Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:36 PM GMT

PDB ID	:	3U7D
Title	:	Crystal structure of the KRIT1/CCM1 FERM domain in complex with the heart of glass (HEG1) cytoplasmic tail
Authors	:	Gingras, A.R.; Liu, J.J.; Ginsberg, M.H.; Assembly, Dynamics and Evolution of Cell-Cell and Cell-Matrix Adhesions (CELLMAT)
Deposited on	:	2011-10-13
Resolution	:	2.49 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:

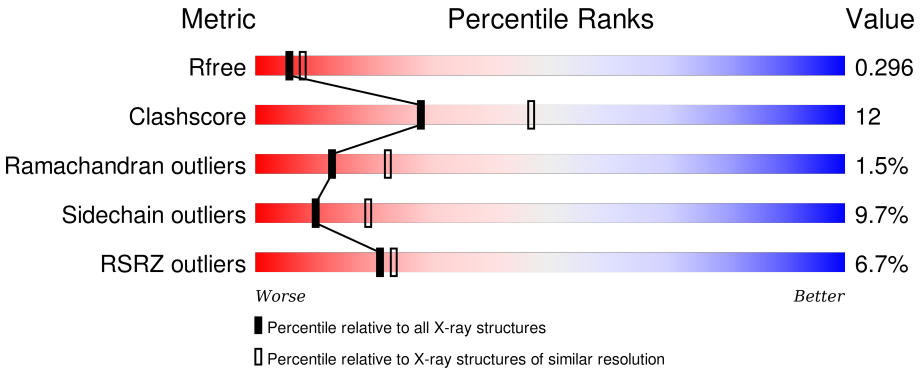
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.49 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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	322	7% 68% 23% • 5%
1	C	322	6% 66% 24% • 5%
2	B	26	4% 8% 12% 8% 73%
2	D	26	12% • 8% 77%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5136 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 Krev interaction trapped protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	305	Total	C	N	O	S	0	0	0
			2493	1608	427	444	14			
1	C	305	Total	C	N	O	S	0	1	0
			2499	1612	427	446	14			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	415	GLY	-	EXPRESSION TAG	UNP O00522
A	416	ALA	-	EXPRESSION TAG	UNP O00522
C	415	GLY	-	EXPRESSION TAG	UNP O00522
C	416	ALA	-	EXPRESSION TAG	UNP O00522

- Molecule 2 is a protein called Protein HEG homolog 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	7	Total	C	N	O	0	0	0
			70	43	16	11			
2	D	6	Total	C	N	O	0	0	0
			64	40	15	9			

- Molecule 3 is water.

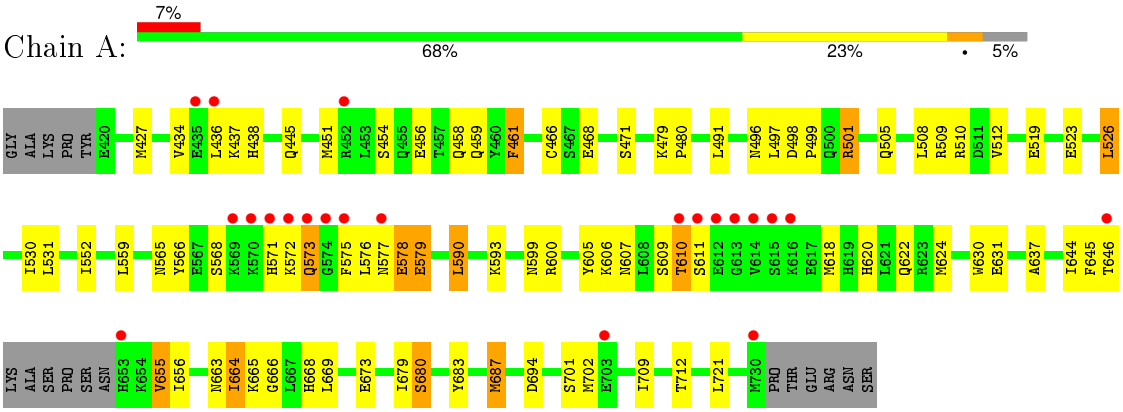
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	8	Total	O	0	0
			8	8		
3	C	2	Total	O	0	0
			2	2		

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.

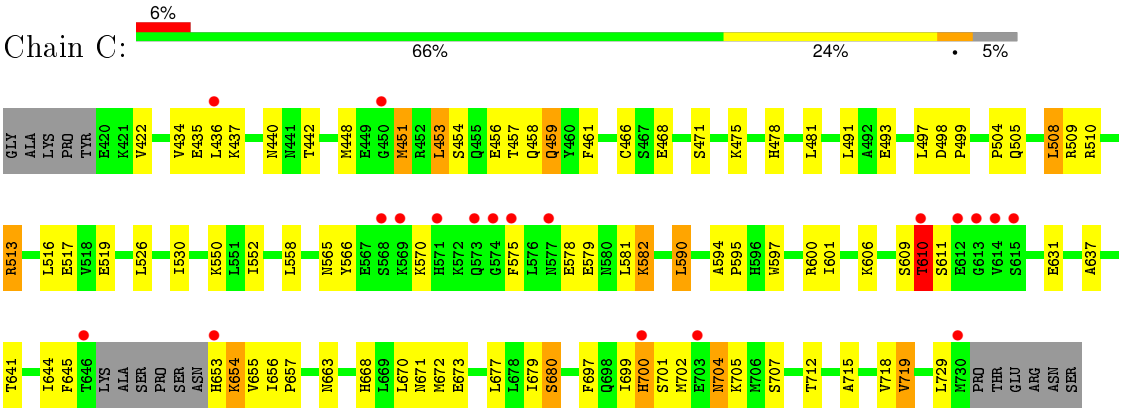
- Molecule 1: Krev interaction trapped protein 1

Chain A:



- Molecule 1: Krev interaction trapped protein 1

Chain C:



- Molecule 2: Protein HEG homolog 1

Chain B:

- Molecule 2: Protein HEG homolog 1

Chain D:


SER
ARG
HIS
SER
CYS
ILE
PHE
PRO
GLY
GLN
TYR
ASN
PRO
SER
PHE
ILE
SER
ASP
GLU
SER
R1376
R1377
R1378
F1381

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	73.05Å 76.82Å 79.18Å 90.00° 113.62° 90.00°	Depositor
Resolution (Å)	72.55 – 2.49 48.93 – 2.49	Depositor EDS
% Data completeness (in resolution range)	98.3 (72.55-2.49) 98.3 (48.93-2.49)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.38 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.234 , 0.309 0.227 , 0.296	Depositor DCC
R_{free} test set	1407 reflections (5.33%)	DCC
Wilson B-factor (Å^2)	51.3	Xtriage
Anisotropy	0.148	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 47.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 27827 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	5136	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.06% 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

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	0.81	1/2549 (0.0%)	0.81	0/3445
1	C	0.81	1/2558 (0.0%)	0.84	0/3457
2	B	0.69	0/71	0.93	0/92
2	D	0.85	0/65	1.19	0/84
All	All	0.81	2/5243 (0.0%)	0.83	0/7078

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	C	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	631	GLU	CG-CD	6.29	1.61	1.51
1	A	523	GLU	CG-CD	5.78	1.60	1.51

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	654	LYS	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	2493	0	2530	49	0
1	C	2499	0	2536	61	0
2	B	70	0	65	7	0
2	D	64	0	60	8	0
3	A	8	0	0	1	0
3	C	2	0	0	0	0
All	All	5136	0	5191	121	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 12.

All (121) 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:D:1377:ARG:HG2	2:D:1377:ARG:HH11	1.25	0.97
2:D:1376:ARG:HG3	2:D:1376:ARG:HH11	1.31	0.94
1:A:456:GLU:O	1:A:459:GLN:HG2	1.71	0.91
1:C:701:SER:HB2	1:C:704:ASN:HB3	1.55	0.89
2:B:1377:ARG:HH21	2:B:1377:ARG:HG2	1.38	0.87
1:A:552:ILE:HG21	1:A:600:ARG:HG2	1.57	0.86
2:B:1376:ARG:HH11	2:B:1376:ARG:HG2	1.41	0.86
1:A:620:HIS:O	1:A:624:MET:HG3	1.79	0.81
1:A:668:HIS:HD2	1:A:680:SER:OG	1.67	0.77
1:A:526:LEU:O	1:A:530:ILE:HD12	1.86	0.76
1:C:491:LEU:HD22	1:C:497:LEU:HD12	1.66	0.75
1:A:498:ASP:HB3	1:A:501:ARG:HG3	1.70	0.74
1:A:573:GLN:NE2	1:A:599:ASN:OD1	2.22	0.72
1:C:451:MET:HB2	1:C:453:LEU:HD22	1.74	0.70
1:A:590:LEU:O	1:A:590:LEU:HD22	1.91	0.70
1:A:427:MET:SD	1:A:509:ARG:HD2	2.31	0.70
1:C:700:HIS:CD2	1:C:700:HIS:N	2.60	0.69
1:A:510:ARG:NH2	1:A:519:GLU:OE1	2.26	0.68
2:B:1376:ARG:NH1	2:B:1376:ARG:HG2	2.00	0.68
2:B:1377:ARG:NH2	2:B:1377:ARG:HG2	2.09	0.67
1:A:454:SER:O	1:A:458:GLN:HG3	1.94	0.66
1:C:671:ASN:OD1	1:C:673:GLU:N	2.28	0.66
1:C:448:MET:HE2	1:C:458:GLN:HG2	1.76	0.66
1:C:701:SER:CB	1:C:704:ASN:HB3	2.26	0.65
1:A:578:GLU:O	1:A:579:GLU:HB2	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:663:ASN:OD1	1:C:668:HIS:HE1	1.82	0.63
2:B:1376:ARG:HH11	2:B:1376:ARG:CG	2.09	0.63
2:D:1376:ARG:CG	2:D:1376:ARG:HH11	2.08	0.62
1:C:579:GLU:OE1	1:C:579:GLU:HA	2.00	0.62
1:C:641:THR:HG22	1:C:672:MET:HE2	1.82	0.61
1:C:448:MET:CE	1:C:458:GLN:HG2	2.30	0.61
1:C:701:SER:HB2	1:C:704:ASN:CB	2.30	0.60
1:A:468:GLU:H	1:A:468:GLU:CD	2.06	0.60
1:A:644:ILE:HG22	1:A:709:ILE:O	2.02	0.58
1:C:475:LYS:H	1:C:478:HIS:HD2	1.50	0.58
1:A:456:GLU:O	1:A:459:GLN:CG	2.48	0.58
2:D:1377:ARG:HG2	2:D:1377:ARG:NH1	2.00	0.57
1:C:475:LYS:H	1:C:478:HIS:CD2	2.22	0.57
1:C:700:HIS:HD2	1:C:700:HIS:N	2.03	0.57
1:C:668:HIS:HD2	1:C:680:SER:OG	1.88	0.57
1:C:701:SER:CB	1:C:704:ASN:CB	2.83	0.56
1:A:630:TRP:O	1:A:665:LYS:NZ	2.39	0.56
1:A:644:ILE:HG13	1:A:656:ILE:HB	1.87	0.56
1:C:461:PHE:CZ	1:C:530:ILE:HD13	2.40	0.56
1:A:663:ASN:OD1	1:A:668:HIS:HE1	1.89	0.55
1:C:456:GLU:O	1:C:459:GLN:HG3	2.06	0.55
1:C:461:PHE:HB2	1:C:509:ARG:O	2.07	0.54
1:A:669:LEU:HD12	1:A:679:ILE:HG22	1.90	0.54
1:A:668:HIS:CD2	1:A:680:SER:OG	2.57	0.53
1:C:637:ALA:HA	1:C:663:ASN:HB3	1.91	0.52
1:A:437:LYS:HE3	1:A:438:HIS:CE1	2.44	0.52
1:A:607:ASN:O	1:A:611:SER:HB2	2.11	0.51
1:C:510:ARG:NH2	1:C:519:GLU:OE1	2.42	0.51
1:A:606:LYS:O	1:A:610:THR:HB	2.11	0.50
1:C:552:ILE:HG21	1:C:600:ARG:HG2	1.94	0.50
1:A:572:LYS:O	1:A:573:GLN:HB2	2.12	0.50
2:D:1376:ARG:NH1	2:D:1376:ARG:HG3	2.12	0.49
1:C:597:TRP:O	1:C:601:ILE:HG13	2.11	0.49
1:A:496:ASN:HB3	1:C:657:PRO:HG3	1.93	0.49
1:A:566:TYR:H	1:A:609:SER:CB	2.25	0.49
1:C:697:PHE:CZ	1:C:718:VAL:HG11	2.48	0.49
1:C:526:LEU:O	1:C:530:ILE:HD12	2.13	0.48
1:C:466:CYS:SG	1:C:471:SER:HB3	2.54	0.48
1:C:609:SER:O	1:C:611:SER:N	2.47	0.48
2:B:1375:SER:HB3	2:B:1376:ARG:NH1	2.29	0.48
1:C:582:LYS:HB3	1:C:590:LEU:HD11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:456:GLU:O	1:C:459:GLN:CG	2.62	0.47
1:A:434:VAL:HG21	1:A:451:MET:HG2	1.96	0.47
1:A:646:THR:HG22	1:A:656:ILE:HD11	1.95	0.47
1:A:618:MET:HG3	1:A:622:GLN:NE2	2.29	0.47
1:A:577:ASN:O	1:A:579:GLU:N	2.48	0.47
1:C:436:LEU:HB3	1:C:442:THR:OG1	2.15	0.47
1:A:607:ASN:HA	1:A:610:THR:HG22	1.96	0.47
1:C:517[B]:GLU:CD	1:C:517[B]:GLU:H	2.16	0.46
1:A:479:LYS:HA	1:A:480:PRO:HD2	1.73	0.46
1:A:559:LEU:HD13	1:A:605:TYR:CD2	2.50	0.46
1:C:699:ILE:O	1:C:707:SER:HA	2.15	0.46
1:A:491:LEU:HD22	1:A:497:LEU:HD12	1.98	0.46
1:A:501:ARG:CZ	1:C:468:GLU:O	2.64	0.46
1:C:565:ASN:HD22	1:C:609:SER:CA	2.29	0.46
1:C:581:LEU:HB3	1:C:590:LEU:HD21	1.96	0.46
1:A:645:PHE:CE2	1:A:655:VAL:HG13	2.51	0.45
1:C:645:PHE:CE2	1:C:655:VAL:HG22	2.52	0.45
1:C:516:LEU:HD12	1:C:516:LEU:HA	1.86	0.45
1:A:721:LEU:HD13	2:B:1381:PHE:HB3	1.98	0.45
1:C:565:ASN:HD22	1:C:609:SER:HA	1.81	0.45
1:A:637:ALA:HA	1:A:663:ASN:HB3	1.98	0.45
1:C:641:THR:HG22	1:C:672:MET:CE	2.44	0.45
1:C:508:LEU:HA	1:C:508:LEU:HD12	1.67	0.45
1:A:666:GLY:HA2	1:A:683:TYR:CZ	2.52	0.45
1:C:457:THR:C	1:C:459:GLN:H	2.20	0.44
1:C:565:ASN:ND2	1:C:609:SER:HA	2.32	0.44
1:A:461:PHE:CD1	1:A:461:PHE:N	2.85	0.44
1:C:670:LEU:CD2	1:C:677:LEU:HD12	2.48	0.44
2:D:1376:ARG:CG	2:D:1376:ARG:NH1	2.75	0.44
2:D:1377:ARG:NH1	2:D:1377:ARG:CG	2.77	0.44
1:A:593:LYS:N	1:A:593:LYS:HD2	2.32	0.43
1:C:498:ASP:HA	1:C:499:PRO:HD2	1.51	0.43
1:C:654:LYS:HD2	1:C:655:VAL:H	1.83	0.43
1:C:558:LEU:HA	1:C:558:LEU:HD23	1.87	0.43
1:C:606:LYS:O	1:C:610:THR:HB	2.18	0.43
1:C:440:ASN:HB2	1:C:481:LEU:HB2	2.01	0.42
1:C:513:ARG:HE	1:C:513:ARG:HB2	1.50	0.42
1:C:491:LEU:CD2	1:C:497:LEU:HD12	2.44	0.42
1:C:700:HIS:H	1:C:700:HIS:CD2	2.34	0.42
1:C:668:HIS:CD2	1:C:680:SER:OG	2.71	0.42
1:C:700:HIS:H	1:C:700:HIS:HD2	1.66	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:715:ALA:O	1:C:719:VAL:HB	2.20	0.41
1:A:498:ASP:HA	1:A:499:PRO:HD2	1.54	0.41
1:A:526:LEU:HD12	1:A:530:ILE:CD1	2.50	0.41
1:C:654:LYS:HD2	1:C:655:VAL:N	2.35	0.41
1:C:594:ALA:N	1:C:595:PRO:CD	2.84	0.41
1:C:504:PRO:O	1:C:505:GLN:HG3	2.19	0.41
1:C:566:TYR:H	1:C:609:SER:CB	2.33	0.41
1:A:466:CYS:SG	1:A:471:SER:HB3	2.61	0.41
1:A:664:ILE:HG13	3:A:2:HOH:O	2.19	0.41
1:A:526:LEU:O	1:A:530:ILE:CD1	2.62	0.41
1:A:637:ALA:CA	1:A:663:ASN:HB3	2.51	0.40
1:A:687:MET:HB3	1:A:687:MET:HE2	1.83	0.40
1:C:493:GLU:OE1	2:D:1378:ARG:NH1	2.53	0.40
1:A:497:LEU:O	1:A:499:PRO:HD3	2.21	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	301/322 (94%)	280 (93%)	16 (5%)	5 (2%)	11 19
1	C	302/322 (94%)	269 (89%)	29 (10%)	4 (1%)	15 26
2	B	5/26 (19%)	4 (80%)	1 (20%)	0	100 100
2	D	4/26 (15%)	3 (75%)	1 (25%)	0	100 100
All	All	612/696 (88%)	556 (91%)	47 (8%)	9 (2%)	13 22

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	578	GLU

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Mol	Chain	Res	Type
1	A	579	GLU
1	C	610	THR
1	C	705	LYS
1	A	571	HIS
1	C	578	GLU
1	A	573	GLN
1	A	664	ILE
1	C	437	LYS

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	277/293 (94%)	253 (91%)	24 (9%)	13 24
1	C	278/293 (95%)	252 (91%)	26 (9%)	11 20
2	B	7/25 (28%)	4 (57%)	3 (43%)	0 0
2	D	6/25 (24%)	4 (67%)	2 (33%)	0 0
All	All	568/636 (89%)	513 (90%)	55 (10%)	10 19

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	436	LEU
1	A	445	GLN
1	A	461	PHE
1	A	501	ARG
1	A	505	GLN
1	A	508	LEU
1	A	512	VAL
1	A	526	LEU
1	A	531	LEU
1	A	565	ASN
1	A	568	SER
1	A	575	PHE
1	A	576	LEU

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Mol	Chain	Res	Type
1	A	590	LEU
1	A	610	THR
1	A	631	GLU
1	A	655	VAL
1	A	673	GLU
1	A	680	SER
1	A	687	MET
1	A	694	ASP
1	A	701	SER
1	A	702	MET
1	A	712	THR
2	B	1376	ARG
2	B	1377	ARG
2	B	1378	ARG
1	C	422	VAL
1	C	434	VAL
1	C	435	GLU
1	C	451	MET
1	C	453	LEU
1	C	454	SER
1	C	459	GLN
1	C	508	LEU
1	C	513	ARG
1	C	550	LYS
1	C	570	LYS
1	C	575	PHE
1	C	582	LYS
1	C	590	LEU
1	C	610	THR
1	C	644	ILE
1	C	653	HIS
1	C	656	ILE
1	C	679	ILE
1	C	680	SER
1	C	700	HIS
1	C	702	MET
1	C	704	ASN
1	C	712	THR
1	C	719	VAL
1	C	729	LEU
2	D	1376	ARG
2	D	1377	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	483	HIS
1	A	580	ASN
1	A	622	GLN
1	A	643	GLN
1	A	668	HIS
1	A	711	HIS
1	C	459	GLN
1	C	478	HIS
1	C	482	GLN
1	C	560	GLN
1	C	565	ASN
1	C	571	HIS
1	C	643	GLN
1	C	668	HIS
1	C	689	GLN
1	C	698	GLN
1	C	700	HIS
1	C	704	ASN
1	C	711	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

There are no ligands in this entry.

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	305/322 (94%)	0.38	22 (7%) 18 20	26, 45, 82, 92	0
1	C	305/322 (94%)	0.40	19 (6%) 24 27	24, 46, 82, 100	0
2	B	7/26 (26%)	0.38	1 (14%) 4 3	40, 53, 71, 71	0
2	D	6/26 (23%)	0.87	0 100 100	45, 59, 73, 76	0
All	All	623/696 (89%)	0.40	42 (6%) 21 23	24, 46, 82, 100	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	575	PHE	12.6
1	C	574	GLY	12.3
1	A	614	VAL	8.5
1	C	613	GLY	8.2
1	C	612	GLU	5.9
1	A	730	MET	5.8
1	C	575	PHE	5.6
1	A	615	SER	5.3
1	C	571	HIS	4.6
1	C	577	ASN	4.4
1	A	613	GLY	4.2
1	A	611	SER	4.1
1	C	436	LEU	3.9
1	A	610	THR	3.8
1	C	573	GLN	3.8
1	C	646	THR	3.6
1	A	574	GLY	3.6
1	A	435	GLU	3.5
1	A	436	LEU	3.3
1	C	703	GLU	3.3
1	A	703	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	730	MET	3.2
1	C	653	HIS	3.2
1	C	450	GLY	3.2
1	C	610	THR	3.1
1	A	571	HIS	2.9
1	A	616	LYS	2.9
1	A	577	ASN	2.8
1	C	614	VAL	2.8
1	A	612	GLU	2.7
1	C	615	SER	2.7
1	A	452	ARG	2.6
1	A	572	LYS	2.5
1	C	700	HIS	2.4
1	A	569	LYS	2.4
1	A	573	GLN	2.3
2	B	1375	SER	2.2
1	A	570	LYS	2.2
1	C	568	SER	2.2
1	A	653	HIS	2.1
1	C	569	LYS	2.1
1	A	646	THR	2.1

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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.