Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:24 AM GMT

PDB ID	:	2CX9
Title	:	Crystal structure of acyl-CoA dehydrogenase
Authors	:	Murayama, K.; Kinebuchi, T.; Shirouzu, M.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on	:	2005-06-28
Resolution	:	2.00 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 ⓘ symbol.

The following versions of software and data (see references ①) were used in the production of this report:

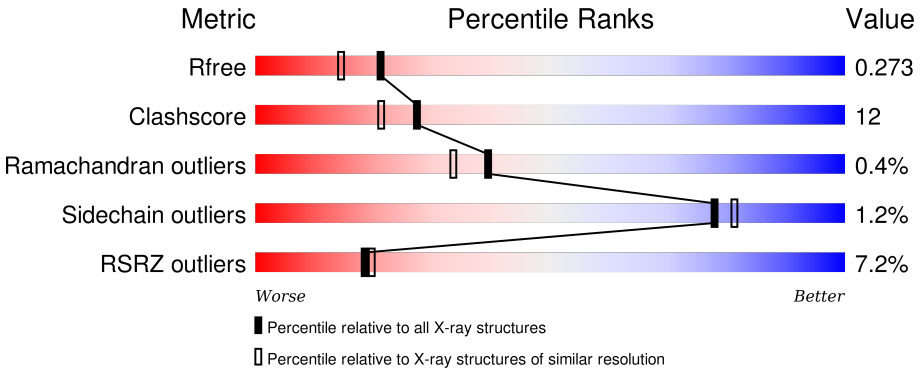
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.00 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	387	5% 80% 19%
1	B	387	4% 81% 18%
1	C	387	16% 66% 33%
1	D	387	5% 77% 22%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12199 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 acyl-CoA dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	385	Total	C	N	O	S	0	0	0
			2924	1872	506	542	4			
1	B	385	Total	C	N	O	S	0	0	0
			2924	1872	506	542	4			
1	C	385	Total	C	N	O	S	0	0	0
			2924	1872	506	542	4			
1	D	385	Total	C	N	O	S	0	0	0
			2924	1872	506	542	4			

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Cl	0	0
			1	1		
2	A	1	Total	Cl	0	0
			1	1		
2	D	2	Total	Cl	0	0
			2	2		

- Molecule 3 is water.

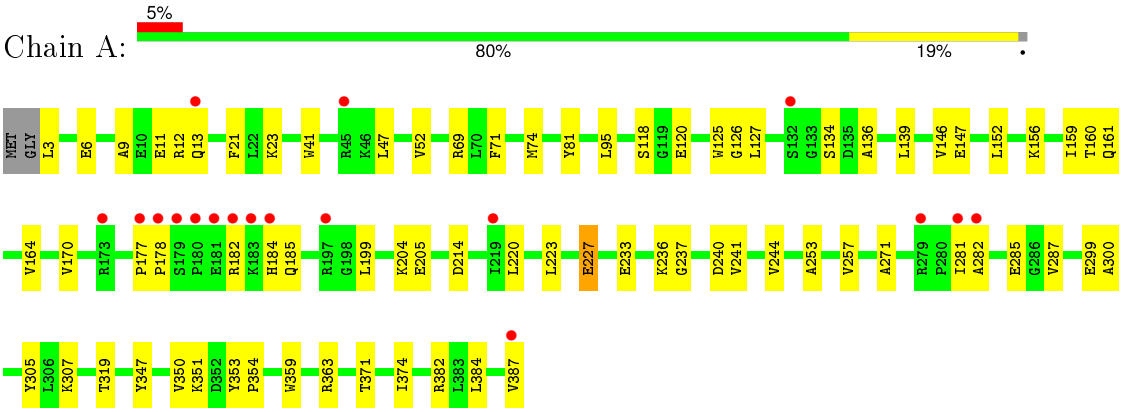
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	132	Total	O	0	0
			132	132		
3	B	161	Total	O	0	0
			161	161		
3	C	85	Total	O	0	0
			85	85		
3	D	121	Total	O	0	0
			121	121		

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.

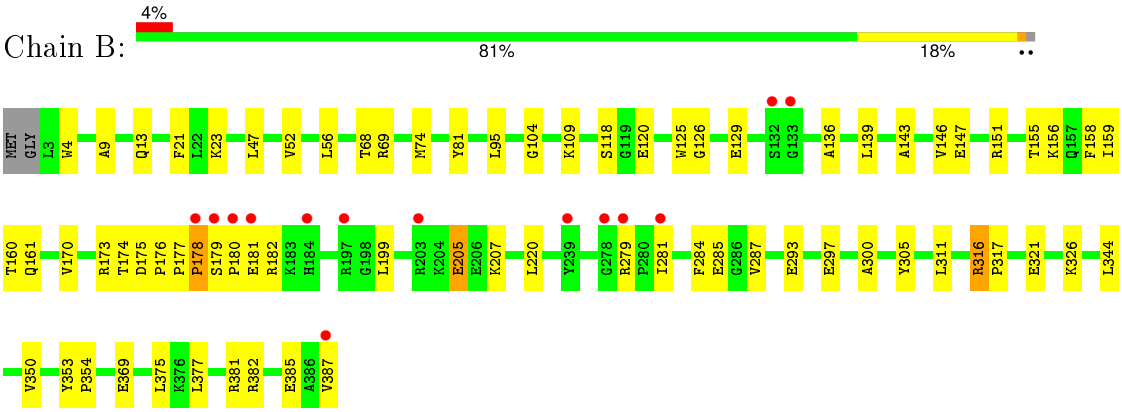
- Molecule 1: acyl-CoA dehydrogenase

Chain A:



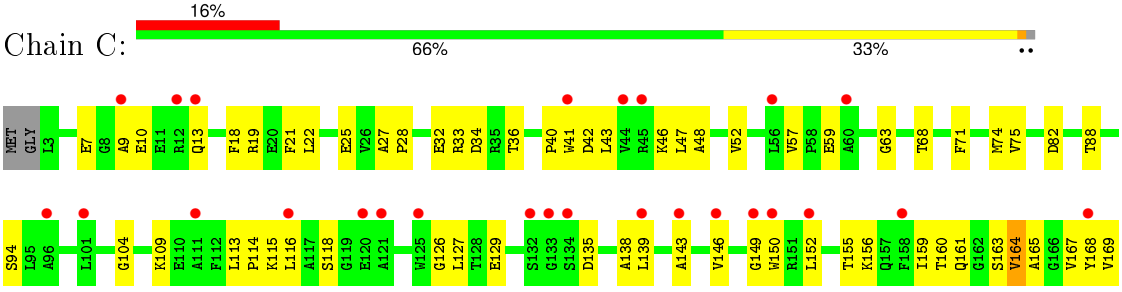
- Molecule 1: acyl-CoA dehydrogenase

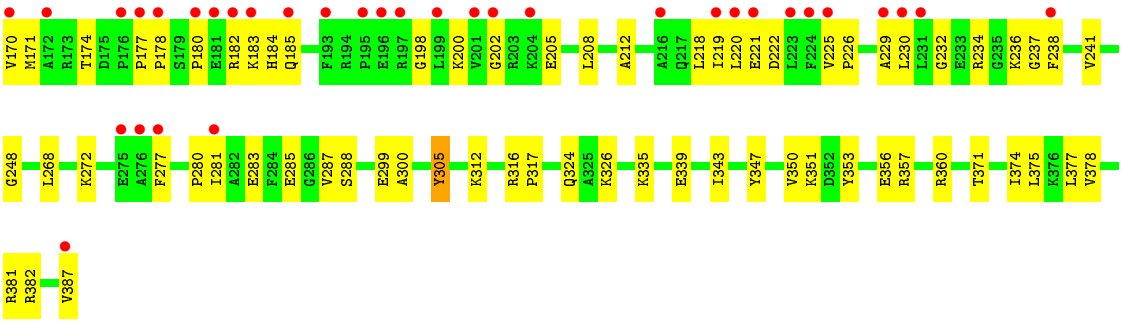
Chain B:



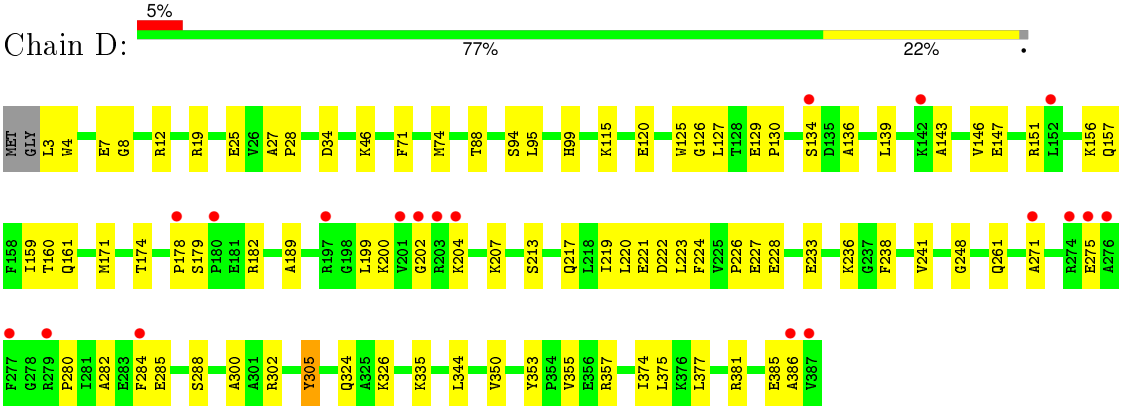
- Molecule 1: acyl-CoA dehydrogenase

Chain C:





- Molecule 1: acyl-CoA dehydrogenase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	75.69Å 88.64Å 119.56Å 90.00° 91.15° 90.00°	Depositor
Resolution (Å)	49.55 – 2.00 49.55 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.5 (49.55-2.00) 92.3 (49.55-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.80	Depositor
$< I/\sigma(I) >$ [1]	3.98 (at 2.00Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.237 , 0.272 0.237 , 0.273	Depositor DCC
R_{free} test set	5258 reflections (5.05%)	DCC
Wilson B-factor (Å^2)	26.7	Xtriage
Anisotropy	0.482	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 32.4	EDS
Estimated twinning fraction	0.220 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 104146 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	12199	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.16% 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: CL

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	0.34	0/2982	0.54	0/4027
1	B	0.36	0/2982	0.54	0/4027
1	C	0.31	0/2982	0.52	0/4027
1	D	0.32	0/2982	0.53	0/4027
All	All	0.33	0/11928	0.53	0/16108

There are no bond length outliers.

There are no bond angle outliers.

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	2924	0	2940	60	0
1	B	2924	0	2940	51	0
1	C	2924	0	2940	117	0
1	D	2924	0	2940	67	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	D	2	0	0	0	0
3	A	132	0	0	2	0
3	B	161	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	85	0	0	5	0
3	D	121	0	0	1	0
All	All	12199	0	11760	278	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 (278) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:387:VAL:HG21	1:C:272:LYS:HD2	1.47	0.96
1:C:281:ILE:HG12	1:C:287:VAL:HG21	1.48	0.95
1:D:130:PRO:HG3	1:D:157:GLN:HG3	1.47	0.94
1:B:281:ILE:HG22	1:B:287:VAL:HG21	1.50	0.94
1:D:146:VAL:HG22	1:D:147:GLU:H	1.40	0.86
1:A:281:ILE:HG22	1:A:287:VAL:HG21	1.60	0.83
1:D:71:PHE:HA	1:D:74:MET:HE3	1.63	0.81
1:C:33:ARG:HD2	3:C:426:HOH:O	1.83	0.78
1:B:143:ALA:HB3	1:B:174:THR:HG22	1.66	0.77
1:C:127:LEU:HD12	1:C:139:LEU:HD11	1.64	0.77
1:D:143:ALA:HB3	1:D:174:THR:HG22	1.65	0.76
1:A:152:LEU:HD12	1:A:223:LEU:HD23	1.66	0.76
1:B:160:THR:HG22	1:B:161:GLN:NE2	2.02	0.75
1:C:163:SER:O	1:C:164:VAL:HG22	1.86	0.75
1:A:160:THR:HG22	1:A:161:GLN:NE2	2.03	0.74
1:C:68:THR:HG21	1:C:312:LYS:HD3	1.70	0.72
1:B:281:ILE:CG2	1:B:287:VAL:HG21	2.19	0.72
1:A:134:SER:HB2	1:A:374:ILE:HD11	1.73	0.71
1:D:160:THR:HG22	1:D:161:GLN:NE2	2.05	0.70
1:C:326:LYS:HD2	1:C:375:LEU:HD11	1.73	0.70
1:B:178:PRO:HB2	1:B:182:ARG:NE	2.07	0.69
1:C:114:PRO:HG2	3:C:412:HOH:O	1.92	0.69
1:D:228:GLU:H	1:D:228:GLU:CD	1.97	0.68
1:C:238:PHE:O	1:C:241:VAL:HB	1.94	0.67
1:A:71:PHE:HA	1:A:74:MET:HE2	1.75	0.67
1:A:134:SER:CB	1:A:374:ILE:HD11	2.25	0.67
1:A:384:LEU:O	1:A:387:VAL:HG23	1.95	0.67
1:C:104:GLY:O	1:C:109:LYS:HE3	1.94	0.67
1:D:285:GLU:HA	1:D:288:SER:OG	1.95	0.66
1:C:143:ALA:HB3	1:C:174:THR:HG22	1.76	0.66
1:B:173:ARG:NH1	1:B:177:PRO:HG3	2.11	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:178:PRO:HB2	1:B:182:ARG:HE	1.60	0.65
1:C:161:GLN:O	1:C:165:ALA:HB2	1.97	0.65
1:A:387:VAL:HG22	1:C:268:LEU:HD11	1.78	0.64
1:B:146:VAL:HG21	1:B:151:ARG:HG2	1.79	0.64
1:D:326:LYS:HD2	1:D:375:LEU:HD11	1.79	0.64
1:D:271:ALA:HB1	1:D:282:ALA:HB2	1.79	0.64
1:A:177:PRO:HB2	1:A:178:PRO:C	2.17	0.64
1:A:160:THR:O	1:A:161:GLN:HB2	1.98	0.63
1:B:146:VAL:HG12	1:B:147:GLU:N	2.14	0.62
1:B:160:THR:O	1:B:161:GLN:HB2	2.00	0.62
1:C:88:THR:HA	1:C:161:GLN:HE22	1.65	0.62
1:D:261:GLN:HE21	1:D:302:ARG:HH22	1.46	0.62
1:D:377:LEU:O	1:D:381:ARG:HG3	1.99	0.61
1:C:351:LYS:HD3	1:C:356:GLU:OE2	1.99	0.61
1:C:285:GLU:HA	1:C:288:SER:OG	2.00	0.61
1:C:225:VAL:HG12	1:C:226:PRO:HD2	1.80	0.61
1:C:33:ARG:HG2	1:C:212:ALA:HB2	1.83	0.61
1:C:59:GLU:HA	1:C:63:GLY:O	2.02	0.60
1:A:387:VAL:HG22	1:C:268:LEU:CD1	2.30	0.60
1:B:118:SER:OG	1:B:120:GLU:HG2	2.02	0.60
1:D:151:ARG:NH1	1:D:224:PHE:HB2	2.16	0.60
1:A:233:GLU:HB2	1:A:236:LYS:HB2	1.84	0.59
1:C:230:LEU:HD11	1:C:234:ARG:HB2	1.84	0.59
1:D:202:GLY:N	1:D:217:GLN:O	2.34	0.59
1:A:3:LEU:HD23	1:A:6:GLU:OE1	2.02	0.59
1:C:88:THR:HG23	1:C:161:GLN:NE2	2.18	0.59
1:C:177:PRO:HG2	1:C:178:PRO:O	2.02	0.58
1:D:261:GLN:NE2	1:D:302:ARG:HH22	2.02	0.58
1:C:350:VAL:HG23	1:C:353:TYR:HD1	1.68	0.58
1:C:27:ALA:N	1:C:28:PRO:HD2	2.18	0.58
1:D:179:SER:HB3	1:D:182:ARG:HG2	1.86	0.58
1:C:280:PRO:HD2	1:C:283:GLU:OE2	2.03	0.58
1:A:205:GLU:HG2	3:A:711:HOH:O	2.04	0.57
1:D:344:LEU:HD12	1:D:355:VAL:HG21	1.86	0.57
1:C:326:LYS:HD2	1:C:375:LEU:CD1	2.34	0.57
1:B:326:LYS:HD2	1:B:375:LEU:HD11	1.87	0.57
1:A:204:LYS:HE2	1:A:214:ASP:OD2	2.03	0.56
1:B:279:ARG:HD2	1:B:284:PHE:CE2	2.40	0.56
1:B:129:GLU:HG2	1:B:155:THR:O	2.05	0.56
1:C:41:TRP:CZ2	1:C:164:VAL:HB	2.41	0.56
1:A:182:ARG:HB2	1:A:184:HIS:CE1	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:134:SER:OG	1:D:374:ILE:HD11	2.04	0.56
1:C:160:THR:O	1:C:161:GLN:HB2	2.05	0.55
1:C:160:THR:HG22	1:C:161:GLN:NE2	2.21	0.55
1:C:41:TRP:CH2	1:C:164:VAL:HB	2.41	0.55
1:B:126:GLY:HA2	1:B:159:ILE:HD12	1.89	0.55
1:C:351:LYS:HD3	1:C:356:GLU:CD	2.27	0.55
1:C:225:VAL:HG12	1:C:229:ALA:HB2	1.88	0.55
1:A:136:ALA:O	1:A:139:LEU:HG	2.07	0.54
1:B:146:VAL:HG12	1:B:147:GLU:H	1.72	0.54
1:C:180:PRO:O	1:C:183:LYS:HG3	2.07	0.54
3:A:686:HOH:O	1:D:285:GLU:HG3	2.07	0.54
1:C:200:LYS:HB2	1:C:219:ILE:HB	1.89	0.54
1:D:27:ALA:N	1:D:28:PRO:HD2	2.23	0.54
1:A:127:LEU:O	1:A:139:LEU:HD21	2.07	0.54
1:A:199:LEU:HD13	1:A:220:LEU:CD2	2.37	0.54
1:A:285:GLU:OE2	1:C:377:LEU:HD11	2.07	0.53
1:C:225:VAL:CG1	1:C:226:PRO:HD2	2.38	0.53
1:D:350:VAL:HG23	1:D:353:TYR:HD1	1.72	0.53
1:A:21:PHE:HE2	1:A:47:LEU:HD23	1.74	0.53
1:C:155:THR:HG23	1:C:218:LEU:O	2.08	0.53
1:C:185:GLN:HE21	1:C:236:LYS:NZ	2.07	0.53
1:C:57:VAL:HB	1:C:63:GLY:HA3	1.91	0.53
1:A:9:ALA:HA	1:A:12:ARG:NH1	2.24	0.53
1:D:157:GLN:HG2	1:D:217:GLN:HG3	1.92	0.52
1:D:344:LEU:HD12	1:D:355:VAL:CG2	2.39	0.52
1:C:115:LYS:O	1:C:118:SER:HB3	2.08	0.52
1:A:300:ALA:HB1	1:C:300:ALA:HB1	1.92	0.52
1:D:202:GLY:HA3	1:D:217:GLN:HB3	1.90	0.52
1:C:156:LYS:HE3	1:C:170:VAL:HG13	1.90	0.52
1:A:285:GLU:OE1	1:D:284:PHE:HB3	2.10	0.52
1:A:95:LEU:HB3	1:A:125:TRP:CG	2.45	0.52
1:C:378:VAL:O	1:C:382:ARG:HG2	2.10	0.52
1:C:277:PHE:HE1	1:D:134:SER:HG	1.58	0.52
1:D:227:GLU:HB2	1:D:228:GLU:OE2	2.09	0.52
1:C:156:LYS:HB2	1:C:218:LEU:HB2	1.91	0.52
1:C:18:PHE:O	1:C:22:LEU:HG	2.09	0.52
1:C:163:SER:C	1:C:165:ALA:H	2.13	0.52
1:B:382:ARG:HG2	1:B:382:ARG:HH11	1.75	0.52
1:D:146:VAL:HG22	1:D:147:GLU:N	2.18	0.51
1:C:177:PRO:HG2	1:C:178:PRO:C	2.30	0.51
1:B:293:GLU:O	1:B:297:GLU:HG3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:GLY:O	1:A:241:VAL:HG23	2.09	0.51
1:D:7:GLU:OE2	1:D:19:ARG:NH2	2.30	0.51
1:C:33:ARG:HD3	1:C:40:PRO:HB3	1.92	0.51
1:B:9:ALA:O	1:B:13:GLN:HG3	2.10	0.51
1:D:381:ARG:O	1:D:385:GLU:HG3	2.10	0.51
1:A:199:LEU:HD13	1:A:220:LEU:HD23	1.92	0.51
1:D:115:LYS:HG2	1:D:120:GLU:CD	2.31	0.51
1:D:136:ALA:O	1:D:139:LEU:HG	2.11	0.51
1:C:129:GLU:HG3	1:C:139:LEU:HD22	1.92	0.51
1:B:136:ALA:O	1:B:139:LEU:HG	2.11	0.50
1:A:182:ARG:HB2	1:A:184:HIS:NE2	2.27	0.50
1:A:146:VAL:HG22	1:A:147:GLU:N	2.26	0.50
1:A:146:VAL:HG22	1:A:147:GLU:H	1.76	0.50
1:C:198:GLY:O	1:C:220:LEU:HA	2.10	0.50
1:D:127:LEU:HD13	1:D:171:MET:HG3	1.93	0.50
1:C:139:LEU:CD1	1:C:171:MET:HB2	2.42	0.49
1:D:99:HIS:HE1	1:D:171:MET:HE1	1.76	0.49
1:B:311:LEU:CD1	1:B:321:GLU:HG2	2.42	0.49
1:C:116:LEU:HD21	1:C:167:VAL:HB	1.93	0.49
1:C:205:GLU:HA	1:C:205:GLU:OE1	2.13	0.49
1:D:381:ARG:HG2	1:D:381:ARG:HH11	1.77	0.49
1:C:180:PRO:O	1:C:183:LYS:HE3	2.13	0.49
1:A:9:ALA:O	1:A:13:GLN:HG3	2.12	0.49
1:A:23:LYS:HG3	1:A:81:TYR:OH	2.13	0.49
3:B:644:HOH:O	1:C:285:GLU:HG3	2.13	0.49
1:C:377:LEU:O	1:C:381:ARG:HG3	2.12	0.49
1:D:8:GLY:O	1:D:12:ARG:HG3	2.12	0.49
1:C:163:SER:O	1:C:165:ALA:N	2.46	0.49
1:C:387:VAL:HG22	1:C:387:VAL:O	2.13	0.49
1:D:171:MET:HE3	1:D:189:ALA:HB2	1.95	0.48
1:B:350:VAL:HG23	1:B:353:TYR:HD1	1.77	0.48
1:C:135:ASP:OD2	1:C:138:ALA:HB2	2.13	0.48
1:C:182:ARG:HB2	1:C:184:HIS:CE1	2.49	0.48
1:B:316:ARG:HG3	1:B:317:PRO:HD2	1.94	0.48
1:C:184:HIS:HB2	1:C:238:PHE:HD2	1.79	0.48
1:A:126:GLY:HA2	1:A:159:ILE:HD12	1.95	0.48
1:D:94:SER:HB3	1:D:248:GLY:HA2	1.96	0.48
1:A:319:THR:HG21	1:A:382:ARG:NH2	2.29	0.48
1:C:126:GLY:HA2	1:C:159:ILE:HD12	1.95	0.48
1:C:230:LEU:HD22	1:C:232:GLY:O	2.13	0.48
1:B:316:ARG:HH12	1:D:3:LEU:HD12	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:VAL:HG22	1:B:74:MET:CE	2.43	0.47
1:C:7:GLU:CD	1:C:19:ARG:HH22	2.16	0.47
1:D:228:GLU:N	1:D:228:GLU:CD	2.67	0.47
1:A:156:LYS:HE3	1:A:170:VAL:HG13	1.96	0.47
1:D:130:PRO:HG3	1:D:157:GLN:CG	2.33	0.47
1:D:200:LYS:HB2	1:D:219:ILE:HB	1.96	0.47
1:C:9:ALA:O	1:C:13:GLN:HG3	2.15	0.47
1:B:377:LEU:HD11	1:D:285:GLU:OE2	2.15	0.47
1:C:155:THR:HA	1:C:218:LEU:O	2.15	0.47
1:B:381:ARG:O	1:B:385:GLU:HG3	2.14	0.47
1:D:34:ASP:HB2	1:D:357:ARG:HD2	1.96	0.46
1:B:199:LEU:HD13	1:B:220:LEU:CD2	2.45	0.46
1:C:10:GLU:HB2	3:C:415:HOH:O	2.16	0.46
1:C:32:GLU:O	1:C:36:THR:HG23	2.15	0.46
1:D:199:LEU:HD23	1:D:199:LEU:C	2.36	0.46
1:C:21:PHE:HE2	1:C:47:LEU:HD23	1.80	0.46
1:A:351:LYS:HE2	1:B:207:LYS:O	2.15	0.46
1:B:179:SER:OG	1:B:180:PRO:HD2	2.16	0.46
1:D:238:PHE:O	1:D:241:VAL:HB	2.16	0.46
1:B:160:THR:HG22	1:B:161:GLN:HE22	1.79	0.46
1:A:387:VAL:HG21	1:C:272:LYS:CD	2.32	0.46
1:B:285:GLU:HB2	1:C:285:GLU:HB2	1.97	0.46
1:B:21:PHE:HE2	1:B:47:LEU:HD23	1.81	0.46
1:C:34:ASP:HB2	1:C:357:ARG:HD2	1.97	0.46
1:B:23:LYS:HG2	1:B:81:TYR:OH	2.16	0.46
1:C:237:GLY:O	1:C:241:VAL:HG23	2.15	0.46
1:B:95:LEU:HB3	1:B:125:TRP:CG	2.52	0.45
1:A:350:VAL:HG23	1:A:353:TYR:HD1	1.81	0.45
1:D:178:PRO:HG2	1:D:182:ARG:NE	2.31	0.45
1:D:207:LYS:NZ	1:D:213:SER:OG	2.49	0.45
1:C:21:PHE:HE1	1:C:46:LYS:HZ3	1.64	0.45
1:C:33:ARG:NH1	1:C:82:ASP:OD2	2.50	0.45
1:B:146:VAL:HG21	1:B:151:ARG:CG	2.43	0.45
1:C:161:GLN:O	1:C:163:SER:O	2.35	0.45
1:B:179:SER:C	1:B:181:GLU:H	2.20	0.45
1:D:160:THR:O	1:D:161:GLN:HB2	2.16	0.45
1:C:25:GLU:HG3	1:C:46:LYS:NZ	2.32	0.45
1:C:94:SER:HB3	1:C:248:GLY:HA2	1.98	0.45
1:D:126:GLY:HA2	1:D:159:ILE:HD12	1.98	0.45
1:D:220:LEU:HD22	1:D:223:LEU:HD22	1.99	0.45
1:C:387:VAL:HG13	1:C:387:VAL:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:71:PHE:O	1:C:75:VAL:HG23	2.17	0.45
1:D:130:PRO:CG	1:D:157:GLN:HG3	2.33	0.45
1:C:182:ARG:O	1:C:182:ARG:HG3	2.17	0.45
1:C:127:LEU:HD13	1:C:171:MET:HG3	1.99	0.44
1:C:347:TYR:O	1:C:350:VAL:HG22	2.17	0.44
1:D:305:TYR:CD1	1:D:305:TYR:C	2.91	0.44
1:C:350:VAL:HG23	1:C:353:TYR:CD1	2.50	0.44
1:A:371:THR:H	1:A:374:ILE:HD12	1.82	0.44
1:A:9:ALA:HA	1:A:12:ARG:HH12	1.81	0.44
1:A:382:ARG:HH11	1:A:382:ARG:HG2	1.82	0.44
1:C:42:ASP:CG	1:C:43:LEU:N	2.71	0.44
1:B:4:TRP:O	1:B:69:ARG:NH2	2.43	0.44
1:D:129:GLU:HG2	1:D:156:LYS:HD3	2.00	0.44
1:C:88:THR:HG23	1:C:161:GLN:HE21	1.83	0.44
1:B:146:VAL:CG1	1:B:147:GLU:N	2.81	0.44
1:D:171:MET:CE	1:D:189:ALA:HB2	2.48	0.43
1:C:156:LYS:HB3	1:C:159:ILE:HG13	2.00	0.43
1:C:113:LEU:N	1:C:114:PRO:HD2	2.32	0.43
1:D:233:GLU:OE1	1:D:236:LYS:HG3	2.17	0.43
1:D:226:PRO:HB2	1:D:228:GLU:OE1	2.19	0.43
1:A:11:GLU:OE2	1:A:69:ARG:NE	2.48	0.43
1:B:387:VAL:HG13	1:B:387:VAL:OXT	2.18	0.43
1:A:118:SER:OG	1:A:120:GLU:HG2	2.18	0.43
1:C:371:THR:OG1	1:C:374:ILE:HG12	2.18	0.43
1:B:4:TRP:CE3	1:D:4:TRP:CE3	3.07	0.43
1:A:240:ASP:O	1:A:244:VAL:HG23	2.18	0.43
1:A:182:ARG:HG3	1:A:182:ARG:O	2.19	0.43
1:A:41:TRP:CZ2	1:A:164:VAL:HB	2.54	0.43
1:D:326:LYS:HD2	1:D:375:LEU:CD1	2.47	0.43
1:D:160:THR:HG22	1:D:161:GLN:CD	2.38	0.43
1:A:184:HIS:ND1	1:A:185:GLN:N	2.66	0.43
1:D:221:GLU:O	1:D:222:ASP:C	2.58	0.43
1:B:104:GLY:O	1:B:109:LYS:HE3	2.19	0.42
1:B:158:PHE:HE2	1:B:205:GLU:OE2	2.01	0.42
1:A:299:GLU:HG3	1:C:324:GLN:HE22	1.83	0.42
1:A:139:LEU:HD22	1:A:156:LYS:NZ	2.35	0.42
1:A:160:THR:HG22	1:A:161:GLN:HE22	1.81	0.42
1:C:149:GLY:HA3	1:C:225:VAL:O	2.19	0.42
1:B:56:LEU:HD21	1:B:68:THR:HA	2.02	0.42
1:A:253:ALA:O	1:A:257:VAL:HG23	2.19	0.42
1:C:184:HIS:HB2	1:C:238:PHE:CD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:220:LEU:HD12	1:C:220:LEU:N	2.35	0.42
1:C:185:GLN:HE21	1:C:236:LYS:HZ2	1.67	0.42
1:C:152:LEU:HD13	1:C:225:VAL:HG23	2.01	0.42
1:C:339:GLU:O	1:C:343:ILE:HG13	2.20	0.42
1:A:227:GLU:HA	1:A:227:GLU:OE1	2.20	0.42
1:C:305:TYR:CD1	1:C:305:TYR:C	2.92	0.42
1:C:163:SER:C	1:C:165:ALA:N	2.73	0.42
1:C:165:ALA:HB3	1:C:168:TYR:CZ	2.55	0.42
1:D:88:THR:HA	1:D:161:GLN:HE22	1.85	0.42
1:B:156:LYS:HB3	1:B:159:ILE:HD11	2.02	0.42
1:C:48:ALA:HB1	1:C:118:SER:O	2.20	0.42
1:B:176:PRO:HA	1:B:177:PRO:HD3	1.87	0.41
1:A:307:LYS:NZ	1:C:299:GLU:OE1	2.47	0.41
1:A:347:TYR:O	1:A:350:VAL:HG22	2.20	0.41
1:C:21:PHE:CE2	1:C:47:LEU:HD23	2.55	0.41
1:A:271:ALA:HB1	1:A:282:ALA:HB2	2.02	0.41
1:C:156:LYS:HB3	1:C:159:ILE:CG1	2.49	0.41
1:D:25:GLU:OE1	1:D:46:LYS:HE3	2.21	0.41
1:D:95:LEU:HB3	1:D:125:TRP:CG	2.55	0.41
1:D:178:PRO:HG2	1:D:182:ARG:HE	1.86	0.41
1:D:324:GLN:NE2	3:D:618:HOH:O	2.52	0.41
1:C:169:VAL:HG12	1:C:171:MET:CE	2.50	0.41
1:C:353:TYR:CD1	1:C:353:TYR:N	2.89	0.41
1:C:198:GLY:HA2	1:C:221:GLU:O	2.20	0.41
1:B:316:ARG:HG3	1:B:317:PRO:CD	2.50	0.41
1:C:208:LEU:O	1:C:360:ARG:HD2	2.20	0.41
1:B:175:ASP:HA	1:B:176:PRO:HD3	1.90	0.41
1:C:374:ILE:HG13	3:C:453:HOH:O	2.20	0.41
1:C:335:LYS:HE2	3:C:443:HOH:O	2.21	0.41
1:B:300:ALA:HB1	1:D:300:ALA:HB1	2.03	0.41
1:B:156:LYS:HE3	1:B:170:VAL:HG13	2.03	0.41
1:A:95:LEU:HB3	1:A:125:TRP:CD2	2.56	0.41
1:C:74:MET:HE3	1:C:74:MET:HB2	1.92	0.41
1:A:359:TRP:CZ2	1:A:363:ARG:HD3	2.56	0.41
1:A:6:GLU:OE1	1:C:316:ARG:NH1	2.54	0.40
1:A:21:PHE:CE2	1:A:47:LEU:HD23	2.54	0.40
1:C:146:VAL:HG12	1:C:150:TRP:CA	2.50	0.40
1:C:21:PHE:HE2	1:C:47:LEU:CD2	2.34	0.40
1:C:316:ARG:HB3	1:C:317:PRO:HD2	2.02	0.40
1:C:221:GLU:O	1:C:222:ASP:C	2.60	0.40
1:B:143:ALA:HB3	1:B:174:THR:CG2	2.44	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:275:GLU:HA	1:D:280:PRO:HA	2.04	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	383/387 (99%)	372 (97%)	11 (3%)	0	100	100
1	B	383/387 (99%)	372 (97%)	10 (3%)	1 (0%)	46	41
1	C	383/387 (99%)	357 (93%)	23 (6%)	3 (1%)	24	15
1	D	383/387 (99%)	367 (96%)	14 (4%)	2 (0%)	34	26
All	All	1532/1548 (99%)	1468 (96%)	58 (4%)	6 (0%)	39	33

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	164	VAL
1	D	386	ALA
1	B	178	PRO
1	D	204	LYS
1	C	52	VAL
1	C	202	GLY

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	279/280 (100%)	275 (99%)	4 (1%)	74 77
1	B	279/280 (100%)	273 (98%)	6 (2%)	60 62
1	C	279/280 (100%)	278 (100%)	1 (0%)	93 95
1	D	279/280 (100%)	277 (99%)	2 (1%)	88 91
All	All	1116/1120 (100%)	1103 (99%)	13 (1%)	78 81

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	VAL
1	A	227	GLU
1	A	305	TYR
1	A	354	PRO
1	B	205	GLU
1	B	305	TYR
1	B	316	ARG
1	B	344	LEU
1	B	354	PRO
1	B	369	GLU
1	C	305	TYR
1	D	305	TYR
1	D	335	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	161	GLN
1	A	324	GLN
1	B	161	GLN
1	B	324	GLN
1	C	161	GLN
1	C	185	GLN
1	C	324	GLN
1	D	161	GLN
1	D	261	GLN
1	D	324	GLN

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

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	385/387 (99%)	0.30	18 (4%)	35 37	13, 29, 54, 83	0
1	B	385/387 (99%)	0.24	14 (3%)	46 48	12, 26, 54, 82	0
1	C	385/387 (99%)	0.90	60 (15%)	3 3	17, 42, 68, 80	0
1	D	385/387 (99%)	0.34	19 (4%)	33 35	15, 31, 59, 71	0
All	All	1540/1548 (99%)	0.45	111 (7%)	18 20	12, 31, 63, 83	0

All (111) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	387	VAL	7.1
1	C	133	GLY	5.8
1	C	281	ILE	5.7
1	C	387	VAL	5.7
1	B	180	PRO	5.6
1	C	177	PRO	5.5
1	A	180	PRO	5.0
1	C	132	SER	5.0
1	A	181	GLU	4.9
1	D	277	PHE	4.9
1	C	56	LEU	4.8
1	D	279	ARG	4.8
1	D	203	ARG	4.7
1	D	202	GLY	4.5
1	D	276	ALA	4.4
1	C	204	LYS	4.3
1	B	179	SER	4.3
1	C	230	LEU	4.1
1	C	13	GLN	4.0
1	D	204	LYS	4.0
1	A	178	PRO	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	278	GLY	3.9
1	C	219	ILE	3.8
1	A	387	VAL	3.7
1	C	181	GLU	3.6
1	C	150	TRP	3.6
1	A	279	ARG	3.6
1	B	281	ILE	3.6
1	B	133	GLY	3.5
1	C	178	PRO	3.5
1	C	45	ARG	3.5
1	D	275	GLU	3.4
1	C	134	SER	3.3
1	C	276	ALA	3.3
1	C	195	PRO	3.3
1	A	183	LYS	3.2
1	C	139	LEU	3.2
1	D	178	PRO	3.2
1	C	152	LEU	3.1
1	A	281	ILE	3.0
1	D	271	ALA	3.0
1	A	13	GLN	3.0
1	C	182	ARG	2.9
1	A	179	SER	2.9
1	C	121	ALA	2.9
1	D	386	ALA	2.9
1	B	178	PRO	2.9
1	C	225	VAL	2.9
1	B	184	HIS	2.8
1	A	182	ARG	2.8
1	C	180	PRO	2.8
1	C	120	GLU	2.8
1	A	282	ALA	2.8
1	C	229	ALA	2.8
1	D	387	VAL	2.8
1	C	202	GLY	2.8
1	B	203	ARG	2.8
1	C	44	VAL	2.8
1	B	132	SER	2.7
1	D	134	SER	2.7
1	A	219	ILE	2.7
1	C	223	LEU	2.7
1	D	152	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	9	ALA	2.7
1	B	181	GLU	2.7
1	A	197	ARG	2.6
1	C	231	LEU	2.6
1	C	60	ALA	2.5
1	C	143	ALA	2.5
1	D	201	VAL	2.5
1	C	193	PHE	2.5
1	C	224	PHE	2.5
1	D	197	ARG	2.5
1	C	220	LEU	2.5
1	C	158	PHE	2.5
1	A	45	ARG	2.5
1	D	274	ARG	2.5
1	C	185	GLN	2.5
1	C	183	LYS	2.5
1	C	201	VAL	2.4
1	B	279	ARG	2.4
1	C	197	ARG	2.4
1	C	196	GLU	2.4
1	A	132	SER	2.4
1	C	168	TYR	2.3
1	C	277	PHE	2.3
1	C	149	GLY	2.3
1	C	238	PHE	2.3
1	C	176	PRO	2.3
1	D	180	PRO	2.3
1	C	101	LEU	2.3
1	B	197	ARG	2.3
1	C	111	ALA	2.3
1	C	41	TRP	2.2
1	C	146	VAL	2.2
1	A	177	PRO	2.2
1	B	239	TYR	2.2
1	C	221	GLU	2.2
1	C	172	ALA	2.2
1	A	173	ARG	2.2
1	C	170	VAL	2.2
1	C	199	LEU	2.2
1	C	216	ALA	2.1
1	A	184	HIS	2.1
1	C	96	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	275	GLU	2.1
1	C	116	LEU	2.1
1	C	125	TRP	2.0
1	C	12	ARG	2.0
1	D	142	LYS	2.0
1	D	284	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
2	CL	B	604	1/1	0.98	0.11	-	47,47,47,47	0
2	CL	D	603	1/1	0.96	0.18	-	47,47,47,47	0
2	CL	D	601	1/1	0.94	0.14	-	42,42,42,42	0
2	CL	A	602	1/1	0.95	0.14	-	48,48,48,48	0

6.5 Other polymers (i)

There are no such residues in this entry.