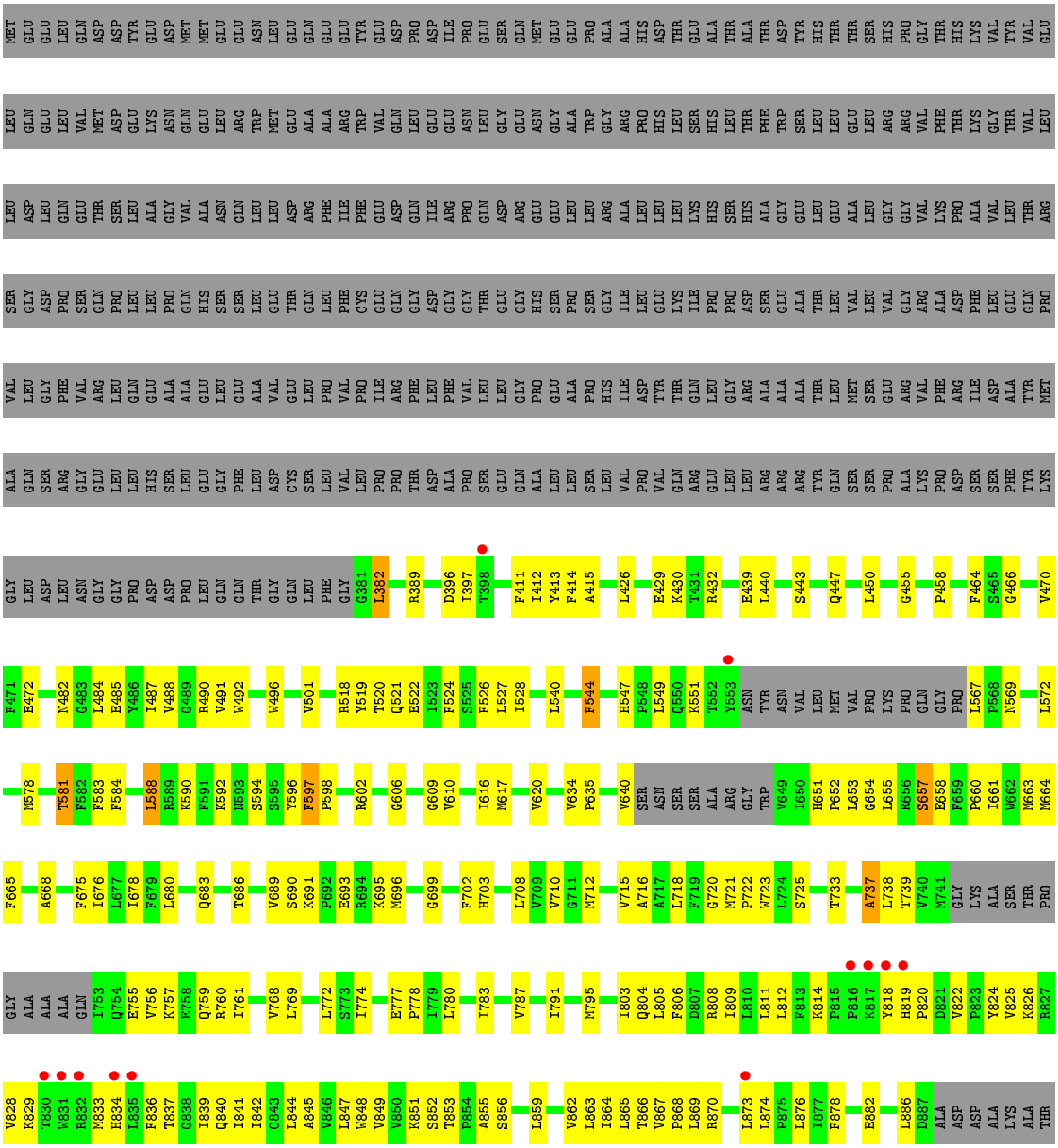
3 Residue-property plots (i)

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: Band 3 anion transport protein

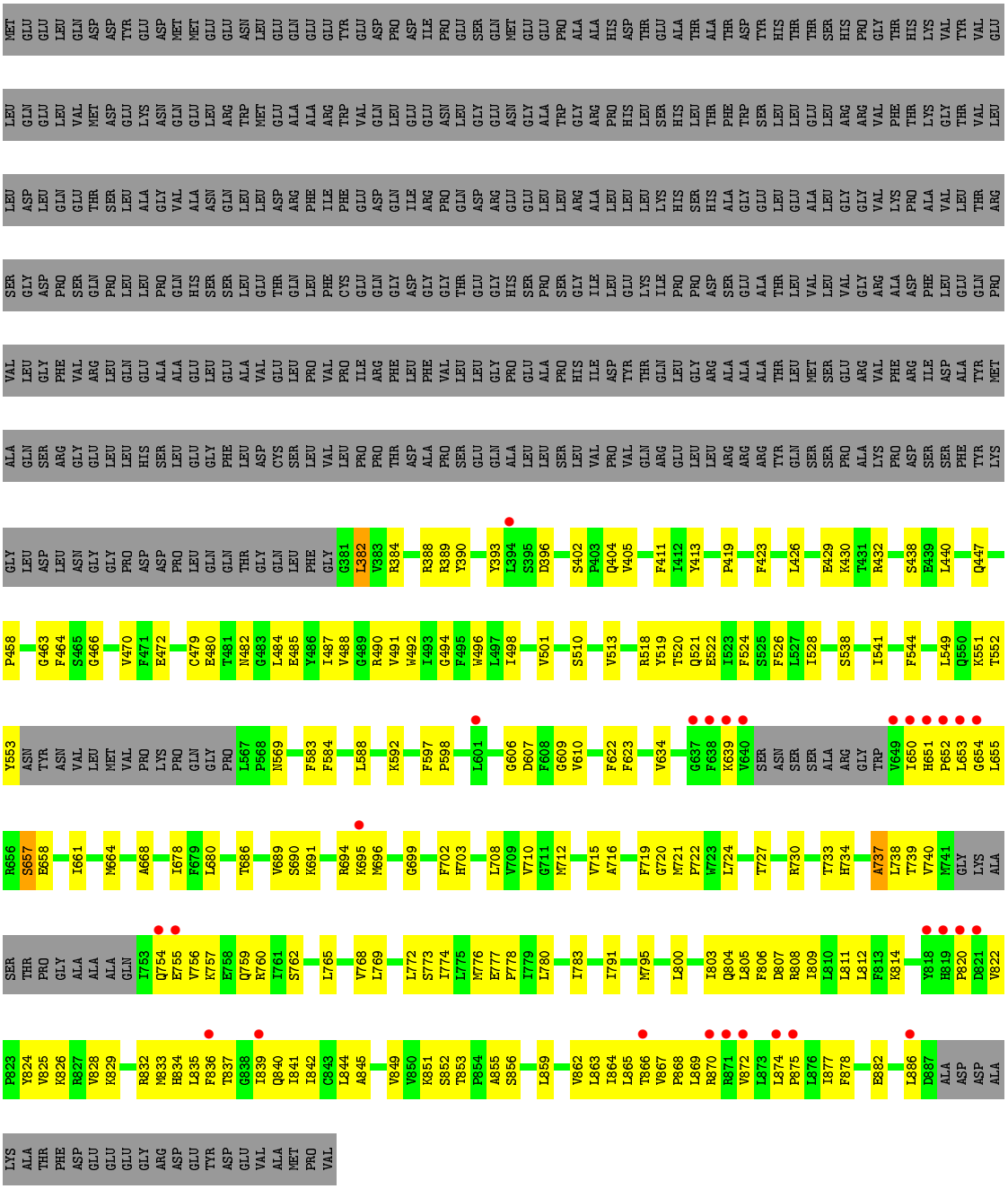
Chain A:





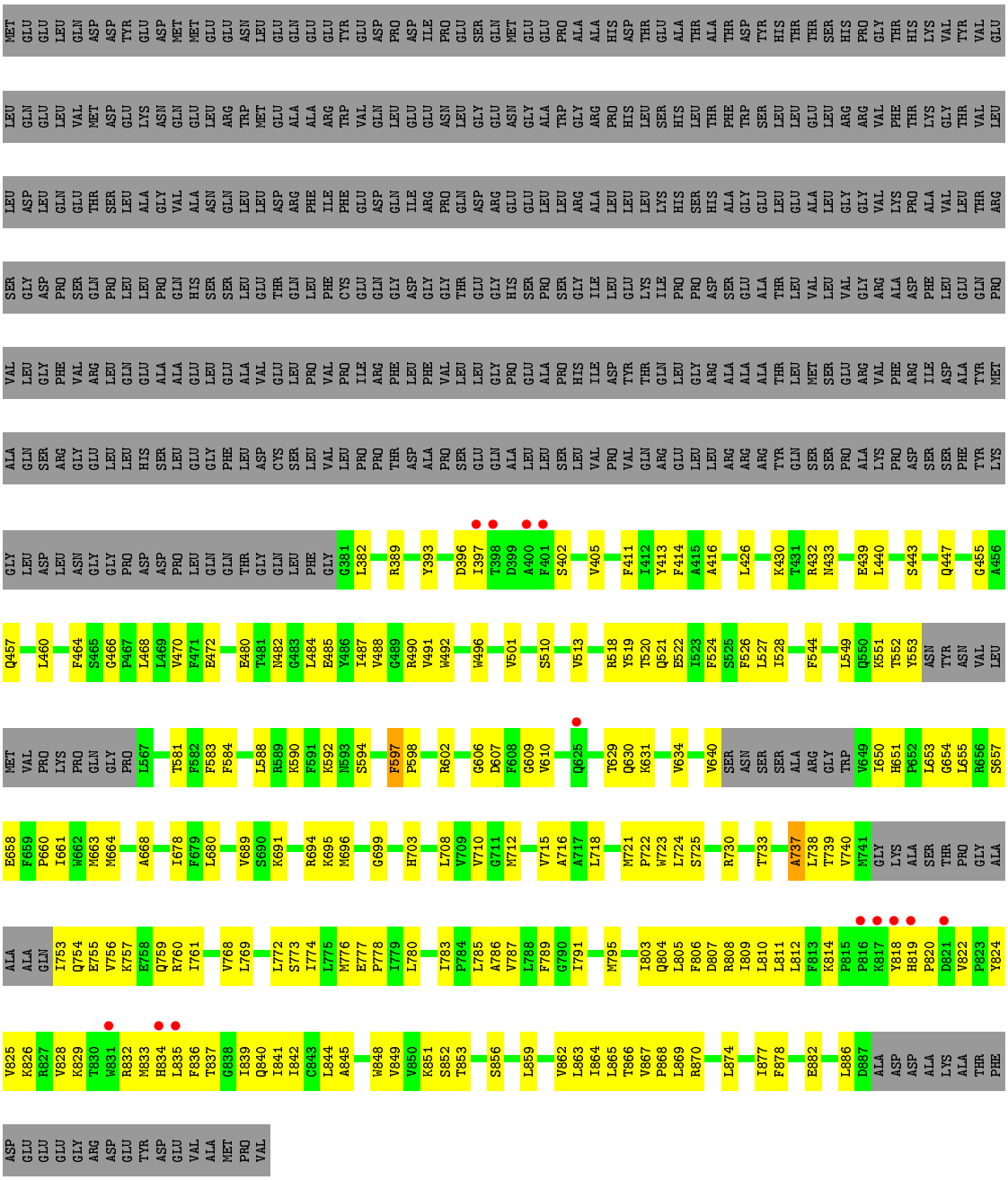
- Molecule 1: Band 3 anion transport protein

Chain B:



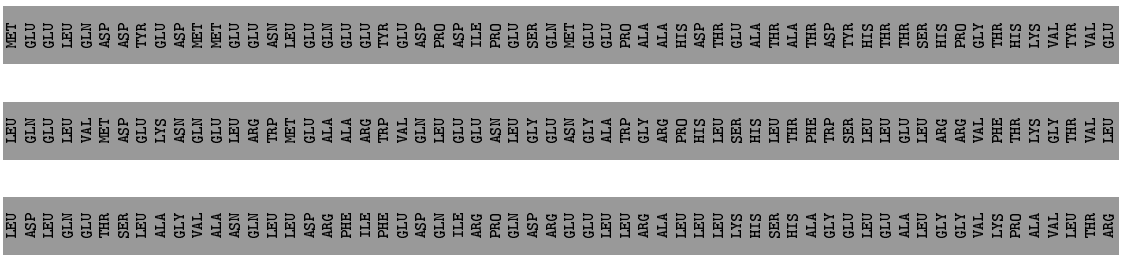
- Molecule 1: Band 3 anion transport protein

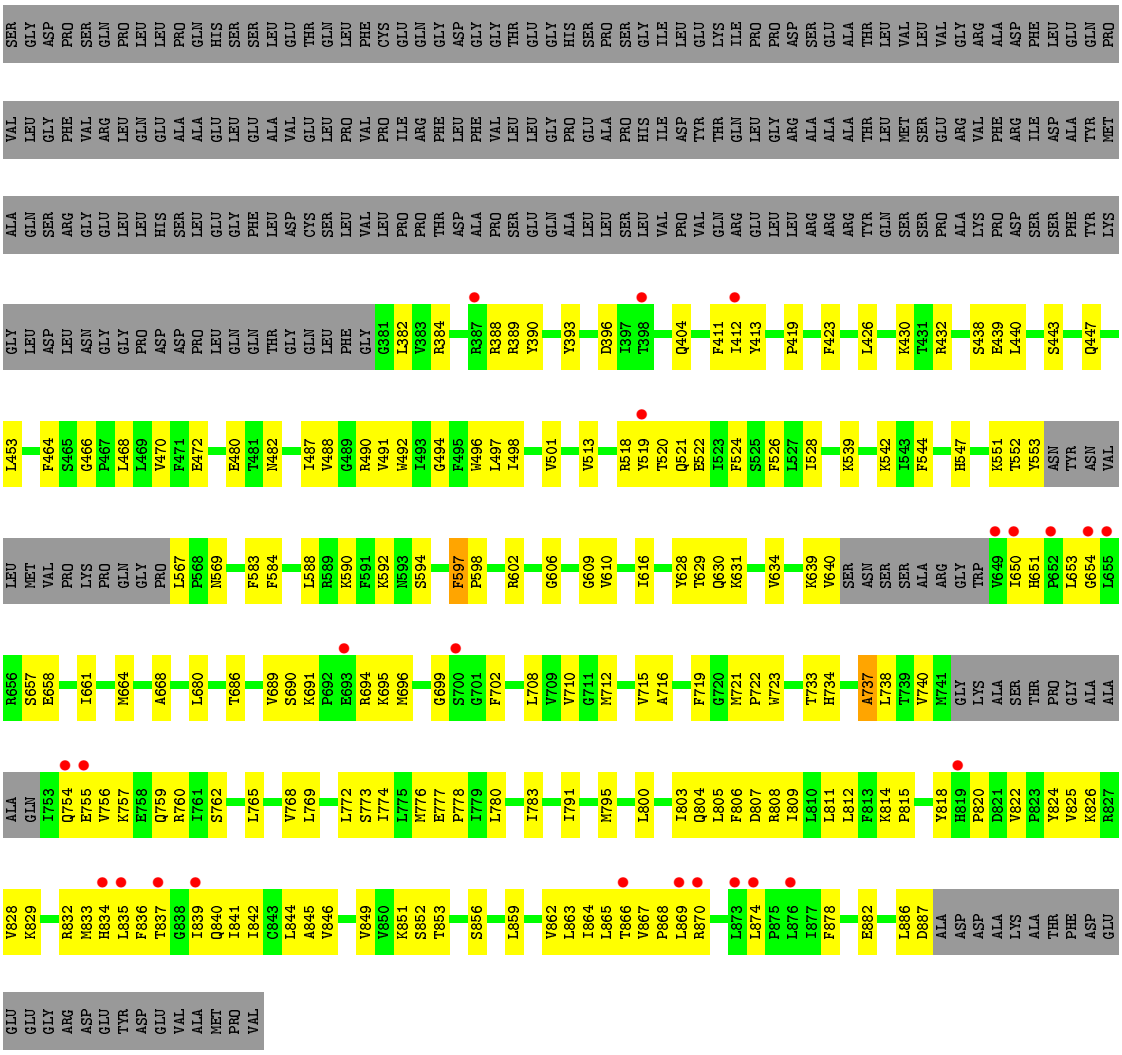
Chain C:



• Molecule 1: Band 3 anion transport protein

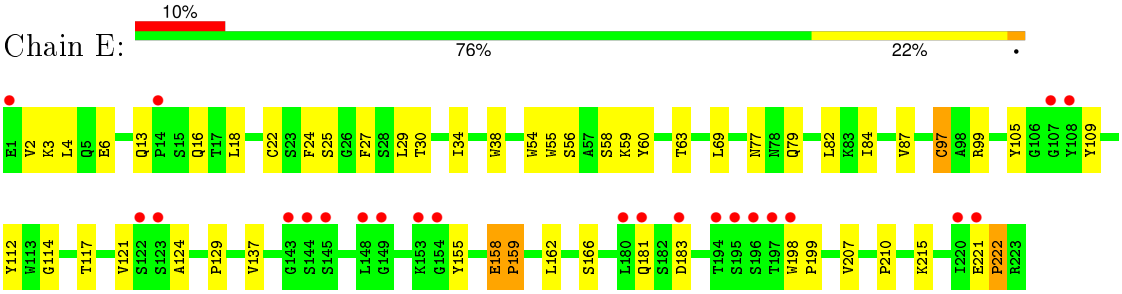
Chain D:





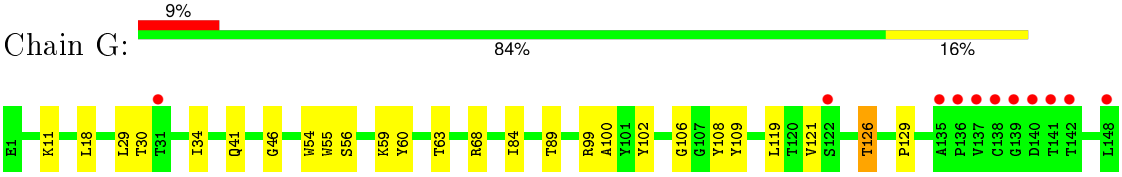
• Molecule 2: FAB fragment of Immunoglobulin (IgG) molecule

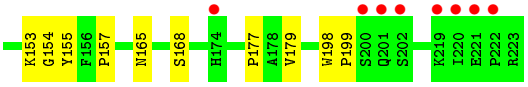
Chain E:



• Molecule 2: FAB fragment of Immunoglobulin (IgG) molecule

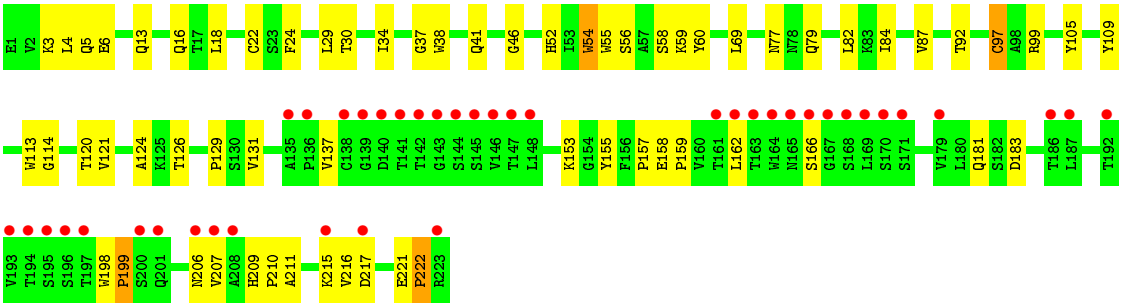
Chain G:





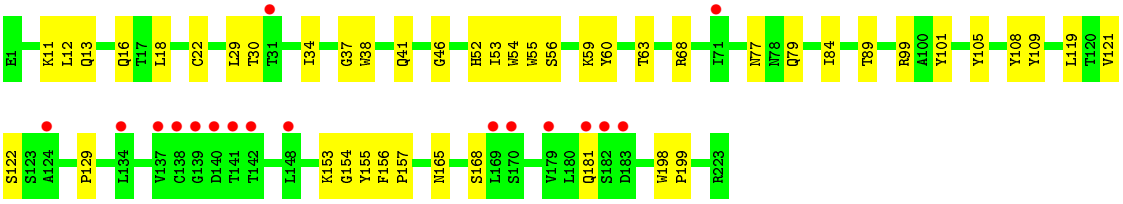
• Molecule 2: FAB fragment of Immunoglobulin (IgG) molecule

Chain I:



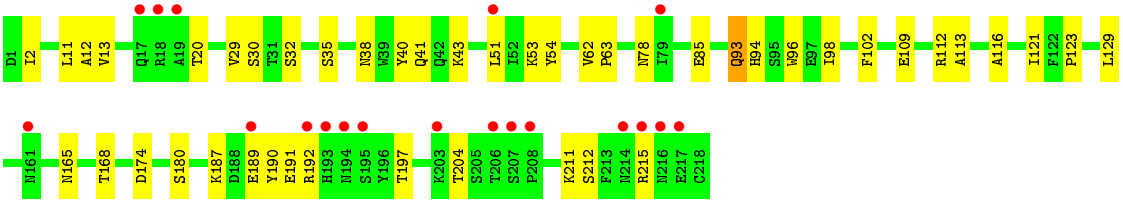
• Molecule 2: FAB fragment of Immunoglobulin (IgG) molecule

Chain K:



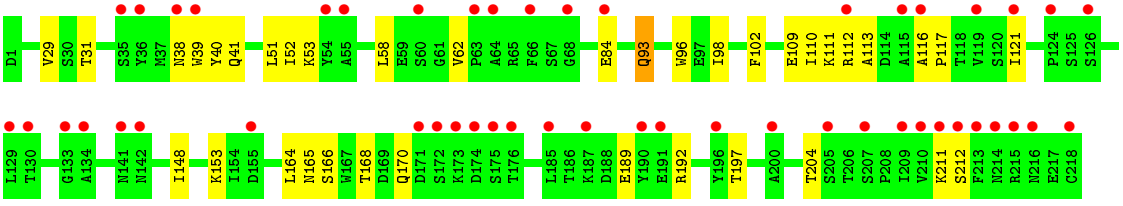
• Molecule 3: FAB fragment of Immunoglobulin (IgG) molecule

Chain F:



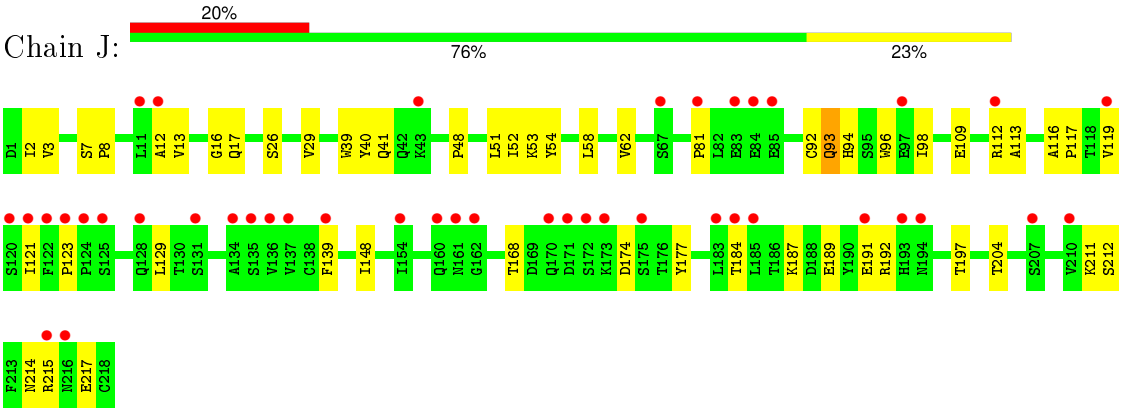
• Molecule 3: FAB fragment of Immunoglobulin (IgG) molecule

Chain H:



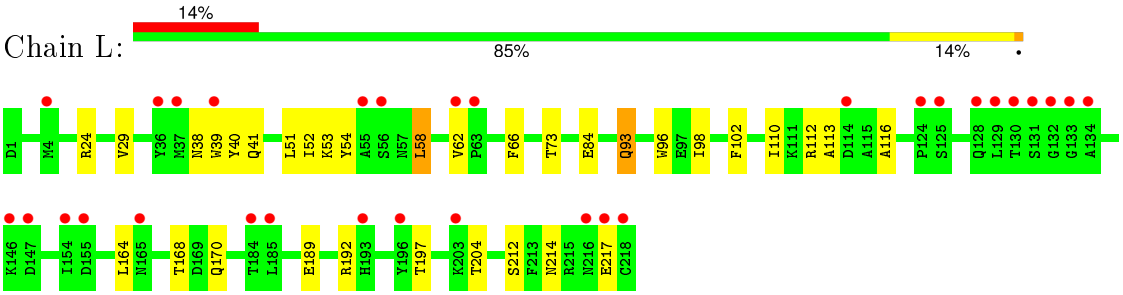
• Molecule 3: FAB fragment of Immunoglobulin (IgG) molecule

Chain J:



• Molecule 3: FAB fragment of Immunoglobulin (IgG) molecule

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	152.82Å 171.96Å 271.70Å 90.00° 101.16° 90.00°	Depositor
Resolution (Å)	37.72 – 3.50 48.84 – 3.50	Depositor EDS
% Data completeness (in resolution range)	94.6 (37.72-3.50) 94.7 (48.84-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.59 (at 3.48Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1951)	Depositor
R, R_{free}	0.274 , 0.290 0.287 , 0.303	Depositor DCC
R_{free} test set	4133 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	115.1	Xtriage
Anisotropy	0.214	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 67.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.24$	Xtriage
Outliers	5 of 82522 reflections (0.006%)	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	28724	wwPDB-VP
Average B, all atoms (Å^2)	145.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 51.75 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 5.3662e-05.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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

Bond lengths and bond angles in the following residue types are not validated in this section: 4KU

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	0.42	0/3862	0.62	2/5246 (0.0%)
1	B	0.37	0/3862	0.59	2/5246 (0.0%)
1	C	0.40	0/3862	0.60	1/5246 (0.0%)
1	D	0.37	0/3862	0.57	1/5246 (0.0%)
2	E	0.48	0/1737	0.90	3/2377 (0.1%)
2	G	0.39	0/1737	0.67	1/2377 (0.0%)
2	I	0.43	0/1737	0.81	3/2377 (0.1%)
2	K	0.37	0/1737	0.66	1/2377 (0.0%)
3	F	0.44	0/1736	0.64	0/2360
3	H	0.37	0/1736	0.57	1/2360 (0.0%)
3	J	0.37	0/1736	0.60	0/2360
3	L	0.34	0/1736	0.55	0/2360
All	All	0.40	0/29340	0.64	15/39932 (0.0%)

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
3	H	0	1

There are no bond length outliers.

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	68	ARG	NE-CZ-NH1	-7.19	116.70	120.30
2	E	158	GLU	C-N-CD	-6.51	106.27	120.60
2	K	68	ARG	NE-CZ-NH1	-5.98	117.31	120.30
2	I	158	GLU	C-N-CD	-5.73	107.99	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	737	ALA	C-N-CA	5.63	135.79	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	H	111	LYS	Mainchain

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	3769	0	3990	150	0
1	B	3769	0	3990	141	0
1	C	3769	0	3988	138	0
1	D	3769	0	3989	144	0
2	E	1690	0	1645	40	0
2	G	1690	0	1645	28	0
2	I	1690	0	1645	45	0
2	K	1690	0	1645	33	0
3	F	1694	0	1609	33	0
3	H	1694	0	1609	28	0
3	J	1694	0	1609	40	0
3	L	1694	0	1609	26	0
4	A	28	0	15	1	0
4	B	28	0	14	2	0
4	C	28	0	15	3	0
4	D	28	0	15	2	0
All	All	28724	0	29032	798	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 14.

The worst 5 of 798 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:828:VAL:HG23	1:A:829:LYS:HG3	1.48	0.94
1:D:851:LYS:HE3	1:D:859:LEU:HD22	1.51	0.92
1:C:828:VAL:HG23	1:C:829:LYS:HG3	1.49	0.92
1:D:828:VAL:HG23	1:D:829:LYS:HG3	1.54	0.90
1:D:737:ALA:HB3	1:D:738:LEU:HB2	1.55	0.89

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	467/911 (51%)	435 (93%)	31 (7%)	1 (0%)	52 88
1	B	467/911 (51%)	436 (93%)	30 (6%)	1 (0%)	52 88
1	C	467/911 (51%)	436 (93%)	30 (6%)	1 (0%)	52 88
1	D	467/911 (51%)	436 (93%)	30 (6%)	1 (0%)	52 88
2	E	221/223 (99%)	211 (96%)	7 (3%)	3 (1%)	14 58
2	G	221/223 (99%)	214 (97%)	7 (3%)	0	100 100
2	I	221/223 (99%)	212 (96%)	6 (3%)	3 (1%)	14 58
2	K	221/223 (99%)	213 (96%)	8 (4%)	0	100 100
3	F	216/218 (99%)	208 (96%)	8 (4%)	0	100 100
3	H	216/218 (99%)	209 (97%)	7 (3%)	0	100 100
3	J	216/218 (99%)	209 (97%)	7 (3%)	0	100 100
3	L	216/218 (99%)	211 (98%)	5 (2%)	0	100 100
All	All	3616/5408 (67%)	3430 (95%)	176 (5%)	10 (0%)	46 84

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	166	SER

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Mol	Chain	Res	Type
2	I	166	SER
2	E	159	PRO
2	I	159	PRO
2	E	210	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	417/786 (53%)	411 (99%)	6 (1%)	74	91
1	B	417/786 (53%)	413 (99%)	4 (1%)	82	93
1	C	417/786 (53%)	412 (99%)	5 (1%)	78	92
1	D	417/786 (53%)	413 (99%)	4 (1%)	82	93
2	E	190/190 (100%)	188 (99%)	2 (1%)	80	92
2	G	190/190 (100%)	188 (99%)	2 (1%)	80	92
2	I	190/190 (100%)	187 (98%)	3 (2%)	70	89
2	K	190/190 (100%)	189 (100%)	1 (0%)	92	97
3	F	193/193 (100%)	191 (99%)	2 (1%)	82	93
3	H	193/193 (100%)	191 (99%)	2 (1%)	82	93
3	J	193/193 (100%)	191 (99%)	2 (1%)	82	93
3	L	193/193 (100%)	190 (98%)	3 (2%)	70	89
All	All	3200/4676 (68%)	3164 (99%)	36 (1%)	80	92

5 of 36 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	544	PHE
2	E	222	PRO
3	L	58	LEU
1	D	723	TRP
3	F	93	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	447	GLN
1	C	651	HIS
1	D	840	GLN
1	B	569	ASN
1	C	834	HIS

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 (i)

4 ligands 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	$\#\|Z\| > 2$
4	4KU	A	1000	1	29,29,29	1.65	2 (6%)	32,42,42	3.68	12 (37%)
4	4KU	B	1000	1	29,29,29	1.63	4 (13%)	32,42,42	3.18	12 (37%)
4	4KU	C	1000	1	29,29,29	1.64	2 (6%)	32,42,42	3.00	10 (31%)
4	4KU	D	1000	1	29,29,29	1.67	3 (10%)	32,42,42	2.96	10 (31%)

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
4	4KU	A	1000	1	-	0/21/23/23	0/2/2/2
4	4KU	B	1000	1	-	0/21/23/23	0/2/2/2
4	4KU	C	1000	1	-	0/21/23/23	0/2/2/2
4	4KU	D	1000	1	-	0/21/23/23	0/2/2/2

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1000	4KU	CAI-SAG	-5.95	1.66	1.81
4	D	1000	4KU	CAI-SAG	-5.79	1.66	1.81
4	C	1000	4KU	CAI-SAG	-5.68	1.66	1.81
4	B	1000	4KU	CAI-SAG	-5.60	1.67	1.81
4	D	1000	4KU	CAJ-SAH	-5.59	1.67	1.81

The worst 5 of 44 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1000	4KU	CAR-CAQ-CAW	-8.22	99.98	112.77
4	A	1000	4KU	CAO-CAY-CAW	-5.90	117.80	121.79
4	B	1000	4KU	CAO-CAY-CAW	-5.22	118.25	121.79
4	C	1000	4KU	CAR-CAQ-CAW	-4.74	105.39	112.77
4	C	1000	4KU	CAO-CAY-CAW	-4.59	118.68	121.79

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1000	4KU	1	0
4	B	1000	4KU	2	0
4	C	1000	4KU	3	0
4	D	1000	4KU	2	0

5.7 Other polymers (i)

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	475/911 (52%)	-0.20	12 (2%) 61 50	71, 103, 169, 208	0
1	B	475/911 (52%)	-0.03	28 (5%) 26 20	90, 142, 202, 249	0
1	C	475/911 (52%)	-0.16	13 (2%) 58 47	79, 114, 184, 226	0
1	D	475/911 (52%)	-0.02	24 (5%) 32 24	103, 151, 219, 259	0
2	E	223/223 (100%)	0.30	23 (10%) 9 8	79, 105, 150, 177	0
2	G	223/223 (100%)	0.26	19 (8%) 13 12	124, 152, 211, 250	0
2	I	223/223 (100%)	1.13	41 (18%) 2 2	79, 112, 310, 355	0
2	K	223/223 (100%)	0.30	17 (7%) 17 14	126, 152, 209, 248	0
3	F	218/218 (100%)	0.11	19 (8%) 13 12	81, 111, 141, 179	0
3	H	218/218 (100%)	0.84	49 (22%) 1 1	125, 181, 255, 268	0
3	J	218/218 (100%)	0.83	43 (19%) 1 2	90, 164, 292, 310	0
3	L	218/218 (100%)	0.52	31 (14%) 4 4	127, 169, 242, 253	0
All	All	3664/5408 (67%)	0.20	319 (8%) 13 12	71, 139, 238, 355	0

The worst 5 of 319 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	143	GLY	18.2
2	I	135	ALA	17.2
2	I	195	SER	14.6
2	I	144	SER	13.2
2	I	140	ASP	11.3

6.2 Non-standard residues in protein, DNA, RNA chains

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)

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
4	4KU	C	1000	28/28	0.76	0.32	1.21	113,118,123,125	0
4	4KU	A	1000	28/28	0.78	0.29	0.27	105,108,112,114	0
4	4KU	B	1000	28/28	0.80	0.27	-0.13	143,146,152,155	0
4	4KU	D	1000	28/28	0.81	0.25	-0.21	148,152,159,163	0

6.5 Other polymers (i)

There are no such residues in this entry.