wwPDB X-ray Structure Validation Summary Report (i)

Feb 19, 2016 – 08:22 PM GMT

PDB ID	:	4XH2
Title	:	Crystal structure of human paxillin LD4 motif in complex with Fab fragment
Authors	:	Nocula-Lugowska, M.; Lugowski, M.; Salgia, R.; Kossiakoff, A.A.
Deposited on	:	2015-01-04
Resolution	:	2.00 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:

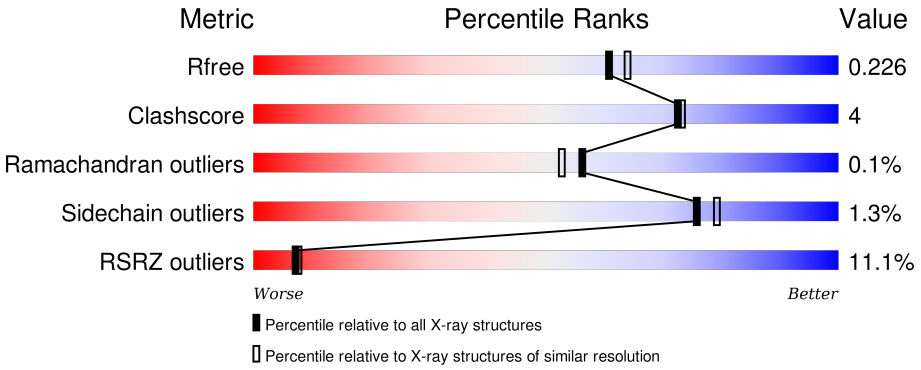
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.00 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	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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	228	7% 90% 6% ·
1	C	228	21% 86% 10% ·
1	E	228	4% 89% 7% ·
1	G	228	10% 85% 11% · ·
1	H	228	11% 88% 5% 7%

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Mol	Chain	Length	Quality of chain
1	J	228	9% 88% 10%
2	B	217	7% 89% 7%
2	D	217	12% 86% 10%
2	F	217	4% 87% 9%
2	I	217	10% 91% 5%
2	K	217	9% 91% 6%
2	L	217	8% 90% 5%
3	a	18	22% 89% 11%
3	c	18	56% 56% 6% 39%
3	e	18	28% 89% 6% 6%
3	g	18	44% 78% 22%
3	h	18	44% 67% 33%
3	j	18	61% 61% 6% 33%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	B	301	-	-	-	X
4	GOL	C	301	-	-	-	X
4	GOL	C	302	-	-	-	X
4	GOL	F	302	-	-	-	X
4	GOL	G	301	-	-	-	X
4	GOL	H	302	-	-	-	X
4	GOL	I	301	-	-	-	X
4	GOL	I	302	-	-	-	X
4	GOL	I	303	-	-	-	X
4	GOL	K	301	-	-	-	X
4	GOL	L	301	-	-	X	X
4	GOL	L	302	-	-	-	X
6	ACT	F	305	-	-	-	X
7	LDA	F	306	-	-	-	X
8	ACE	L	303	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 21729 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 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	220	Total	C	N	O	S	0	0	0
			1640	1038	270	327	5			
1	C	220	Total	C	N	O	S	0	0	0
			1642	1040	270	326	6			
1	E	220	Total	C	N	O	S	0	0	0
			1644	1043	270	326	5			
1	G	220	Total	C	N	O	S	0	1	0
			1646	1042	271	328	5			
1	H	213	Total	C	N	O	S	0	0	0
			1599	1017	262	315	5			
1	J	222	Total	C	N	O	S	0	0	0
			1658	1050	273	329	6			

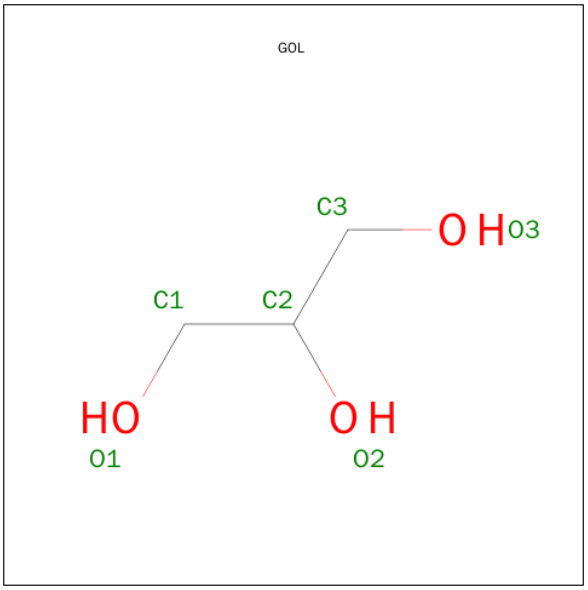
- Molecule 2 is a protein called Fab Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	210	Total	C	N	O	S	0	0	0
			1608	1007	271	324	6			
2	D	210	Total	C	N	O	S	0	0	0
			1608	1007	271	324	6			
2	F	209	Total	C	N	O	S	0	0	0
			1606	1005	273	323	5			
2	I	209	Total	C	N	O	S	0	0	0
			1602	1004	270	322	6			
2	K	210	Total	C	N	O	S	0	0	0
			1605	1005	271	324	5			
2	L	209	Total	C	N	O	S	0	0	0
			1588	996	265	321	6			

- Molecule 3 is a protein called paxillin LD4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	a	16	Total	C	N	O	S	0	0	0
			113	67	19	26	1			
3	c	11	Total	C	N	O	S	0	0	0
			78	47	11	19	1			
3	e	17	Total	C	N	O	S	0	0	0
			120	70	20	29	1			
3	g	14	Total	C	N	O	S	0	0	0
			98	60	14	23	1			
3	h	12	Total	C	N	O	S	0	0	0
			82	50	13	18	1			
3	j	12	Total	C	N	O	S	0	0	0
			80	51	12	16	1			

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	F	1	Total	C	O	0	0
			6	3	3		

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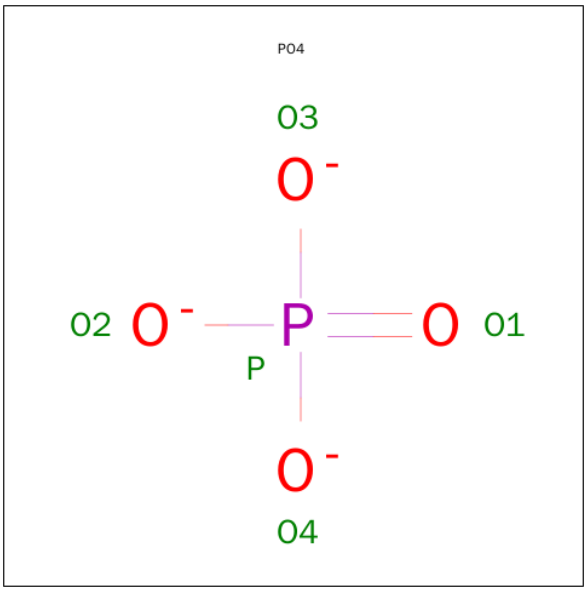
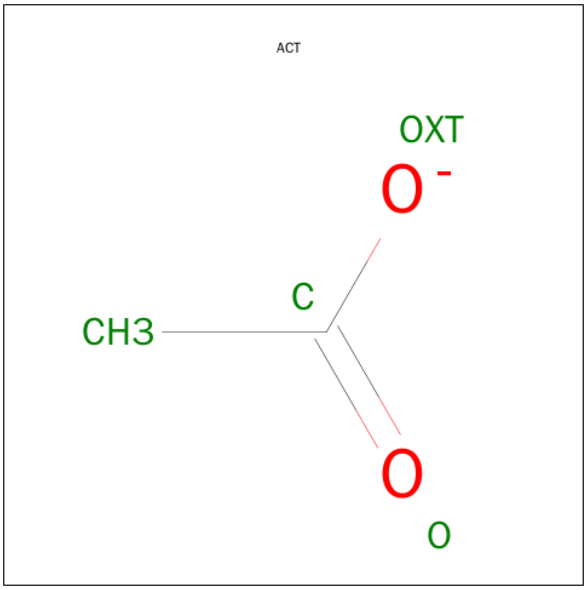
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	F	1	Total	C	O	0	0
			6	3	3		
4	F	1	Total	C	O	0	0
			6	3	3		
4	F	1	Total	C	O	0	0
			6	3	3		
4	G	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		
4	I	1	Total	C	O	0	0
			6	3	3		
4	I	1	Total	C	O	0	0
			6	3	3		
4	I	1	Total	C	O	0	0
			6	3	3		
4	K	1	Total	C	O	0	0
			6	3	3		
4	K	1	Total	C	O	0	0
			6	3	3		
4	K	1	Total	C	O	0	0
			6	3	3		
4	L	1	Total	C	O	0	0
			6	3	3		
4	L	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total O P 5 4 1	0	0
5	F	1	Total O P 5 4 1	0	0

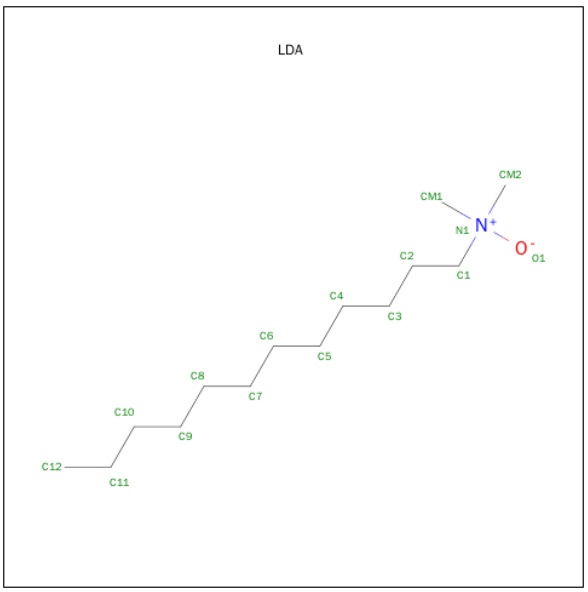
- Molecule 6 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	F	1	Total C O 4 2 2	0	0

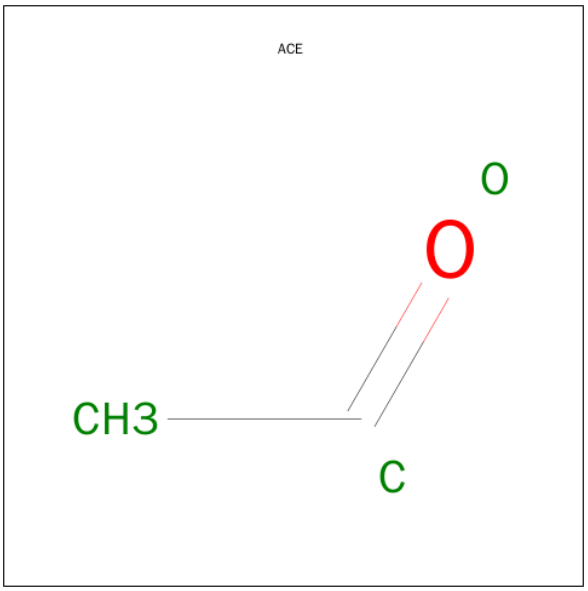
- Molecule 7 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula:

$C_{14}H_{31}NO$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	F	1	Total C N O 16 14 1 1	0	0

- Molecule 8 is ACETYL GROUP (three-letter code: ACE) (formula: C_2H_4O).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	J	1	Total C O 3 2 1	0	0
8	L	1	Total C O 3 2 1	0	0

- Molecule 9 is water.

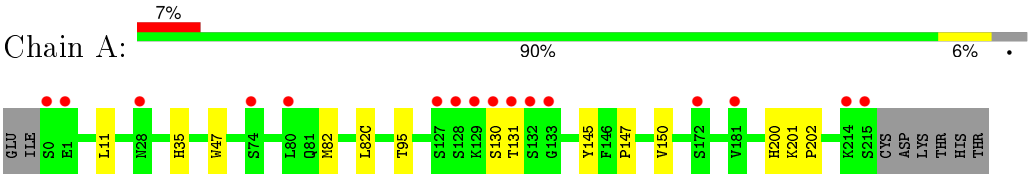
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	117	Total O 117 117	0	0
9	B	133	Total O 133 133	0	0
9	C	110	Total O 110 110	0	0
9	D	118	Total O 118 118	0	0
9	E	174	Total O 174 174	0	0
9	F	173	Total O 173 173	0	0
9	G	99	Total O 99 99	0	0
9	H	92	Total O 92 92	0	0
9	I	118	Total O 118 118	0	0
9	J	143	Total O 143 143	0	0
9	K	154	Total O 154 154	0	0
9	L	101	Total O 101 101	0	0
9	a	7	Total O 7 7	0	0
9	c	1	Total O 1 1	0	0
9	e	6	Total O 6 6	0	0
9	g	5	Total O 5 5	0	0
9	h	3	Total O 3 3	0	0
9	j	2	Total O 2 2	0	0

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.

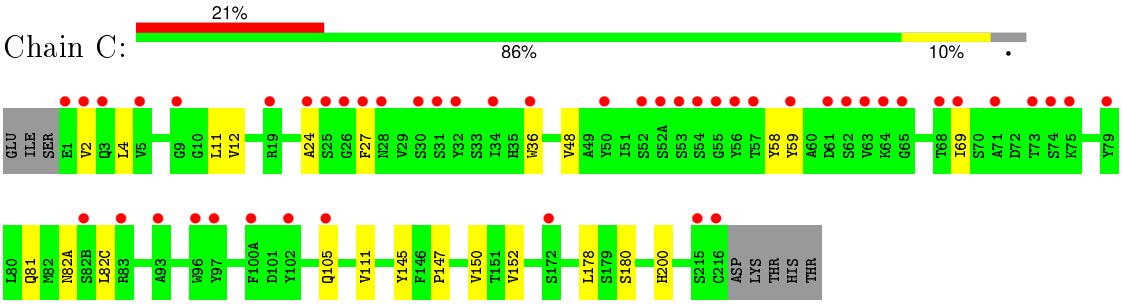
- Molecule 1: Fab Heavy Chain

Chain A:



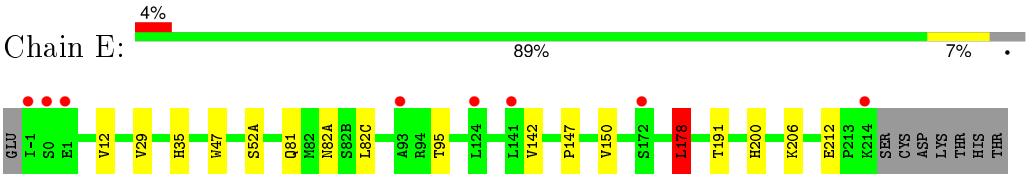
- Molecule 1: Fab Heavy Chain

Chain C:



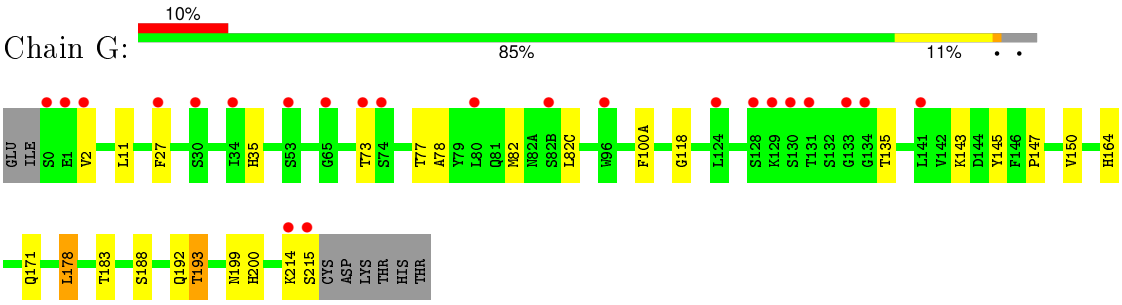
- Molecule 1: Fab Heavy Chain

Chain E:



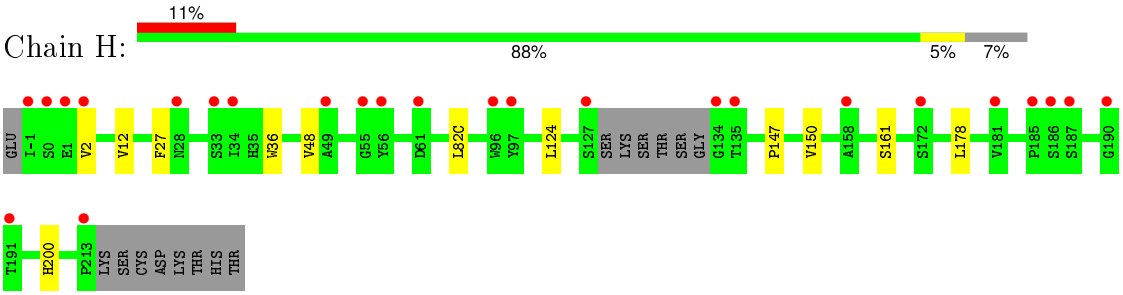
- Molecule 1: Fab Heavy Chain

Chain G:



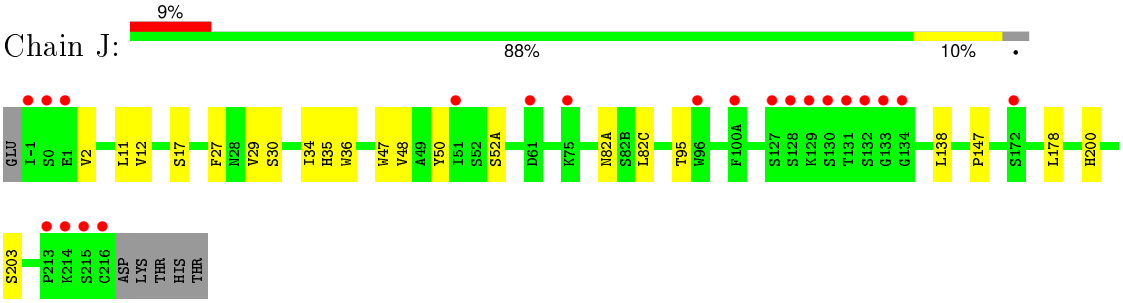
- Molecule 1: Fab Heavy Chain

Chain H:



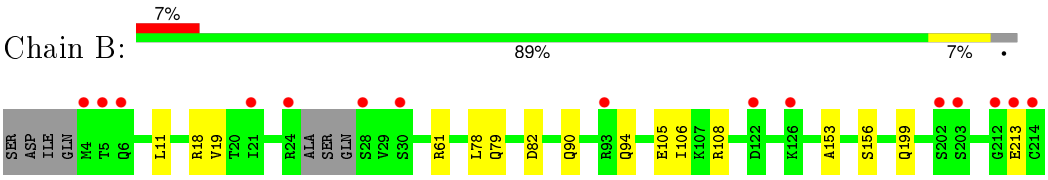
• Molecule 1: Fab Heavy Chain

Chain J:



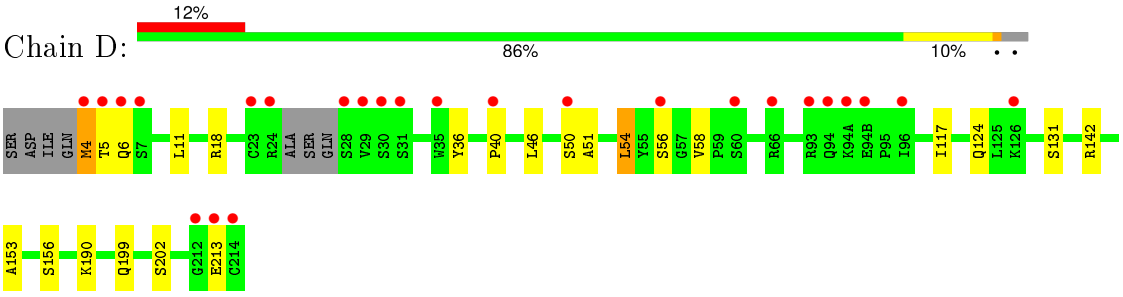
• Molecule 2: Fab Light Chain

Chain B:



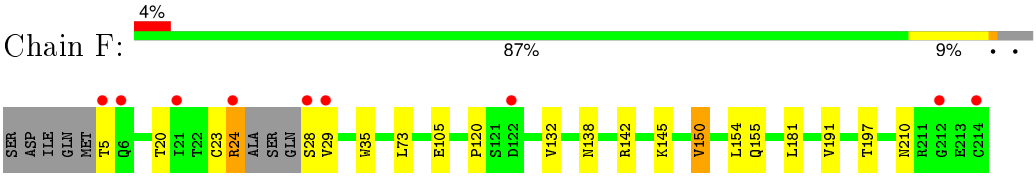
• Molecule 2: Fab Light Chain

Chain D:



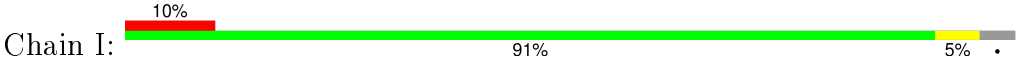
• Molecule 2: Fab Light Chain

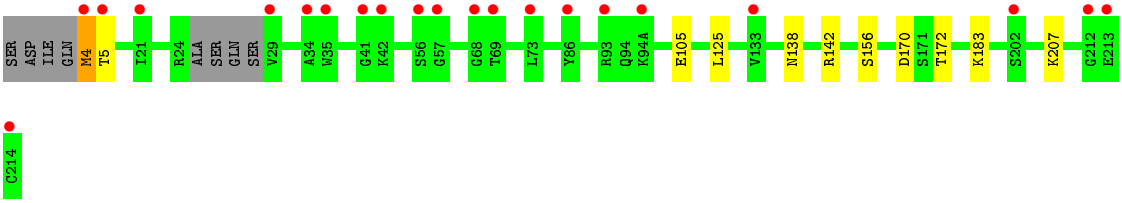
Chain F:



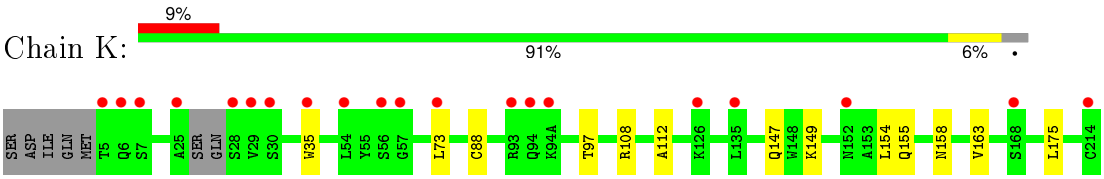
• Molecule 2: Fab Light Chain

Chain I:

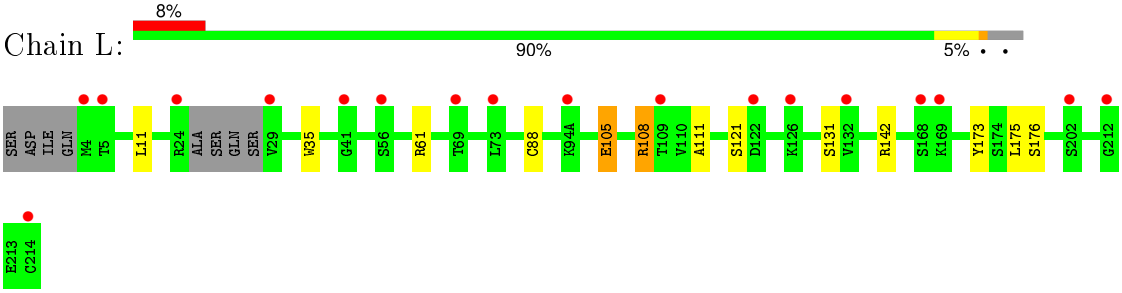




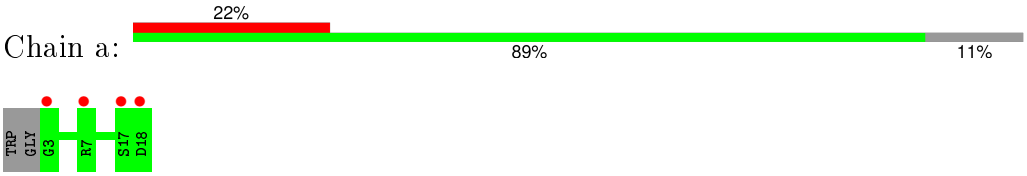
• Molecule 2: Fab Light Chain



• Molecule 2: Fab Light Chain



• Molecule 3: paxillin LD4



• Molecule 3: paxillin LD4

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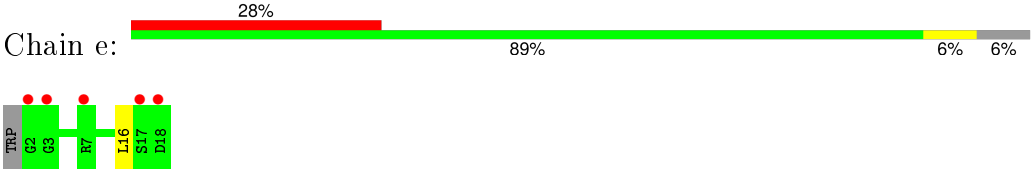
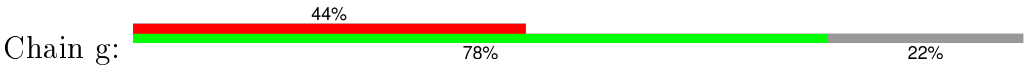
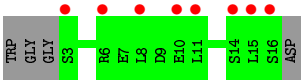


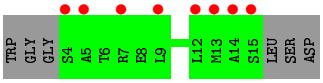
• Molecule 3: paxillin LD4





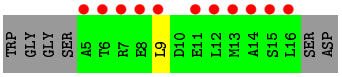
- Molecule 3: paxillin LD4

Chain h:



- Molecule 3: paxillin LD4

Chain j:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	117.58Å 138.12Å 223.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	117.50 – 2.00 20.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	93.2 (117.50-2.00) 93.3 (20.00-2.00)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.31 (at 2.01Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.224 , 0.258 0.224 , 0.226	Depositor DCC
R_{free} test set	11454 reflections (5.29%)	DCC
Wilson B-factor (Å^2)	30.8	Xtriage
Anisotropy	0.177	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 44.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	1 of 228060 reflections (0.000%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	21729	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.33% 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

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, LDA, PO4, ACE, ACT

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	0.49	0/1683	0.58	0/2298
1	C	0.49	0/1685	0.55	0/2300
1	E	0.50	0/1687	0.61	1/2303 (0.0%)
1	G	0.48	0/1692	0.56	0/2310
1	H	0.47	0/1641	0.55	0/2241
1	J	0.50	1/1701 (0.1%)	0.55	0/2321
2	B	0.42	0/1641	0.59	0/2223
2	D	0.42	0/1641	0.58	0/2223
2	F	0.45	0/1639	0.64	0/2220
2	I	0.40	0/1635	0.57	0/2215
2	K	0.44	0/1638	0.58	0/2220
2	L	0.41	0/1621	0.56	0/2199
3	a	0.48	0/112	0.59	0/149
3	c	0.34	0/77	0.40	0/103
3	e	0.42	0/119	0.51	0/158
3	g	0.40	0/97	0.49	0/129
3	h	0.40	0/81	0.44	0/107
3	j	0.41	0/79	0.51	0/106
All	All	0.46	1/20469 (0.0%)	0.58	1/27825 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	36	TRP	CD2-CE2	5.19	1.47	1.41

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	178	LEU	CA-CB-CG	5.36	127.63	115.30

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	1640	0	1582	9	0
1	C	1642	0	1585	17	0
1	E	1644	0	1592	12	0
1	G	1646	0	1590	22	0
1	H	1599	0	1547	10	0
1	J	1658	0	1608	13	0
2	B	1608	0	1573	11	0
2	D	1608	0	1572	18	0
2	F	1606	0	1575	17	0
2	I	1602	0	1568	11	0
2	K	1605	0	1568	12	0
2	L	1588	0	1540	12	0
3	a	113	0	107	0	0
3	c	78	0	70	0	0
3	e	120	0	112	0	0
3	g	98	0	91	0	0
3	h	82	0	75	0	0
3	j	80	0	77	0	0
4	B	12	0	16	0	0
4	C	12	0	16	1	0
4	D	6	0	8	0	0
4	F	24	0	32	0	0
4	G	6	0	8	0	0
4	H	12	0	16	0	0
4	I	18	0	24	1	0
4	K	18	0	24	1	0
4	L	12	0	16	7	0
5	D	5	0	0	0	0
5	F	5	0	0	0	0
6	F	4	0	3	0	0
7	F	16	0	31	5	0
8	J	3	0	3	0	0
8	L	3	0	3	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	A	117	0	0	0	0
9	B	133	0	0	2	0
9	C	110	0	0	0	0
9	D	118	0	0	1	0
9	E	174	0	0	4	0
9	F	173	0	0	5	0
9	G	99	0	0	3	0
9	H	92	0	0	0	0
9	I	118	0	0	3	0
9	J	143	0	0	2	0
9	K	154	0	0	1	0
9	L	101	0	0	1	0
9	a	7	0	0	0	0
9	c	1	0	0	0	0
9	e	6	0	0	0	0
9	g	5	0	0	0	0
9	h	3	0	0	0	0
9	j	2	0	0	0	0
All	All	21729	0	19632	157	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 4.

The worst 5 of 157 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)
9:E:396:HOH:O	1:G:193:THR:HG21	1.72	0.90
2:L:142:ARG:NH1	9:L:401:HOH:O	2.10	0.83
7:F:306:LDA:HM11	9:F:424:HOH:O	1.85	0.76
2:K:155:GLN:HE21	2:K:158:ASN:HD21	1.35	0.74
1:J:138:LEU:HD13	9:J:439:HOH:O	1.88	0.73

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	218/228 (96%)	206 (94%)	12 (6%)	0	100	100
1	C	218/228 (96%)	212 (97%)	6 (3%)	0	100	100
1	E	218/228 (96%)	214 (98%)	4 (2%)	0	100	100
1	G	219/228 (96%)	215 (98%)	4 (2%)	0	100	100
1	H	209/228 (92%)	207 (99%)	2 (1%)	0	100	100
1	J	220/228 (96%)	215 (98%)	5 (2%)	0	100	100
2	B	206/217 (95%)	201 (98%)	5 (2%)	0	100	100
2	D	206/217 (95%)	199 (97%)	5 (2%)	2 (1%)	19	11
2	F	205/217 (94%)	197 (96%)	8 (4%)	0	100	100
2	I	205/217 (94%)	197 (96%)	8 (4%)	0	100	100
2	K	206/217 (95%)	200 (97%)	6 (3%)	0	100	100
2	L	205/217 (94%)	198 (97%)	7 (3%)	0	100	100
3	a	14/18 (78%)	14 (100%)	0	0	100	100
3	c	9/18 (50%)	9 (100%)	0	0	100	100
3	e	15/18 (83%)	14 (93%)	1 (7%)	0	100	100
3	g	12/18 (67%)	12 (100%)	0	0	100	100
3	h	10/18 (56%)	10 (100%)	0	0	100	100
3	j	10/18 (56%)	8 (80%)	2 (20%)	0	100	100
All	All	2605/2778 (94%)	2528 (97%)	75 (3%)	2 (0%)	56	53

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	56	SER
2	D	40	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	182/191 (95%)	182 (100%)	0	100 100
1	C	182/191 (95%)	180 (99%)	2 (1%)	80 83
1	E	182/191 (95%)	180 (99%)	2 (1%)	80 83
1	G	183/191 (96%)	179 (98%)	4 (2%)	60 62
1	H	177/191 (93%)	176 (99%)	1 (1%)	90 93
1	J	185/191 (97%)	182 (98%)	3 (2%)	70 73
2	B	185/192 (96%)	181 (98%)	4 (2%)	60 62
2	D	185/192 (96%)	183 (99%)	2 (1%)	80 83
2	F	185/192 (96%)	181 (98%)	4 (2%)	60 62
2	I	184/192 (96%)	182 (99%)	2 (1%)	80 83
2	K	184/192 (96%)	183 (100%)	1 (0%)	92 94
2	L	181/192 (94%)	179 (99%)	2 (1%)	80 83
3	a	12/14 (86%)	12 (100%)	0	100 100
3	c	8/14 (57%)	7 (88%)	1 (12%)	6 3
3	e	13/14 (93%)	12 (92%)	1 (8%)	16 10
3	g	10/14 (71%)	10 (100%)	0	100 100
3	h	7/14 (50%)	7 (100%)	0	100 100
3	j	7/14 (50%)	6 (86%)	1 (14%)	4 2
All	All	2252/2382 (94%)	2222 (99%)	30 (1%)	76 79

5 of 30 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	154	LEU
1	G	178	LEU
3	c	6	THR
1	G	77	THR
1	G	193	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
2	F	210	ASN
1	G	200	HIS
2	K	155	GLN
1	G	82(A)	ASN

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Mol	Chain	Res	Type
1	H	35	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

26 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	GOL	B	301	-	5,5,5	0.32	0	5,5,5	0.23	0
4	GOL	B	302	-	5,5,5	0.34	0	5,5,5	0.32	0
4	GOL	C	301	-	5,5,5	0.23	0	5,5,5	0.53	0
4	GOL	C	302	-	5,5,5	0.26	0	5,5,5	0.12	0
4	GOL	D	301	-	5,5,5	0.16	0	5,5,5	0.35	0
5	PO4	D	302	-	4,4,4	0.98	0	6,6,6	0.24	0
4	GOL	F	301	-	5,5,5	0.31	0	5,5,5	0.24	0
4	GOL	F	302	-	5,5,5	0.25	0	5,5,5	0.21	0
4	GOL	F	303	-	5,5,5	0.15	0	5,5,5	0.45	0
5	PO4	F	304	-	4,4,4	1.11	0	6,6,6	0.23	0
6	ACT	F	305	-	0,3,3	0.00	-	0,3,3	0.00	-
7	LDA	F	306	-	15,15,15	4.00	1 (6%)	16,17,17	0.74	1 (6%)
4	GOL	F	307	-	5,5,5	0.25	0	5,5,5	0.25	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	GOL	G	301	-	5,5,5	0.26	0	5,5,5	0.13	0
4	GOL	H	301	-	5,5,5	0.29	0	5,5,5	0.32	0
4	GOL	H	302	-	5,5,5	0.34	0	5,5,5	0.52	0
4	GOL	I	301	-	5,5,5	0.30	0	5,5,5	0.23	0
4	GOL	I	302	-	5,5,5	0.29	0	5,5,5	0.26	0
4	GOL	I	303	-	5,5,5	0.31	0	5,5,5	0.31	0
8	ACE	J	301	-	2,2,2	0.53	0	0,1,1	0.00	-
4	GOL	K	301	-	5,5,5	0.14	0	5,5,5	0.65	0
4	GOL	K	302	-	5,5,5	0.19	0	5,5,5	0.38	0
4	GOL	K	303	-	5,5,5	0.29	0	5,5,5	0.21	0
4	GOL	L	301	-	5,5,5	0.29	0	5,5,5	0.49	0
4	GOL	L	302	-	5,5,5	0.25	0	5,5,5	0.20	0
8	ACE	L	303	-	2,2,2	0.60	0	0,1,1	0.00	-

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	GOL	B	301	-	-	0/4/4/4	0/0/0/0
4	GOL	B	302	-	-	0/4/4/4	0/0/0/0
4	GOL	C	301	-	-	0/4/4/4	0/0/0/0
4	GOL	C	302	-	-	0/4/4/4	0/0/0/0
4	GOL	D	301	-	-	0/4/4/4	0/0/0/0
5	PO4	D	302	-	-	0/0/0/0	0/0/0/0
4	GOL	F	301	-	-	0/4/4/4	0/0/0/0
4	GOL	F	302	-	-	0/4/4/4	0/0/0/0
4	GOL	F	303	-	-	0/4/4/4	0/0/0/0
5	PO4	F	304	-	-	0/0/0/0	0/0/0/0
6	ACT	F	305	-	-	0/0/0/0	0/0/0/0
7	LDA	F	306	-	-	0/13/13/13	0/0/0/0
4	GOL	F	307	-	-	0/4/4/4	0/0/0/0
4	GOL	G	301	-	-	0/4/4/4	0/0/0/0
4	GOL	H	301	-	-	0/4/4/4	0/0/0/0
4	GOL	H	302	-	-	0/4/4/4	0/0/0/0
4	GOL	I	301	-	-	0/4/4/4	0/0/0/0
4	GOL	I	302	-	-	0/4/4/4	0/0/0/0
4	GOL	I	303	-	-	0/4/4/4	0/0/0/0
8	ACE	J	301	-	-	0/0/0/0	0/0/0/0
4	GOL	K	301	-	-	0/4/4/4	0/0/0/0
4	GOL	K	302	-	-	0/4/4/4	0/0/0/0
4	GOL	K	303	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	L	301	-	-	0/4/4/4	0/0/0/0
4	GOL	L	302	-	-	0/4/4/4	0/0/0/0
8	ACE	L	303	-	-	0/0/0/0	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	F	306	LDA	O1-N1	-15.18	1.25	1.39

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	F	306	LDA	O1-N1-CM1	-2.08	106.28	109.05

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	302	GOL	1	0
7	F	306	LDA	5	0
4	I	301	GOL	1	0
4	K	303	GOL	1	0
4	L	301	GOL	7	0
8	L	303	ACE	2	0

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	220/228 (96%)	0.62	16 (7%) 18 19	17, 26, 52, 90	0
1	C	220/228 (96%)	1.13	48 (21%) 1 1	16, 35, 77, 98	0
1	E	220/228 (96%)	0.24	8 (3%) 46 48	14, 23, 34, 64	0
1	G	220/228 (96%)	0.70	23 (10%) 8 9	18, 32, 54, 82	0
1	H	213/228 (93%)	0.73	25 (11%) 6 7	23, 31, 52, 75	0
1	J	222/228 (97%)	0.72	21 (9%) 10 11	17, 27, 48, 88	0
2	B	210/217 (96%)	0.45	15 (7%) 19 20	18, 26, 46, 81	0
2	D	210/217 (96%)	0.80	25 (11%) 6 6	17, 31, 63, 92	0
2	F	209/217 (96%)	0.44	9 (4%) 39 40	14, 22, 48, 72	0
2	I	209/217 (96%)	0.69	21 (10%) 9 10	19, 30, 50, 100	0
2	K	210/217 (96%)	0.61	20 (9%) 10 11	17, 25, 49, 77	0
2	L	209/217 (96%)	0.75	18 (8%) 13 14	21, 32, 53, 84	0
3	a	16/18 (88%)	1.39	4 (25%) 1 1	24, 29, 52, 53	0
3	c	11/18 (61%)	3.95	10 (90%) 0 0	74, 81, 85, 86	0
3	e	17/18 (94%)	2.05	5 (29%) 1 1	26, 34, 60, 72	0
3	g	14/18 (77%)	2.23	8 (57%) 0 1	44, 50, 56, 58	0
3	h	12/18 (66%)	3.22	8 (66%) 0 1	55, 60, 67, 69	0
3	j	12/18 (66%)	4.39	11 (91%) 0 0	63, 72, 91, 92	0
All	All	2654/2778 (95%)	0.72	295 (11%) 7 8	14, 28, 60, 100	0

The worst 5 of 295 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	131	THR	13.6
2	B	214	CYS	13.2
2	I	4	MET	13.1

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Mol	Chain	Res	Type	RSRZ
1	J	216	CYS	13.0
2	L	4	MET	12.7

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)

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	GOL	I	301	6/6	0.69	0.50	11.59	46,48,50,51	0
4	GOL	L	302	6/6	0.72	0.34	9.40	61,62,63,65	0
4	GOL	C	302	6/6	0.81	0.25	5.82	38,41,42,45	0
6	ACT	F	305	4/4	0.67	0.30	5.76	47,48,50,51	0
4	GOL	G	301	6/6	0.62	0.46	4.55	71,73,75,78	0
4	GOL	C	301	6/6	0.83	0.22	4.26	21,23,25,30	0
7	LDA	F	306	16/16	0.64	0.39	3.98	52,57,61,61	0
4	GOL	I	303	6/6	0.68	0.31	3.92	44,45,46,49	0
4	GOL	F	302	6/6	0.83	0.24	3.71	46,48,49,51	0
4	GOL	K	301	6/6	0.82	0.28	3.10	36,40,43,43	0
4	GOL	I	302	6/6	0.82	0.27	2.73	43,46,47,47	0
4	GOL	H	302	6/6	0.86	0.22	2.22	40,42,42,44	0
4	GOL	L	301	6/6	0.82	0.25	2.12	39,40,41,42	0
4	GOL	F	303	6/6	0.91	0.19	1.98	20,21,21,21	0
4	GOL	B	302	6/6	0.90	0.17	1.81	35,36,37,38	0
4	GOL	B	301	6/6	0.57	0.47	1.75	55,58,59,61	0
4	GOL	F	301	6/6	0.85	0.17	0.99	27,30,30,33	0
4	GOL	K	302	6/6	0.90	0.17	0.78	31,35,37,39	0
4	GOL	D	301	6/6	0.78	0.26	0.38	47,48,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	PO4	D	302	5/5	0.99	0.09	-2.14	22,23,24,25	0
4	GOL	H	301	6/6	0.70	0.32	-	58,60,61,62	0
4	GOL	K	303	6/6	0.30	0.48	-	61,64,67,69	0
5	PO4	F	304	5/5	0.98	0.17	-	29,31,32,34	0
8	ACE	J	301	3/3	0.62	0.28	-	49,49,49,50	0
4	GOL	F	307	6/6	0.68	0.34	-	53,55,57,59	0
8	ACE	L	303	3/3	0.94	0.12	-	38,38,39,39	0

6.5 Other polymers

There are no such residues in this entry.