Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 03:26 PM GMT

PDB ID	:	4CAD
Title	:	Mechanism of farnesylated CAAX protein processing by the integral membrane protease Rce1
Authors	:	Kulkarni, K.; Manolaridis, I.; Dodd, R.B.; Cronin, N.; Ogasawara, S.; Iwata, S.; Barford, D.
Deposited on	:	2013-10-08
Resolution	:	2.50 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:

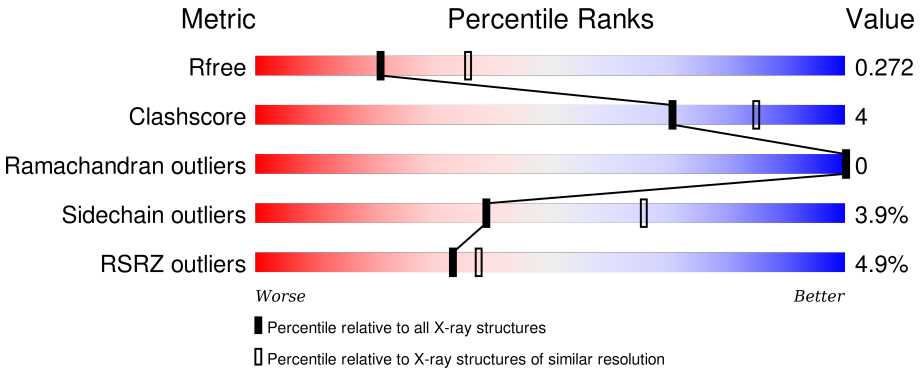
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.50 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	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	214	91% 7% •
1	D	214	87% 11% ••
1	G	214	2% 89% 10% •
1	J	214	2% 87% 12% •
2	B	227	2% 91% 6% •

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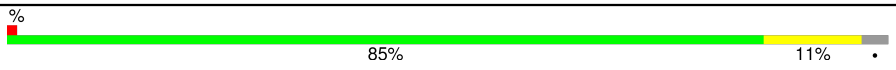
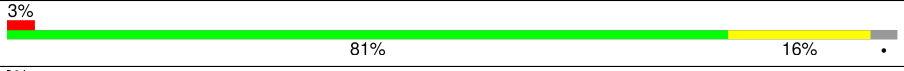
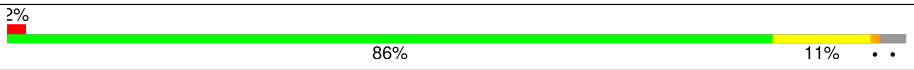
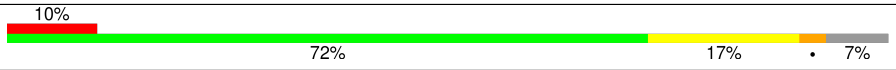
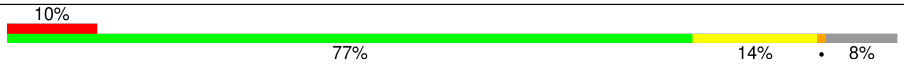
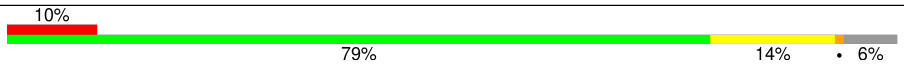
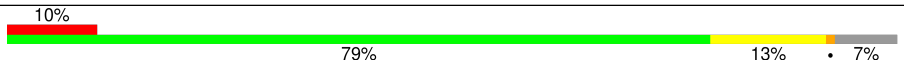
Mol	Chain	Length	Quality of chain
2	E	227	
2	H	227	
2	K	227	
3	C	271	
3	F	271	
3	I	271	
3	L	271	

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
5	LMT	I	301	-	-	-	X
5	LMT	L	301	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 21755 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 ANTIBODY FAB FRAGMENT LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	211	Total	C	N	O	S	0	0	0
			1642	1028	280	329	5			
1	D	211	Total	C	N	O	S	0	0	0
			1642	1028	280	329	5			
1	G	212	Total	C	N	O	S	0	0	0
			1647	1030	280	332	5			
1	J	212	Total	C	N	O	S	0	0	0
			1650	1032	281	332	5			

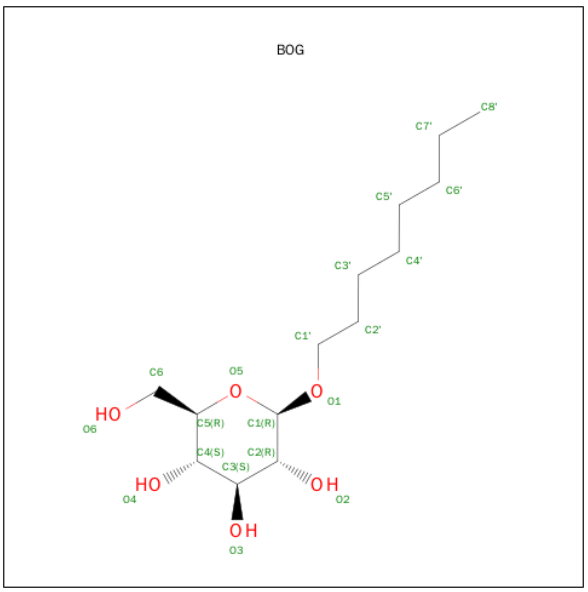
- Molecule 2 is a protein called ANTIBODY FAB FRAGMENT HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	221	Total	C	N	O	S	0	0	0
			1666	1057	270	331	8			
2	E	220	Total	C	N	O	S	0	0	0
			1663	1056	269	330	8			
2	H	221	Total	C	N	O	S	0	0	0
			1668	1059	270	331	8			
2	K	221	Total	C	N	O	S	0	0	0
			1668	1059	270	331	8			

- Molecule 3 is a protein called RAS AND A-FACTOR CONVERTING ENZYME 1, RCE1.

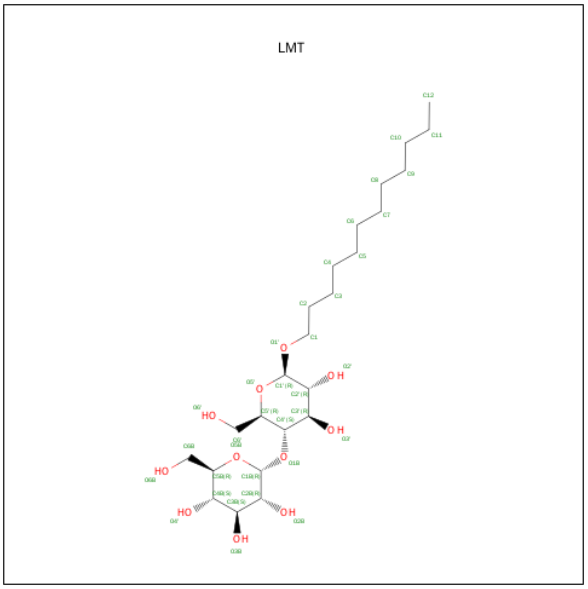
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	251	Total	C	N	O	S	0	0	0
			2020	1386	293	333	8			
3	F	250	Total	C	N	O	S	0	0	0
			2011	1381	290	332	8			
3	I	254	Total	C	N	O	S	0	0	0
			2040	1397	297	339	7			
3	L	253	Total	C	N	O	S	0	0	0
			2041	1398	297	338	8			

- Molecule 4 is SUGAR (B-OCTYLGLUCOSIDE) (three-letter code: BOG) (formula: $C_{14}H_{28}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total C O 13 7 6	0	0
4	F	1	Total C O 13 7 6	0	0

- Molecule 5 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	I	1	Total C O 25 14 11	0	0
5	L	1	Total C O 23 12 11	0	0

- Molecule 6 is water.

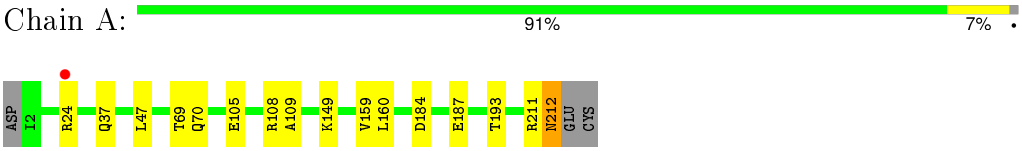
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	39	Total O 39 39	0	0
6	B	46	Total O 46 46	0	0
6	C	7	Total O 7 7	0	0
6	D	37	Total O 37 37	0	0
6	E	51	Total O 51 51	0	0
6	F	7	Total O 7 7	0	0
6	G	32	Total O 32 32	0	0
6	H	33	Total O 33 33	0	0
6	I	2	Total O 2 2	0	0
6	J	31	Total O 31 31	0	0
6	K	36	Total O 36 36	0	0
6	L	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.

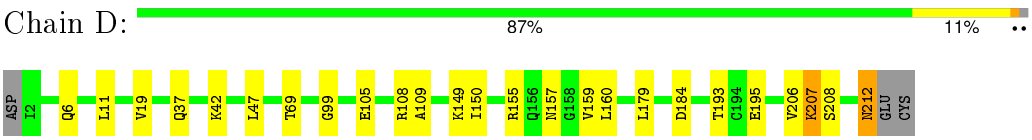
- Molecule 1: ANTIBODY FAB FRAGMENT LIGHT CHAIN

Chain A:



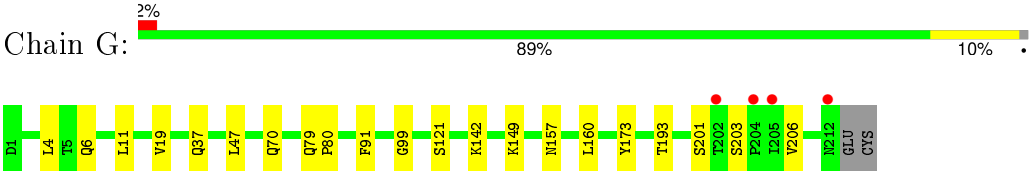
- Molecule 1: ANTIBODY FAB FRAGMENT LIGHT CHAIN

Chain D:



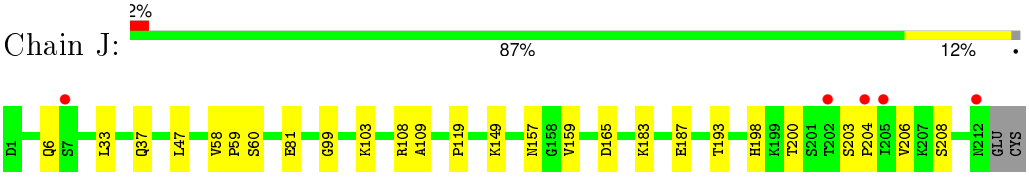
- Molecule 1: ANTIBODY FAB FRAGMENT LIGHT CHAIN

Chain G:



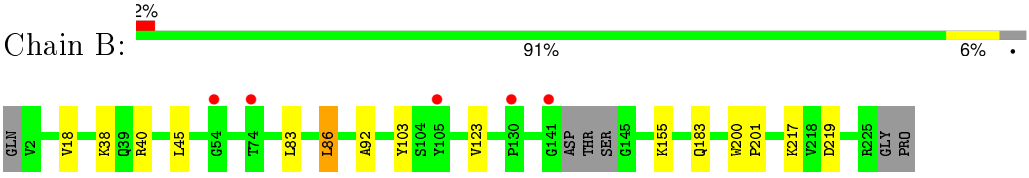
- Molecule 1: ANTIBODY FAB FRAGMENT LIGHT CHAIN

Chain J:



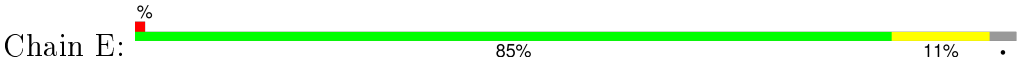
- Molecule 2: ANTIBODY FAB FRAGMENT HEAVY CHAIN

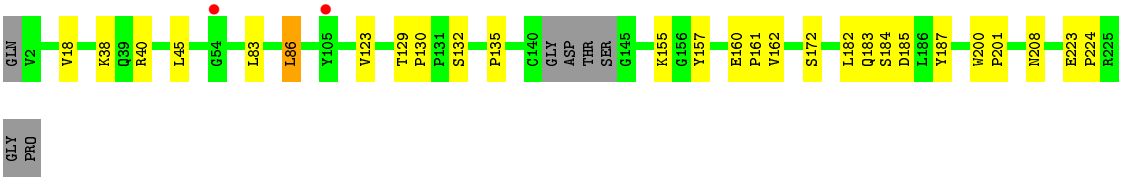
Chain B:



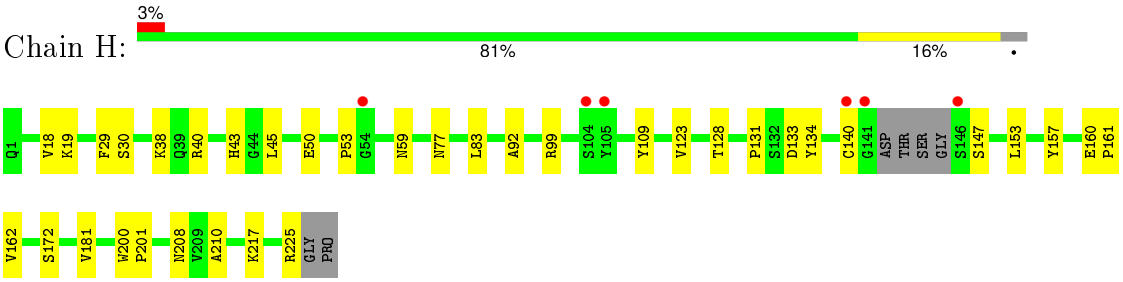
- Molecule 2: ANTIBODY FAB FRAGMENT HEAVY CHAIN

Chain E:

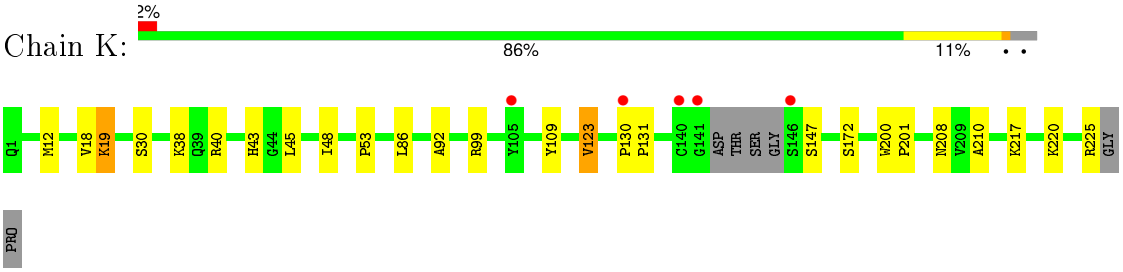




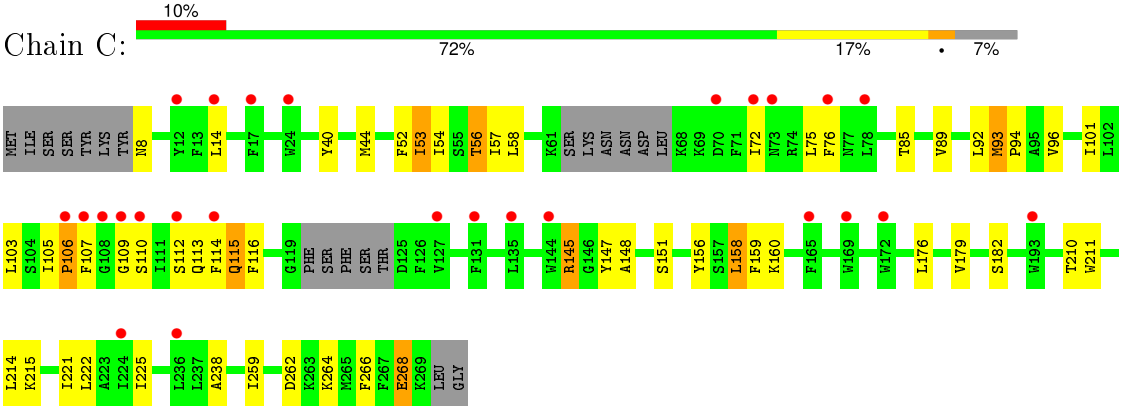
• Molecule 2: ANTIBODY FAB FRAGMENT HEAVY CHAIN



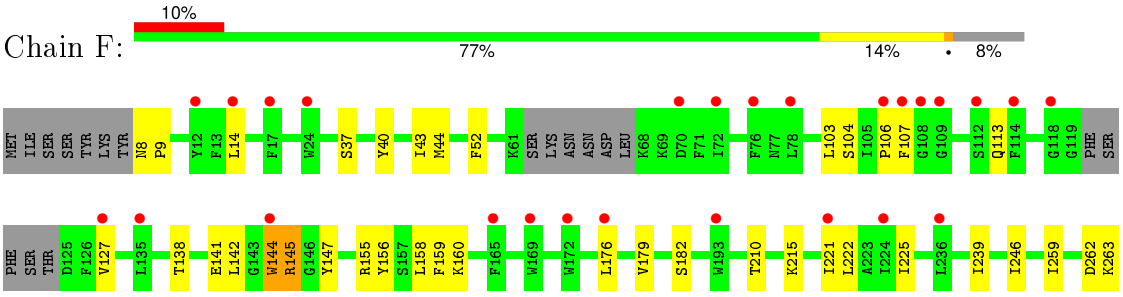
• Molecule 2: ANTIBODY FAB FRAGMENT HEAVY CHAIN

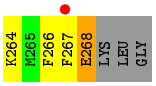


• Molecule 3: RAS AND A-FACTOR CONVERTING ENZYME 1, RCE1

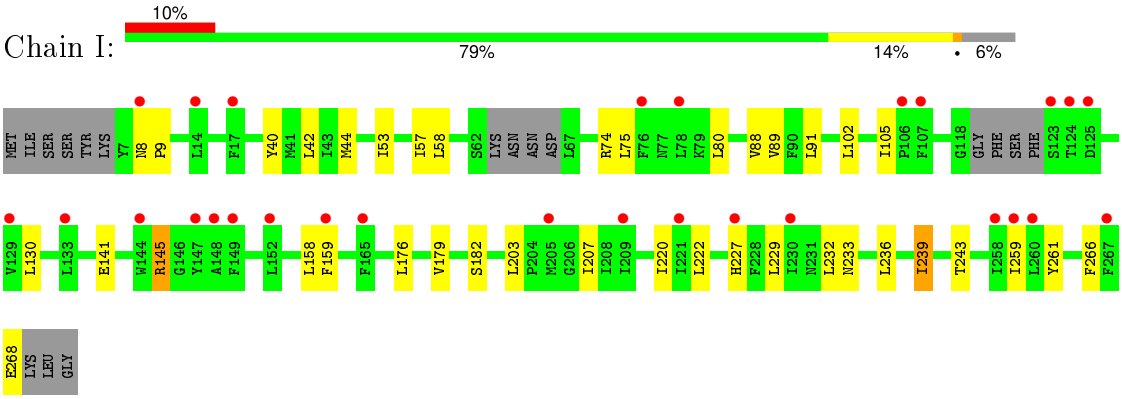


• Molecule 3: RAS AND A-FACTOR CONVERTING ENZYME 1, RCE1

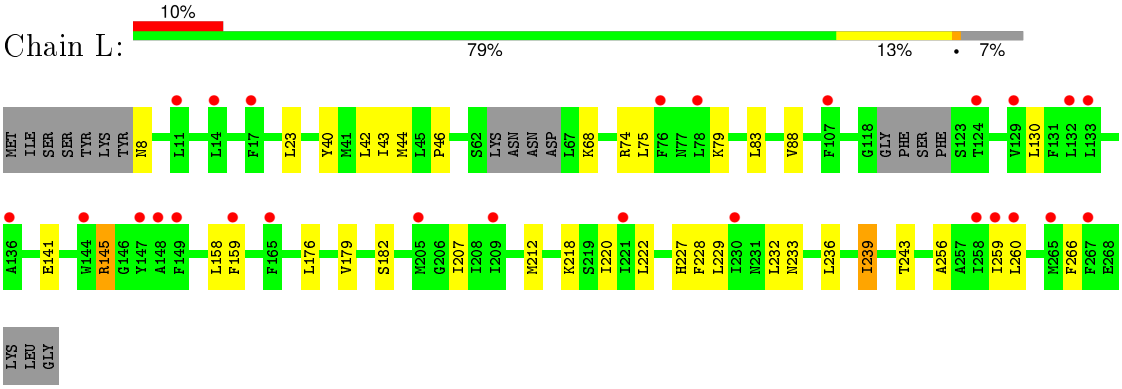




• Molecule 3: RAS AND A-FACTOR CONVERTING ENZYME 1, RCE1



• Molecule 3: RAS AND A-FACTOR CONVERTING ENZYME 1, RCE1



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	113.06Å 90.09Å 99.30Å 89.06° 102.29° 90.00°	Depositor
Resolution (Å)	42.34 – 2.50 43.01 – 2.48	Depositor EDS
% Data completeness (in resolution range)	97.0 (42.34-2.50) 95.9 (43.01-2.48)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.43 (at 2.48Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.226 , 0.267 0.235 , 0.272	Depositor DCC
R_{free} test set	6514 reflections (5.29%)	DCC
Wilson B-factor (Å^2)	43.0	Xtriage
Anisotropy	0.311	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 44.8	EDS
Estimated twinning fraction	0.085 for -h,k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.37$, $< L^2 > = 0.21$	Xtriage
Outliers	0 of 130235 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	21755	wwPDB-VP
Average B, all atoms (Å^2)	70.0	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 99.25 % 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 1.9210e-12.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: LMT, BOG

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	0.24	0/1683	0.44	0/2288
1	D	0.28	0/1683	0.44	0/2288
1	G	0.28	1/1688 (0.1%)	0.45	1/2296 (0.0%)
1	J	0.27	1/1691 (0.1%)	0.43	0/2299
2	B	0.24	0/1712	0.44	0/2334
2	E	0.46	3/1709 (0.2%)	0.56	4/2330 (0.2%)
2	H	0.30	1/1714 (0.1%)	0.47	2/2337 (0.1%)
2	K	0.24	0/1714	0.44	0/2337
3	C	0.33	2/2079 (0.1%)	0.46	2/2830 (0.1%)
3	F	0.25	0/2070	0.39	0/2818
3	I	0.28	1/2099 (0.0%)	0.42	1/2859 (0.0%)
3	L	0.24	0/2100	0.39	0/2858
All	All	0.29	9/21942 (0.0%)	0.44	10/29874 (0.0%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	130	PRO	N-CD	5.29	1.55	1.47
1	J	204	PRO	N-CD	5.27	1.55	1.47
2	E	135	PRO	N-CD	5.20	1.55	1.47
3	I	9	PRO	N-CD	5.18	1.55	1.47
1	G	80	PRO	N-CD	5.15	1.55	1.47
3	C	106	PRO	N-CD	5.07	1.54	1.47
2	H	161	PRO	N-CD	5.06	1.54	1.47
2	E	161	PRO	N-CD	5.03	1.54	1.47
3	C	94	PRO	N-CD	5.03	1.54	1.47

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	130	PRO	C-N-CD	5.79	140.56	128.40
3	C	105	ILE	C-N-CD	5.77	140.51	128.40
2	H	161	PRO	CA-N-CD	-5.71	103.50	111.50
3	I	8	ASN	C-N-CD	5.63	140.22	128.40
1	G	79	GLN	C-N-CD	5.62	140.21	128.40
2	E	129	THR	C-N-CD	5.61	140.19	128.40
3	C	93	MET	C-N-CD	5.56	140.08	128.40
2	E	161	PRO	CA-N-CD	-5.50	103.80	111.50
2	H	160	GLU	C-N-CD	5.33	139.60	128.40
2	E	160	GLU	C-N-CD	5.12	139.15	128.40

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	1642	0	1567	8	0
1	D	1642	0	1567	13	0
1	G	1647	0	1565	11	0
1	J	1650	0	1574	10	0
2	B	1666	0	1594	9	0
2	E	1663	0	1593	11	0
2	H	1668	0	1598	18	0
2	K	1668	0	1598	18	0
3	C	2020	0	2052	35	0
3	F	2011	0	2046	26	0
3	I	2040	0	2073	17	0
3	L	2041	0	2087	19	0
4	C	13	0	11	0	0
4	F	13	0	11	0	0
5	I	25	0	23	2	0
5	L	23	0	21	3	0
6	A	39	0	0	0	0
6	B	46	0	0	0	0
6	C	7	0	0	0	0
6	D	37	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	E	51	0	0	0	0
6	F	7	0	0	0	0
6	G	32	0	0	1	0
6	H	33	0	0	0	0
6	I	2	0	0	0	0
6	J	31	0	0	0	0
6	K	36	0	0	0	0
6	L	2	0	0	0	0
All	All	21755	0	20980	188	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.

All (188) 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:C:158:LEU:HD23	3:C:266:PHE:HA	1.08	1.07
3:C:158:LEU:HD23	3:C:266:PHE:CA	2.00	0.90
1:D:160:LEU:HD11	2:E:183:GLN:HB3	1.55	0.88
2:K:18:VAL:HG23	2:K:86:LEU:HD11	1.60	0.83
2:K:12:MET:HG3	2:K:18:VAL:CG2	2.10	0.82
3:C:93:MET:HE2	3:C:93:MET:HA	1.65	0.77
3:C:158:LEU:CD2	3:C:266:PHE:HA	2.04	0.77
2:K:12:MET:HG3	2:K:18:VAL:HG21	1.68	0.75
3:F:8:ASN:N	3:F:147:TYR:HH	1.82	0.75
3:L:228:PHE:CZ	3:L:232:LEU:HD11	2.22	0.74
2:E:155:LYS:NZ	2:E:183:GLN:OE1	2.22	0.72
3:C:93:MET:CE	3:C:93:MET:HA	2.20	0.70
3:F:145:ARG:HD2	3:F:145:ARG:N	2.05	0.69
3:F:9:PRO:HG2	3:F:155:ARG:HD2	1.74	0.69
1:A:108:ARG:NH1	1:A:109:ALA:O	2.25	0.69
2:B:18:VAL:HG13	2:B:86:LEU:HD21	1.74	0.68
2:E:18:VAL:HG13	2:E:86:LEU:HD21	1.75	0.68
1:A:160:LEU:HD11	2:B:183:GLN:HB3	1.75	0.67
1:D:155:ARG:NE	1:D:157:ASN:O	2.27	0.66
2:K:12:MET:SD	2:K:18:VAL:HG22	2.36	0.65
3:C:8:ASN:N	3:C:147:TYR:HH	1.95	0.65
3:L:130:LEU:HD22	3:L:232:LEU:HD21	1.79	0.65
3:F:113:GLN:HE21	3:F:239:ILE:HG22	1.62	0.65
3:I:158:LEU:HB3	3:I:266:PHE:HA	1.80	0.64
2:E:182:LEU:HD13	2:E:187:TYR:CE1	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:229:LEU:O	3:L:233:ASN:ND2	2.29	0.62
3:L:179:VAL:HG22	3:L:182:SER:HB3	1.81	0.62
2:B:38:LYS:HE2	2:B:40:ARG:HD2	1.81	0.61
3:L:233:ASN:OD1	5:L:301:LMT:O4'	2.18	0.61
2:H:133:ASP:HA	2:H:153:LEU:O	2.01	0.60
3:F:113:GLN:NE2	3:F:239:ILE:HG22	2.18	0.59
2:H:50:GLU:HG2	2:H:59:ASN:HB2	1.85	0.59
3:I:179:VAL:HG22	3:I:182:SER:HB3	1.84	0.58
1:J:183:LYS:NZ	1:J:187:GLU:OE2	2.36	0.57
1:G:121:SER:OG	2:H:134:TYR:HB3	2.05	0.57
3:L:158:LEU:HB3	3:L:266:PHE:HA	1.88	0.56
3:C:159:PHE:HE1	3:C:259:ILE:HD13	1.69	0.56
3:L:23:LEU:HD13	3:L:46:PRO:HB2	1.87	0.56
3:C:107:PHE:N	3:C:107:PHE:CD1	2.74	0.56
3:I:141:GLU:OE2	3:I:227:HIS:ND1	2.37	0.55
3:F:156:TYR:HB3	3:F:160:LYS:HG3	1.87	0.55
2:E:38:LYS:HE2	2:E:40:ARG:HD2	1.88	0.55
3:F:263:LYS:O	3:F:267:PHE:HD2	1.90	0.54
2:K:210:ALA:HB2	2:K:217:LYS:HD3	1.89	0.54
2:B:155:LYS:NZ	2:B:183:GLN:OE1	2.41	0.54
2:E:184:SER:OG	2:E:185:ASP:N	2.37	0.54
1:G:160:LEU:HD11	2:H:181:VAL:HG11	1.90	0.53
3:F:264:LYS:O	3:F:268:GLU:HB2	2.08	0.53
1:D:108:ARG:NH1	1:D:109:ALA:O	2.38	0.53
3:C:114:PHE:O	3:C:116:PHE:CD2	2.62	0.53
1:D:149:LYS:HB2	1:D:193:THR:HB	1.90	0.53
3:I:130:LEU:HD22	3:I:232:LEU:HD11	1.91	0.53
3:F:144:TRP:HE3	3:F:144:TRP:HA	1.74	0.52
3:C:52:PHE:O	3:C:56:THR:OG1	2.28	0.51
3:F:144:TRP:CE3	3:F:144:TRP:HA	2.45	0.51
1:G:37:GLN:HB2	1:G:47:LEU:HD11	1.92	0.51
2:K:12:MET:CG	2:K:18:VAL:CG2	2.88	0.51
2:K:40:ARG:HG2	2:K:92:ALA:HB2	1.93	0.50
3:C:112:SER:O	3:C:115:GLN:HB2	2.11	0.50
1:A:187:GLU:O	1:A:211:ARG:NH2	2.44	0.50
3:C:159:PHE:CE1	3:C:259:ILE:HD13	2.46	0.50
3:I:233:ASN:ND2	5:I:301:LMT:O4'	2.43	0.50
2:H:140:CYS:HB3	2:H:225:ARG:HB2	1.92	0.50
2:K:38:LYS:HE2	2:K:40:ARG:HD2	1.94	0.50
2:H:18:VAL:HG12	2:H:83:LEU:HB2	1.93	0.50
1:J:37:GLN:HB2	1:J:47:LEU:HD11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:145:ARG:NH2	3:C:210:THR:OG1	2.45	0.49
3:C:156:TYR:HB3	3:C:160:LYS:HG2	1.95	0.49
2:H:38:LYS:HE2	2:H:40:ARG:HD2	1.93	0.49
3:C:107:PHE:N	3:C:107:PHE:HD1	2.10	0.49
2:H:131:PRO:HB3	2:H:157:TYR:HB3	1.95	0.49
1:J:103:LYS:NZ	1:J:165:ASP:OD1	2.36	0.49
1:D:37:GLN:HB2	1:D:47:LEU:HD11	1.93	0.49
3:C:53:ILE:O	3:C:57:ILE:HG12	2.12	0.49
1:D:157:ASN:N	1:D:157:ASN:OD1	2.44	0.49
1:J:193:THR:HG23	1:J:208:SER:HB2	1.95	0.48
3:I:176:LEU:HA	3:I:179:VAL:HG13	1.95	0.48
2:K:30:SER:HA	2:K:53:PRO:HB2	1.94	0.48
3:C:109:GLY:O	3:C:110:SER:HB3	2.13	0.48
1:G:149:LYS:HB2	1:G:193:THR:HB	1.94	0.48
1:G:70:GLN:NE2	6:G:2019:HOH:O	2.39	0.48
3:F:179:VAL:HG22	3:F:182:SER:HB3	1.95	0.48
3:C:93:MET:CE	3:C:93:MET:CA	2.87	0.48
5:L:301:LMT:O5B	5:L:301:LMT:O6'	2.23	0.48
3:F:176:LEU:HA	3:F:179:VAL:HG13	1.96	0.48
2:B:217:LYS:NZ	2:B:219:ASP:OD1	2.47	0.48
2:B:18:VAL:HG22	2:B:83:LEU:HB2	1.96	0.48
3:L:74:ARG:HD2	3:L:218:LYS:HB3	1.95	0.48
3:C:148:ALA:O	3:C:151:SER:OG	2.28	0.48
1:G:6:GLN:HG3	1:G:99:GLY:HA3	1.95	0.47
3:L:176:LEU:HA	3:L:179:VAL:HG13	1.96	0.47
2:H:157:TYR:CE2	2:H:162:VAL:HG13	2.50	0.47
2:H:133:ASP:OD1	2:H:133:ASP:N	2.46	0.47
3:L:141:GLU:OE2	3:L:227:HIS:ND1	2.37	0.47
3:I:53:ILE:O	3:I:57:ILE:HG12	2.15	0.47
3:C:101:ILE:HG23	3:C:110:SER:OG	2.15	0.47
3:L:233:ASN:CG	5:L:301:LMT:O4'	2.53	0.46
2:H:99:ARG:HD2	2:H:109:TYR:O	2.14	0.46
1:J:108:ARG:NH1	1:J:109:ALA:O	2.45	0.46
3:C:176:LEU:HA	3:C:179:VAL:HG13	1.96	0.46
1:J:149:LYS:HB2	1:J:193:THR:HB	1.98	0.46
1:G:201:SER:OG	1:G:203:SER:O	2.26	0.46
1:D:207:LYS:HD3	1:D:207:LYS:HA	1.56	0.46
1:D:150:ILE:HD11	1:D:179:LEU:HD21	1.98	0.46
2:H:29:PHE:CD2	2:H:77:ASN:HA	2.51	0.46
2:H:40:ARG:HG2	2:H:92:ALA:HB2	1.97	0.46
1:A:212:ASN:OD1	1:A:212:ASN:N	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:40:TYR:O	3:I:44:MET:HG2	2.16	0.46
3:C:158:LEU:CD1	3:C:214:LEU:HD11	2.47	0.45
3:F:141:GLU:O	3:F:145:ARG:HB2	2.16	0.45
2:H:210:ALA:HB2	2:H:217:LYS:HE3	1.98	0.45
1:A:149:LYS:HB2	1:A:193:THR:HB	1.98	0.45
3:I:229:LEU:O	3:I:233:ASN:ND2	2.40	0.45
1:A:70:GLN:HE22	2:H:128:THR:HB	1.82	0.45
3:F:145:ARG:NH2	3:F:210:THR:OG1	2.50	0.45
1:D:11:LEU:HD21	1:D:19:VAL:HB	1.99	0.45
3:C:72:ILE:O	3:C:76:PHE:HD2	1.99	0.45
3:L:40:TYR:O	3:L:44:MET:HG2	2.17	0.44
3:F:221:ILE:O	3:F:225:ILE:HG12	2.17	0.44
3:L:232:LEU:O	3:L:236:LEU:HB2	2.18	0.44
3:I:159:PHE:HE1	3:I:259:ILE:HD13	1.83	0.44
2:K:200:TRP:CG	2:K:201:PRO:HA	2.52	0.44
1:D:160:LEU:HD11	2:E:183:GLN:CB	2.37	0.44
3:F:8:ASN:N	3:F:147:TYR:OH	2.45	0.44
2:B:40:ARG:HG2	2:B:92:ALA:HB2	2.00	0.44
3:L:43:ILE:O	3:L:46:PRO:HD2	2.17	0.44
2:K:220:LYS:HA	2:K:220:LYS:HD3	1.75	0.44
3:I:102:LEU:HA	3:I:105:ILE:HD12	2.00	0.44
1:J:198:HIS:ND1	1:J:200:THR:OG1	2.35	0.44
3:F:144:TRP:C	3:F:145:ARG:HD2	2.38	0.43
1:A:24:ARG:CZ	1:A:70:GLN:HG2	2.47	0.43
1:G:11:LEU:HD21	1:G:19:VAL:HB	1.99	0.43
2:K:130:PRO:HA	2:K:131:PRO:HD3	1.84	0.43
3:C:103:LEU:O	3:C:106:PRO:HD2	2.18	0.43
2:E:200:TRP:CG	2:E:201:PRO:HA	2.53	0.43
2:K:18:VAL:HG23	2:K:86:LEU:CD1	2.39	0.43
3:C:264:LYS:O	3:C:268:GLU:HB2	2.17	0.43
3:F:113:GLN:HE21	3:F:239:ILE:HA	1.83	0.43
2:E:18:VAL:HG22	2:E:83:LEU:HB2	2.00	0.43
1:G:142:LYS:HB3	1:G:173:TYR:CE1	2.53	0.43
3:L:159:PHE:HE1	3:L:259:ILE:HD13	1.84	0.43
3:F:40:TYR:O	3:F:44:MET:HG2	2.18	0.43
1:J:119:PRO:HG2	2:K:225:ARG:CZ	2.48	0.43
2:E:157:TYR:CE2	2:E:162:VAL:HG13	2.54	0.43
2:K:38:LYS:HB2	2:K:48:ILE:HD11	2.01	0.42
3:F:158:LEU:HD23	3:F:266:PHE:HA	2.01	0.42
2:K:12:MET:O	2:K:123:VAL:HA	2.19	0.42
3:I:141:GLU:O	3:I:145:ARG:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:211:TRP:O	3:C:215:LYS:HG2	2.19	0.42
2:B:200:TRP:CG	2:B:201:PRO:HA	2.54	0.42
3:C:40:TYR:O	3:C:44:MET:HG2	2.19	0.42
3:L:256:ALA:O	3:L:260:LEU:HG	2.20	0.42
3:I:74:ARG:HB3	3:I:220:ILE:HG13	2.01	0.42
3:I:239:ILE:HG13	3:I:243:THR:HB	2.01	0.42
3:F:103:LEU:O	3:F:106:PRO:HD2	2.19	0.42
3:C:158:LEU:HD13	3:C:214:LEU:HD11	2.01	0.42
1:D:195:GLU:HG3	1:D:206:VAL:HG12	2.00	0.42
3:C:53:ILE:HG13	3:C:54:ILE:N	2.35	0.42
1:A:37:GLN:HB2	1:A:47:LEU:HD11	2.01	0.42
3:C:221:ILE:O	3:C:225:ILE:HG12	2.20	0.42
3:C:179:VAL:HG22	3:C:182:SER:HB3	2.02	0.41
1:D:212:ASN:OD1	1:D:212:ASN:N	2.53	0.41
3:C:85:THR:O	3:C:89:VAL:HG23	2.20	0.41
2:H:200:TRP:CG	2:H:201:PRO:HA	2.54	0.41
3:F:104:SER:HB3	3:F:246:ILE:HD12	2.01	0.41
3:F:138:THR:O	3:F:142:LEU:HG	2.20	0.41
1:J:58:VAL:HA	1:J:59:PRO:HD3	1.94	0.41
3:C:92:LEU:O	3:C:96:VAL:HG23	2.20	0.41
2:B:103:TYR:CD1	3:C:238:ALA:HB1	2.56	0.41
3:I:207:ILE:HD13	3:I:259:ILE:HD11	2.02	0.41
5:I:301:LMT:H1B	5:I:301:LMT:H5'	1.34	0.41
3:F:37:SER:O	3:F:40:TYR:HD1	2.04	0.41
2:K:19:LYS:HE2	2:K:19:LYS:HB3	1.88	0.41
3:L:239:ILE:HG13	3:L:243:THR:HB	2.02	0.41
3:F:215:LYS:HA	3:F:215:LYS:HD3	1.85	0.41
3:I:232:LEU:O	3:I:236:LEU:HB2	2.21	0.41
1:D:6:GLN:HG3	1:D:99:GLY:HA3	2.02	0.41
3:F:159:PHE:HE1	3:F:259:ILE:HD13	1.86	0.41
1:J:6:GLN:HG3	1:J:99:GLY:HA3	2.02	0.41
3:L:145:ARG:HB3	3:L:220:ILE:HG12	2.03	0.41
3:C:109:GLY:O	3:C:110:SER:CB	2.68	0.41
3:I:159:PHE:HA	3:I:266:PHE:HD1	1.86	0.40
3:L:207:ILE:HD13	3:L:259:ILE:HD11	2.02	0.40
2:H:30:SER:HA	2:H:53:PRO:HB2	2.03	0.40
1:G:91:PHE:CZ	2:H:99:ARG:HD3	2.56	0.40
1:G:142:LYS:HB3	1:G:173:TYR:CD1	2.57	0.40
2:E:223:GLU:HA	2:E:224:PRO:HD3	1.99	0.40
2:K:99:ARG:HD2	2:K:109:TYR:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	209/214 (98%)	205 (98%)	4 (2%)	0	100	100
1	D	209/214 (98%)	205 (98%)	4 (2%)	0	100	100
1	G	210/214 (98%)	207 (99%)	3 (1%)	0	100	100
1	J	210/214 (98%)	206 (98%)	4 (2%)	0	100	100
2	B	217/227 (96%)	214 (99%)	3 (1%)	0	100	100
2	E	216/227 (95%)	213 (99%)	3 (1%)	0	100	100
2	H	217/227 (96%)	214 (99%)	3 (1%)	0	100	100
2	K	217/227 (96%)	212 (98%)	5 (2%)	0	100	100
3	C	245/271 (90%)	242 (99%)	3 (1%)	0	100	100
3	F	244/271 (90%)	242 (99%)	2 (1%)	0	100	100
3	I	248/271 (92%)	244 (98%)	4 (2%)	0	100	100
3	L	247/271 (91%)	245 (99%)	2 (1%)	0	100	100
All	All	2689/2848 (94%)	2649 (98%)	40 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	185/188 (98%)	180 (97%)	5 (3%)	52	79
1	D	185/188 (98%)	177 (96%)	8 (4%)	35	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	G	185/188 (98%)	182 (98%)	3 (2%)	70 90
1	J	186/188 (99%)	179 (96%)	7 (4%)	40 67
2	B	185/192 (96%)	182 (98%)	3 (2%)	70 90
2	E	185/192 (96%)	179 (97%)	6 (3%)	46 74
2	H	185/192 (96%)	178 (96%)	7 (4%)	40 67
2	K	185/192 (96%)	178 (96%)	7 (4%)	40 67
3	C	216/244 (88%)	204 (94%)	12 (6%)	26 47
3	F	216/244 (88%)	206 (95%)	10 (5%)	33 57
3	I	220/244 (90%)	207 (94%)	13 (6%)	24 44
3	L	222/244 (91%)	211 (95%)	11 (5%)	30 53
All	All	2355/2496 (94%)	2263 (96%)	92 (4%)	39 66

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	THR
1	A	105	GLU
1	A	159	VAL
1	A	184	ASP
1	A	212	ASN
2	B	45	LEU
2	B	86	LEU
2	B	123	VAL
3	C	14	LEU
3	C	53	ILE
3	C	56	THR
3	C	58	LEU
3	C	75	LEU
3	C	113	GLN
3	C	115	GLN
3	C	145	ARG
3	C	158	LEU
3	C	222	LEU
3	C	262	ASP
3	C	268	GLU
1	D	42	LYS
1	D	69	THR
1	D	105	GLU

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Mol	Chain	Res	Type
1	D	159	VAL
1	D	184	ASP
1	D	207	LYS
1	D	208	SER
1	D	212	ASN
2	E	45	LEU
2	E	86	LEU
2	E	123	VAL
2	E	132	SER
2	E	172	SER
2	E	208	ASN
3	F	14	LEU
3	F	43	ILE
3	F	52	PHE
3	F	107	PHE
3	F	127	VAL
3	F	144	TRP
3	F	145	ARG
3	F	222	LEU
3	F	262	ASP
3	F	268	GLU
1	G	4	LEU
1	G	157	ASN
1	G	206	VAL
2	H	19	LYS
2	H	43	HIS
2	H	45	LEU
2	H	123	VAL
2	H	147	SER
2	H	172	SER
2	H	208	ASN
3	I	42	LEU
3	I	58	LEU
3	I	75	LEU
3	I	80	LEU
3	I	88	VAL
3	I	89	VAL
3	I	91	LEU
3	I	145	ARG
3	I	203	LEU
3	I	222	LEU
3	I	239	ILE

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Mol	Chain	Res	Type
3	I	261	TYR
3	I	268	GLU
1	J	33	LEU
1	J	60	SER
1	J	81	GLU
1	J	157	ASN
1	J	159	VAL
1	J	203	SER
1	J	206	VAL
2	K	19	LYS
2	K	43	HIS
2	K	45	LEU
2	K	123	VAL
2	K	147	SER
2	K	172	SER
2	K	208	ASN
3	L	8	ASN
3	L	42	LEU
3	L	68	LYS
3	L	75	LEU
3	L	79	LYS
3	L	83	LEU
3	L	88	VAL
3	L	145	ARG
3	L	212	MET
3	L	222	LEU
3	L	239	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
3	F	113	GLN

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	BOG	C	301	-	13,13,20	0.75	0	18,18,25	1.00	2 (11%)
4	BOG	F	301	-	13,13,20	0.55	0	18,18,25	0.63	0
5	LMT	I	301	-	26,26,36	0.48	0	37,37,47	0.66	0
5	LMT	L	301	-	24,24,36	0.36	0	35,35,47	1.87	4 (11%)

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	BOG	C	301	-	-	0/4/24/31	0/1/1/1
4	BOG	F	301	-	-	0/4/24/31	0/1/1/1
5	LMT	I	301	-	-	0/11/51/61	0/2/2/2
5	LMT	L	301	-	-	0/8/48/61	0/2/2/2

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	L	301	LMT	C1B-O1B-C4'	-8.55	95.67	118.01
4	C	301	BOG	C3-C4-C5	-2.11	106.52	110.20
5	L	301	LMT	O1B-C4'-C3'	2.67	114.07	107.17
4	C	301	BOG	O5-C1-C2	2.73	115.87	110.28
5	L	301	LMT	O1B-C1B-O5B	2.76	117.67	110.68
5	L	301	LMT	O1B-C1B-C2B	4.31	118.59	108.10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	I	301	LMT	2	0
5	L	301	LMT	3	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	211/214 (98%)	-0.11	1 (0%) 91 92	36, 58, 88, 101	0
1	D	211/214 (98%)	-0.09	0 100 100	41, 56, 86, 107	0
1	G	212/214 (99%)	-0.04	4 (1%) 70 73	43, 58, 96, 117	0
1	J	212/214 (99%)	-0.04	5 (2%) 62 66	38, 60, 98, 122	0
2	B	221/227 (97%)	0.04	5 (2%) 64 67	38, 59, 81, 106	0
2	E	220/227 (96%)	-0.03	2 (0%) 85 88	42, 57, 83, 109	0
2	H	221/227 (97%)	0.05	6 (2%) 58 62	41, 55, 81, 100	0
2	K	221/227 (97%)	0.04	5 (2%) 64 67	40, 57, 84, 109	0
3	C	251/271 (92%)	0.41	26 (10%) 8 8	50, 83, 133, 156	0
3	F	250/271 (92%)	0.37	27 (10%) 8 8	51, 83, 129, 152	0
3	I	254/271 (93%)	0.38	28 (11%) 7 7	51, 81, 127, 164	0
3	L	253/271 (93%)	0.38	26 (10%) 9 9	52, 82, 129, 159	0
All	All	2737/2848 (96%)	0.13	135 (4%) 33 38	36, 65, 111, 164	0

All (135) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	141	GLY	10.3
3	F	107	PHE	7.4
3	L	267	PHE	7.2
3	I	260	LEU	6.4
3	L	260	LEU	6.2
1	J	204	PRO	6.0
3	F	109	GLY	5.8
3	C	17	PHE	5.8
1	G	204	PRO	5.5
3	C	106	PRO	5.5
3	F	17	PHE	5.4

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Mol	Chain	Res	Type	RSRZ
3	C	108	GLY	5.2
3	C	110	SER	4.8
3	I	267	PHE	4.7
3	I	133	LEU	4.6
2	H	141	GLY	4.6
3	C	107	PHE	4.6
2	E	54	GLY	4.5
2	H	146	SER	4.4
2	H	105	TYR	4.4
1	G	205	ILE	4.3
3	L	133	LEU	4.2
3	F	108	GLY	4.1
2	B	54	GLY	4.1
3	F	106	PRO	4.1
3	I	221	ILE	4.1
1	J	205	ILE	4.0
2	K	105	TYR	4.0
3	L	230	ILE	3.9
3	C	109	GLY	3.9
3	F	169	TRP	3.9
3	L	147	TYR	3.8
3	C	169	TRP	3.8
3	L	209	ILE	3.7
2	E	105	TYR	3.6
3	L	205	MET	3.6
2	B	105	TYR	3.6
3	C	14	LEU	3.6
3	F	78	LEU	3.6
3	L	165	PHE	3.5
3	L	148	ALA	3.5
3	L	221	ILE	3.5
2	H	54	GLY	3.5
3	I	209	ILE	3.5
3	C	78	LEU	3.4
3	C	112	SER	3.4
3	I	205	MET	3.3
3	F	14	LEU	3.3
3	I	147	TYR	3.3
3	C	144	TRP	3.2
3	I	125	ASP	3.2
3	I	17	PHE	3.2
2	H	140	CYS	3.2

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Mol	Chain	Res	Type	RSRZ
3	I	165	PHE	3.1
3	I	124	THR	3.1
3	I	148	ALA	3.1
3	I	144	TRP	3.1
3	L	159	PHE	3.0
3	I	230	ILE	3.0
3	C	76	PHE	3.0
3	L	258	ILE	3.0
3	L	144	TRP	2.9
3	C	224	ILE	2.9
3	I	159	PHE	2.9
3	F	144	TRP	2.8
3	F	114	PHE	2.8
3	C	193	TRP	2.8
3	F	193	TRP	2.7
3	I	259	ILE	2.7
2	B	130	PRO	2.7
2	K	146	SER	2.7
3	F	165	PHE	2.7
2	K	130	PRO	2.7
3	F	76	PHE	2.6
3	L	265	MET	2.6
3	F	127	VAL	2.6
3	C	172	TRP	2.5
3	C	236	LEU	2.5
3	C	165	PHE	2.5
3	F	224	ILE	2.5
3	C	12	TYR	2.5
3	L	107	PHE	2.4
3	C	127	VAL	2.4
2	K	141	GLY	2.4
3	F	172	TRP	2.4
3	F	236	LEU	2.4
3	I	258	ILE	2.4
3	F	12	TYR	2.4
3	C	70	ASP	2.4
1	G	202	THR	2.4
3	C	24	TRP	2.3
2	K	140	CYS	2.3
3	C	135	LEU	2.3
3	F	112	SER	2.3
1	G	212	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
3	I	76	PHE	2.3
3	L	11	LEU	2.3
3	L	14	LEU	2.3
3	F	135	LEU	2.3
3	C	72	ILE	2.3
3	L	136	ALA	2.3
3	I	227	HIS	2.3
3	C	73	ASN	2.3
2	H	104	SER	2.2
3	L	132	LEU	2.2
3	I	129	VAL	2.2
3	L	129	VAL	2.2
1	J	202	THR	2.2
3	I	78	LEU	2.2
3	L	259	ILE	2.2
3	L	76	PHE	2.2
3	I	152	LEU	2.2
3	L	78	LEU	2.2
1	J	7	SER	2.2
3	I	107	PHE	2.2
1	A	24	ARG	2.2
3	F	24	TRP	2.2
3	L	124	THR	2.2
3	I	149	PHE	2.1
3	I	8	ASN	2.1
3	F	70	ASP	2.1
3	F	118	GLY	2.1
3	L	17	PHE	2.1
3	I	106	PRO	2.1
3	I	123	SER	2.1
3	C	114	PHE	2.1
3	F	72	ILE	2.1
3	F	221	ILE	2.1
2	B	74	THR	2.1
1	J	212	ASN	2.1
3	C	131	PHE	2.1
3	L	149	PHE	2.1
3	F	176	LEU	2.0
3	I	14	LEU	2.0
3	F	267	PHE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no 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
5	LMT	I	301	25/35	0.81	0.23	3.14	153,158,163,165	0
5	LMT	L	301	23/35	0.65	0.26	2.26	147,154,160,165	0
4	BOG	C	301	13/20	0.73	0.23	0.99	127,132,136,136	0
4	BOG	F	301	13/20	0.80	0.20	0.65	124,128,133,136	0

6.5 Other polymers (i)

There are no such residues in this entry.