Full wwPDB X-ray Structure Validation Report (i)

Oct 7, 2016 – 01:22 AM EDT

PDB ID	:	5K24
Title	:	Crystal structure of the complex between phosphatase PRL-2 in the oxidized state with the Bateman domain of murine magnesium transporter CNNM3
Authors	:	Kozlov, G.; Gulerez, I.; Gehring, K.
Deposited on	:	2016-05-18
Resolution	:	3.10 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:

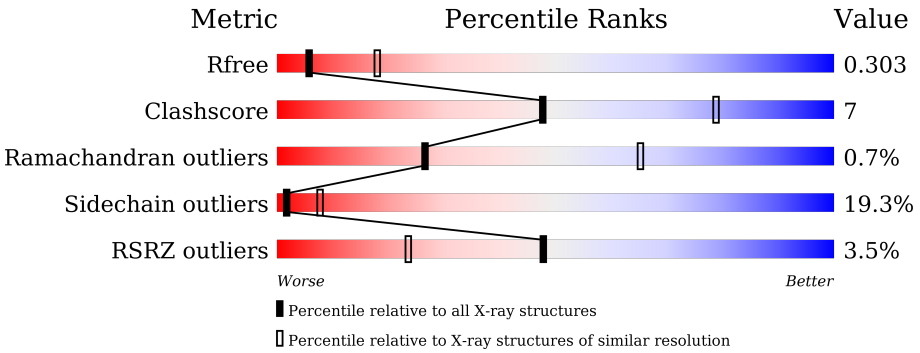
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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	183	51% 28% • 17%
1	B	183	8% 59% 18% • 19%
2	C	153	% 58% 28% • • 10%
2	D	153	3% 58% 24% 6% • 12%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4522 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 Protein tyrosine phosphatase type IVA 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	152	Total	C	N	O	S	0	0	0
			1203	772	206	217	8			
1	B	149	Total	C	N	O	S	0	0	0
			1180	758	203	212	7			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP O70274
A	-18	GLY	-	expression tag	UNP O70274
A	-17	SER	-	expression tag	UNP O70274
A	-16	SER	-	expression tag	UNP O70274
A	-15	HIS	-	expression tag	UNP O70274
A	-14	HIS	-	expression tag	UNP O70274
A	-13	HIS	-	expression tag	UNP O70274
A	-12	HIS	-	expression tag	UNP O70274
A	-11	HIS	-	expression tag	UNP O70274
A	-10	HIS	-	expression tag	UNP O70274
A	-9	SER	-	expression tag	UNP O70274
A	-8	SER	-	expression tag	UNP O70274
A	-7	GLY	-	expression tag	UNP O70274
A	-6	LEU	-	expression tag	UNP O70274
A	-5	VAL	-	expression tag	UNP O70274
A	-4	PRO	-	expression tag	UNP O70274
A	-3	ARG	-	expression tag	UNP O70274
A	-2	GLY	-	expression tag	UNP O70274
A	-1	SER	-	expression tag	UNP O70274
A	0	HIS	-	expression tag	UNP O70274
B	-19	MET	-	initiating methionine	UNP O70274
B	-18	GLY	-	expression tag	UNP O70274
B	-17	SER	-	expression tag	UNP O70274
B	-16	SER	-	expression tag	UNP O70274
B	-15	HIS	-	expression tag	UNP O70274

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	expression tag	UNP O70274
B	-13	HIS	-	expression tag	UNP O70274
B	-12	HIS	-	expression tag	UNP O70274
B	-11	HIS	-	expression tag	UNP O70274
B	-10	HIS	-	expression tag	UNP O70274
B	-9	SER	-	expression tag	UNP O70274
B	-8	SER	-	expression tag	UNP O70274
B	-7	GLY	-	expression tag	UNP O70274
B	-6	LEU	-	expression tag	UNP O70274
B	-5	VAL	-	expression tag	UNP O70274
B	-4	PRO	-	expression tag	UNP O70274
B	-3	ARG	-	expression tag	UNP O70274
B	-2	GLY	-	expression tag	UNP O70274
B	-1	SER	-	expression tag	UNP O70274
B	0	HIS	-	expression tag	UNP O70274

- Molecule 2 is a protein called Metal transporter CNNM3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	137	Total	C	N	O	S	0	0	0
			1074	685	168	216	5			
2	D	135	Total	C	N	O	S	0	0	0
			1052	673	162	212	5			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	304	GLY	-	expression tag	UNP Q32NY4
C	305	PRO	-	expression tag	UNP Q32NY4
C	306	LEU	-	expression tag	UNP Q32NY4
C	307	ASN	-	expression tag	UNP Q32NY4
C	308	MET	-	expression tag	UNP Q32NY4
C	309	ILE	-	expression tag	UNP Q32NY4
C	310	GLN	-	expression tag	UNP Q32NY4
C	311	GLY	-	expression tag	UNP Q32NY4
C	312	VAL	-	expression tag	UNP Q32NY4
C	313	LEU	-	expression tag	UNP Q32NY4
C	314	GLU	-	expression tag	UNP Q32NY4
D	304	GLY	-	expression tag	UNP Q32NY4
D	305	PRO	-	expression tag	UNP Q32NY4
D	306	LEU	-	expression tag	UNP Q32NY4
D	307	ASN	-	expression tag	UNP Q32NY4

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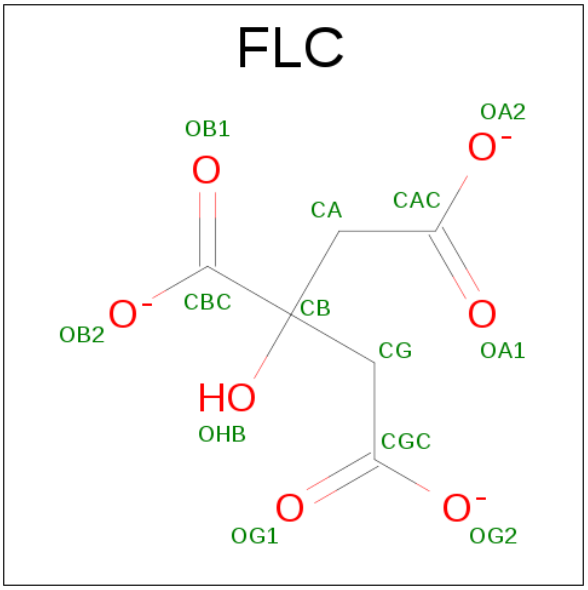
Chain	Residue	Modelled	Actual	Comment	Reference
D	308	MET	-	expression tag	UNP Q32NY4
D	309	ILE	-	expression tag	UNP Q32NY4
D	310	GLN	-	expression tag	UNP Q32NY4
D	311	GLY	-	expression tag	UNP Q32NY4
D	312	VAL	-	expression tag	UNP Q32NY4
D	313	LEU	-	expression tag	UNP Q32NY4
D	314	GLU	-	expression tag	UNP Q32NY4

- Molecule 3 is CITRATE ANION (three-letter code: FLC) (formula: $C_6H_5O_7$).



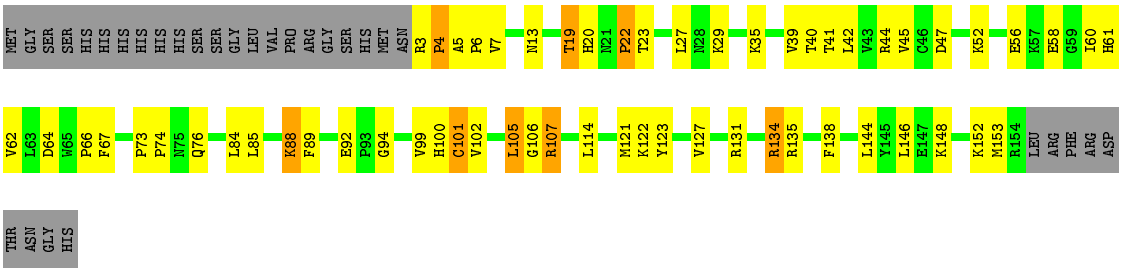
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	C	O	0	0
			13	6	7		

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.

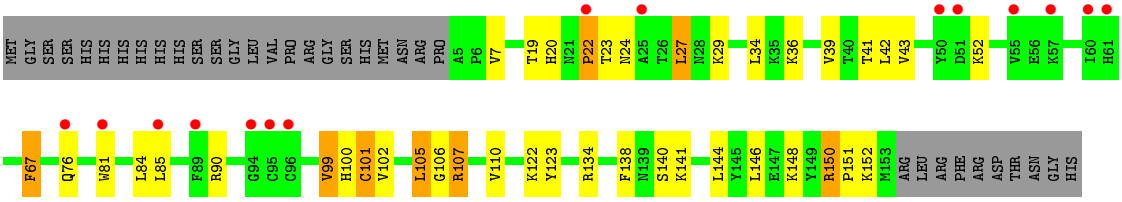
- Molecule 1: Protein tyrosine phosphatase type IVA 2

Chain A:



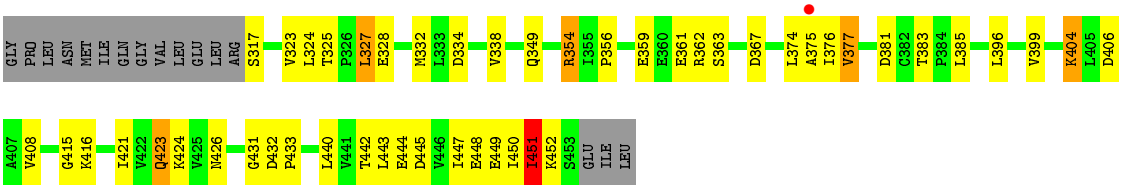
- Molecule 1: Protein tyrosine phosphatase type IVA 2

Chain B:



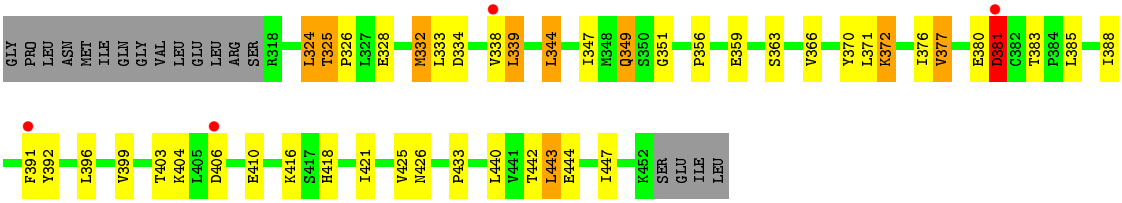
- Molecule 2: Metal transporter CNNM3

Chain C:



- Molecule 2: Metal transporter CNNM3

Chain D:


GLY PRO LEU ASN MET ILE GLN GLY VAL LEU GLU LEU ARG SER R318 L324 T325 P326 L327 E328 M332 L333 D334 V338 L339 L344 I347 N348 Q349 S350 G351 P356 E359 S363 V366 Y370 L371 K372 I376 V377 E380 D381 C382 T383 P384 L385 I388

F391 Y392 L396 V399 T403 K404 L405 D406 E410 K416 S417 H418 I421 V425 N426 P433 L440 V441 T442 L443 E444 I447 K452 SER GLU ILE LEU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	154.22Å 52.12Å 102.86Å 90.00° 106.02° 90.00°	Depositor
Resolution (Å)	50.00 – 3.10 38.35 – 3.10	Depositor EDS
% Data completeness (in resolution range)	98.9 (50.00-3.10) 99.0 (38.35-3.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.38 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.8.0069	Depositor
R, R_{free}	0.252 , 0.303 0.252 , 0.303	Depositor DCC
R_{free} test set	740 reflections (5.41%)	DCC
Wilson B-factor (Å^2)	96.3	Xtriage
Anisotropy	0.181	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 66.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	4522	wwPDB-VP
Average B, all atoms (Å^2)	121.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.88% 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: FLC

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	0.30	0/1232	0.50	0/1674
1	B	0.28	0/1208	0.45	0/1641
2	C	0.29	0/1094	0.49	0/1490
2	D	0.28	0/1072	0.46	0/1463
All	All	0.28	0/4606	0.48	0/6268

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
1	A	0	9
1	B	0	5
2	C	0	8
2	D	0	5
All	All	0	27

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (27) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	100	HIS	Peptide
1	A	101	CYS	Peptide
1	A	152	LYS	Peptide
1	A	19	THR	Peptide
1	A	22	PRO	Peptide

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Mol	Chain	Res	Type	Group
1	A	3	ARG	Peptide
1	A	4	PRO	Peptide
1	A	66	PRO	Peptide
1	A	94	GLY	Peptide
1	B	100	HIS	Peptide
1	B	101	CYS	Peptide
1	B	152	LYS	Peptide
1	B	22	PRO	Peptide
1	B	67	PHE	Peptide
2	C	359	GLU	Peptide
2	C	377	VAL	Peptide
2	C	381	ASP	Peptide
2	C	396	LEU	Peptide
2	C	415	GLY	Peptide
2	C	423	GLN	Peptide
2	C	431	GLY	Peptide
2	C	451	ILE	Peptide
2	D	324	LEU	Peptide
2	D	351	GLY	Peptide
2	D	359	GLU	Peptide
2	D	377	VAL	Peptide
2	D	381	ASP	Peptide

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	1203	0	1198	26	0
1	B	1180	0	1178	12	0
2	C	1074	0	1038	13	0
2	D	1052	0	1006	18	0
3	D	13	0	5	2	0
All	All	4522	0	4425	66	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 7.

All (66) 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:D:501:FLC:OB1	3:D:501:FLC:CAC	2.27	0.79
1:A:105:LEU:HD22	1:A:105:LEU:H	1.49	0.77
1:A:40:THR:HG21	1:A:92:GLU:OE2	1.91	0.71
2:D:332:MET:HB3	2:D:356:PRO:HG2	1.78	0.65
1:A:105:LEU:CD2	1:A:105:LEU:H	2.11	0.63
2:D:418:HIS:HB2	2:D:443:LEU:HB2	1.80	0.62
1:A:101:CYS:SG	1:A:102:VAL:N	2.75	0.60
2:C:376:ILE:O	2:C:376:ILE:HG22	2.02	0.59
1:A:105:LEU:N	1:A:105:LEU:HD22	2.19	0.56
2:D:370:TYR:HB3	2:D:372:LYS:HE3	1.87	0.55
2:D:372:LYS:HE2	2:D:372:LYS:H	1.70	0.55
1:A:44:ARG:HD2	1:A:62:VAL:HG13	1.89	0.55
1:A:84:LEU:O	1:A:88:LYS:HB2	2.07	0.54
3:D:501:FLC:OG1	3:D:501:FLC:OHB	2.23	0.54
1:B:105:LEU:HG	2:D:433:PRO:HB2	1.88	0.54
2:C:399:VAL:HG21	2:C:408:VAL:HG23	1.90	0.53
2:C:375:ALA:HB1	2:D:349:GLN:HA	1.90	0.53
2:D:344:LEU:HA	2:D:347:ILE:HD12	1.91	0.52
2:D:376:ILE:HD12	2:D:392:TYR:OH	2.12	0.50
1:A:22:PRO:HB2	1:A:23:THR:O	2.11	0.49
1:B:81:TRP:O	1:B:85:LEU:HG	2.13	0.49
1:A:7:VAL:HG21	1:A:134:ARG:HD2	1.95	0.48
1:B:106:GLY:O	1:B:110:VAL:HG23	2.13	0.48
2:D:339:LEU:HD21	2:D:385:LEU:HD23	1.95	0.48
2:C:450:ILE:HG22	2:C:450:ILE:O	2.14	0.48
1:B:41:THR:HG21	1:B:84:LEU:HD11	1.95	0.47
2:C:356:PRO:HG3	2:C:440:LEU:HD11	1.95	0.47
1:A:105:LEU:N	1:A:105:LEU:CD2	2.75	0.47
2:C:317:SER:N	2:C:404:LYS:HE3	2.30	0.46
2:C:323:VAL:HG12	2:C:445:ASP:HB3	1.97	0.46
1:A:105:LEU:HG	2:C:433:PRO:HB2	1.98	0.46
2:D:356:PRO:HG3	2:D:440:LEU:HD11	1.98	0.46
1:B:101:CYS:SG	1:B:102:VAL:N	2.89	0.45
1:A:85:LEU:HB3	1:A:89:PHE:CE2	2.52	0.45
1:A:13:ASN:HD22	1:A:89:PHE:HB3	1.81	0.45
2:D:388:ILE:O	2:D:391:PHE:HB2	2.16	0.45
2:C:354:ARG:HH22	2:C:416:LYS:HE2	1.82	0.45
1:B:24:ASN:HA	1:B:27:LEU:HD12	1.98	0.45
2:C:449:GLU:HG3	2:C:449:GLU:O	2.17	0.45
1:A:5:ALA:HA	1:A:6:PRO:HD3	1.73	0.45
1:B:22:PRO:HB2	1:B:23:THR:O	2.18	0.44
2:D:396:LEU:H	2:D:396:LEU:HD23	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:ARG:HA	1:B:151:PRO:HD2	1.78	0.44
1:A:127:VAL:O	1:A:131:ARG:HG3	2.18	0.44
1:A:44:ARG:NH1	1:A:64:ASP:OD1	2.51	0.44
2:D:325:THR:HA	2:D:326:PRO:HD2	1.90	0.44
2:D:418:HIS:HB3	2:D:443:LEU:HD12	1.99	0.44
1:B:43:VAL:HB	1:B:99:VAL:HG13	2.00	0.44
1:A:45:VAL:HB	1:A:101:CYS:HB2	2.00	0.43
1:A:35:LYS:HE3	1:A:58:GLU:HB3	1.99	0.43
1:A:106:GLY:HA3	2:C:432:ASP:CG	2.38	0.43
2:D:406:ASP:O	2:D:410:GLU:HG2	2.18	0.43
1:A:56:GLU:HA	1:A:60:ILE:O	2.19	0.43
1:A:44:ARG:HD3	1:A:64:ASP:OD1	2.19	0.43
2:D:333:LEU:HD11	2:D:347:ILE:HG12	2.01	0.42
2:D:380:GLU:HA	2:D:381:ASP:HA	1.68	0.42
2:C:327:LEU:O	2:C:362:ARG:NH2	2.44	0.42
1:B:34:LEU:HB3	1:B:39:VAL:CG2	2.50	0.42
1:A:114:LEU:HA	1:A:114:LEU:HD12	1.91	0.42
1:A:67:PHE:CE2	1:A:107:ARG:HB2	2.56	0.41
1:A:41:THR:HA	1:A:61:HIS:O	2.21	0.41
1:A:73:PRO:HA	1:A:74:PRO:HD3	1.94	0.41
2:C:447:ILE:HG13	2:D:447:ILE:HD12	2.03	0.41
1:B:7:VAL:HG21	1:B:134:ARG:HD3	2.04	0.40
1:B:67:PHE:CZ	1:B:107:ARG:HB2	2.56	0.40
1:A:88:LYS:HD2	1:A:88:LYS:HA	1.87	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	150/183 (82%)	138 (92%)	10 (7%)	2 (1%)	15 50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	147/183 (80%)	143 (97%)	3 (2%)	1 (1%)	26 65
2	C	135/153 (88%)	125 (93%)	9 (7%)	1 (1%)	26 65
2	D	133/153 (87%)	124 (93%)	9 (7%)	0	100 100
All	All	565/672 (84%)	530 (94%)	31 (6%)	4 (1%)	26 65

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	PRO
1	B	138	PHE
1	A	138	PHE
2	C	451	ILE

5.3.2 Protein sidechains

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	129/159 (81%)	107 (83%)	22 (17%)	2 11
1	B	126/159 (79%)	106 (84%)	20 (16%)	3 13
2	C	123/141 (87%)	95 (77%)	28 (23%)	1 4
2	D	119/141 (84%)	93 (78%)	26 (22%)	1 5
All	All	497/600 (83%)	401 (81%)	96 (19%)	2 8

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	THR
1	A	20	HIS
1	A	27	LEU
1	A	29	LYS
1	A	39	VAL
1	A	42	LEU
1	A	47	ASP

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Mol	Chain	Res	Type
1	A	52	LYS
1	A	76	GLN
1	A	88	LYS
1	A	99	VAL
1	A	105	LEU
1	A	107	ARG
1	A	121	MET
1	A	122	LYS
1	A	123	TYR
1	A	134	ARG
1	A	135	ARG
1	A	144	LEU
1	A	146	LEU
1	A	148	LYS
1	A	153	MET
1	B	19	THR
1	B	20	HIS
1	B	27	LEU
1	B	29	LYS
1	B	36	LYS
1	B	42	LEU
1	B	52	LYS
1	B	76	GLN
1	B	90	ARG
1	B	99	VAL
1	B	105	LEU
1	B	107	ARG
1	B	122	LYS
1	B	123	TYR
1	B	140	SER
1	B	141	LYS
1	B	144	LEU
1	B	146	LEU
1	B	148	LYS
1	B	150	ARG
2	C	324	LEU
2	C	325	THR
2	C	327	LEU
2	C	328	GLU
2	C	332	MET
2	C	334	ASP
2	C	338	VAL

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Mol	Chain	Res	Type
2	C	349	GLN
2	C	354	ARG
2	C	361	GLU
2	C	363	SER
2	C	367	ASP
2	C	374	LEU
2	C	377	VAL
2	C	383	THR
2	C	385	LEU
2	C	404	LYS
2	C	406	ASP
2	C	421	ILE
2	C	423	GLN
2	C	424	LYS
2	C	426	ASN
2	C	442	THR
2	C	443	LEU
2	C	444	GLU
2	C	448	GLU
2	C	451	ILE
2	C	452	LYS
2	D	324	LEU
2	D	325	THR
2	D	328	GLU
2	D	332	MET
2	D	334	ASP
2	D	338	VAL
2	D	339	LEU
2	D	344	LEU
2	D	349	GLN
2	D	363	SER
2	D	366	VAL
2	D	371	LEU
2	D	372	LYS
2	D	377	VAL
2	D	381	ASP
2	D	383	THR
2	D	399	VAL
2	D	403	THR
2	D	404	LYS
2	D	416	LYS
2	D	421	ILE

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Mol	Chain	Res	Type
2	D	425	VAL
2	D	426	ASN
2	D	442	THR
2	D	443	LEU
2	D	444	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	ASN
2	C	349	GLN
2	D	401	ASN

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

1 ligand is 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	$\#\|Z\| > 2$
3	FLC	D	501	-	3,12,12	0.97	0	3,17,17	2.55	2 (66%)

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
3	FLC	D	501	-	-	0/6/16/16	0/0/0/0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	501	FLC	CB-CA-CAC	-3.22	109.93	114.95
3	D	501	FLC	CB-CG-CGC	-3.03	110.22	114.95

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	501	FLC	2	0

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	152/183 (83%)	-0.29	0 100 100	61, 80, 113, 126	0
1	B	149/183 (81%)	0.44	15 (10%) 9 3	82, 145, 236, 287	0
2	C	137/153 (89%)	-0.19	1 (0%) 89 78	69, 110, 159, 175	0
2	D	135/153 (88%)	0.17	4 (2%) 54 29	102, 137, 205, 291	0
All	All	573/672 (85%)	0.03	20 (3%) 48 23	61, 115, 199, 291	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	96	CYS	5.1
1	B	51	ASP	4.0
1	B	81	TRP	3.8
1	B	89	PHE	3.4
2	C	375	ALA	3.3
1	B	50	TYR	3.3
2	D	381	ASP	2.9
1	B	85	LEU	2.8
2	D	406	ASP	2.7
1	B	22	PRO	2.6
1	B	60	ILE	2.5
1	B	55	VAL	2.5
1	B	76	GLN	2.4
1	B	57	LYS	2.3
2	D	338	VAL	2.3
1	B	94	GLY	2.3
1	B	25	ALA	2.2
2	D	391	PHE	2.1
1	B	95	CYS	2.0
1	B	61	HIS	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)

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
3	FLC	D	501	13/13	0.89	0.19	-	136,142,144,147	13

6.5 Other polymers (i)

There are no such residues in this entry.