Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:07 PM GMT

PDB ID	:	4NF0
Title	:	CRYSTAL STRUCTURE OF A TRAP PERIPLASMIC SOLUTE BINDING PROTEIN FROM PSEUDOMONAS AERUGINOSA PAO1 (PA4616), TARGET EFI-510182, WITH BOUND L-Malate
Authors	:	Vetting, M.W.; Patskovsky, Y.; Al Obaidi, N.F.; Morisco, L.L.; Wasserman, S.R.; Sojitra, S.; Stead, M.; Attonito, J.D.; Scott Glenn, A.; Chowdhury, S.; Evans, B.; Hillerich, B.; Love, J.; Seidel, R.D.; Imker, H.J.; Gerlt, J.A.; Almo, S.C.; Enzyme Function Initiative (EFI)
Deposited on	:	2013-10-30
Resolution	:	1.85 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:

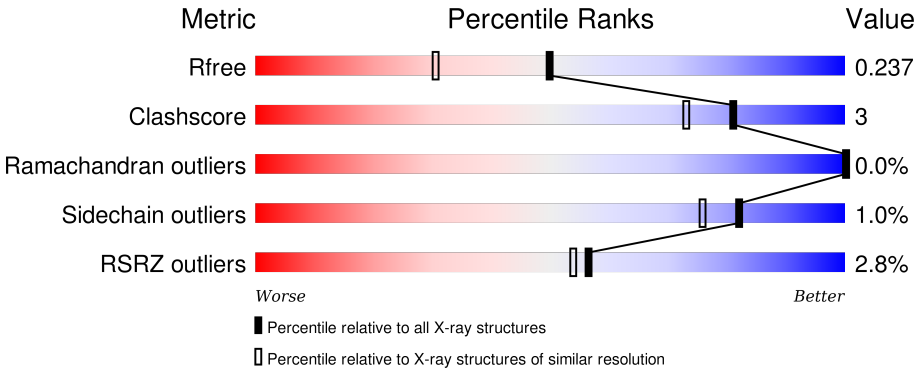
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 1.85 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.



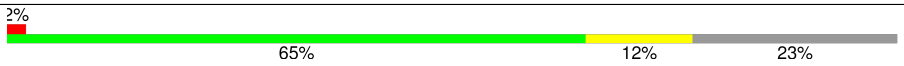
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1745 (1.86-1.86)
Clashscore	102246	1898 (1.86-1.86)
Ramachandran outliers	100387	1875 (1.86-1.86)
Sidechain outliers	100360	1875 (1.86-1.86)
RSRZ outliers	91569	1747 (1.86-1.86)

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	339	80% 6% 14%
1	B	339	76% · 19%
1	C	339	82% · 14%
1	D	339	80% 5% 15%
1	E	339	15% 58% 10% 31%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	339	
1	G	339	
1	H	339	

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
2	LMR	H	401	-	-	-	X
3	SO4	C	402	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 19172 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 Probable c4-dicarboxylate-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	291	Total	C	N	O	S	0	0	0
			2299	1462	395	435	7			
1	B	273	Total	C	N	O	S	0	0	0
			2156	1369	370	410	7			
1	C	291	Total	C	N	O	S	0	1	0
			2297	1464	393	433	7			
1	D	289	Total	C	N	O	S	0	1	0
			2280	1448	391	434	7			
1	E	233	Total	C	N	O	S	0	0	0
			1780	1127	301	346	6			
1	F	288	Total	C	N	O	S	0	0	0
			2281	1451	392	431	7			
1	G	287	Total	C	N	O	S	0	0	0
			2276	1449	392	428	7			
1	H	261	Total	C	N	O	S	0	0	0
			2056	1308	348	393	7			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	334	ALA	-	EXPRESSION TAG	UNP Q9HVH5
A	335	GLU	-	EXPRESSION TAG	UNP Q9HVH5
A	336	ASN	-	EXPRESSION TAG	UNP Q9HVH5
A	337	LEU	-	EXPRESSION TAG	UNP Q9HVH5
A	338	TYR	-	EXPRESSION TAG	UNP Q9HVH5
A	339	PHE	-	EXPRESSION TAG	UNP Q9HVH5
A	340	GLN	-	EXPRESSION TAG	UNP Q9HVH5
B	334	ALA	-	EXPRESSION TAG	UNP Q9HVH5
B	335	GLU	-	EXPRESSION TAG	UNP Q9HVH5
B	336	ASN	-	EXPRESSION TAG	UNP Q9HVH5
B	337	LEU	-	EXPRESSION TAG	UNP Q9HVH5
B	338	TYR	-	EXPRESSION TAG	UNP Q9HVH5
B	339	PHE	-	EXPRESSION TAG	UNP Q9HVH5

Continued on next page...

Continued from previous page...

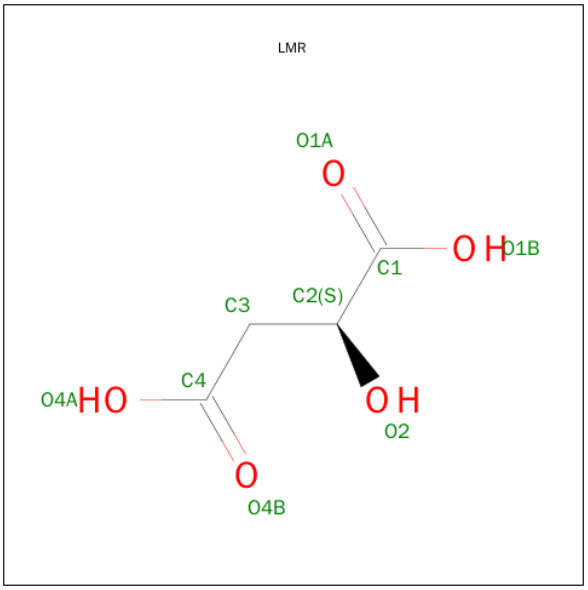
Chain	Residue	Modelled	Actual	Comment	Reference
B	340	GLN	-	EXPRESSION TAG	UNP Q9HVH5
C	334	ALA	-	EXPRESSION TAG	UNP Q9HVH5
C	335	GLU	-	EXPRESSION TAG	UNP Q9HVH5
C	336	ASN	-	EXPRESSION TAG	UNP Q9HVH5
C	337	LEU	-	EXPRESSION TAG	UNP Q9HVH5
C	338	TYR	-	EXPRESSION TAG	UNP Q9HVH5
C	339	PHE	-	EXPRESSION TAG	UNP Q9HVH5
C	340	GLN	-	EXPRESSION TAG	UNP Q9HVH5
D	334	ALA	-	EXPRESSION TAG	UNP Q9HVH5
D	335	GLU	-	EXPRESSION TAG	UNP Q9HVH5
D	336	ASN	-	EXPRESSION TAG	UNP Q9HVH5
D	337	LEU	-	EXPRESSION TAG	UNP Q9HVH5
D	338	TYR	-	EXPRESSION TAG	UNP Q9HVH5
D	339	PHE	-	EXPRESSION TAG	UNP Q9HVH5
D	340	GLN	-	EXPRESSION TAG	UNP Q9HVH5
E	334	ALA	-	EXPRESSION TAG	UNP Q9HVH5
E	335	GLU	-	EXPRESSION TAG	UNP Q9HVH5
E	336	ASN	-	EXPRESSION TAG	UNP Q9HVH5
E	337	LEU	-	EXPRESSION TAG	UNP Q9HVH5
E	338	TYR	-	EXPRESSION TAG	UNP Q9HVH5
E	339	PHE	-	EXPRESSION TAG	UNP Q9HVH5
E	340	GLN	-	EXPRESSION TAG	UNP Q9HVH5
F	334	ALA	-	EXPRESSION TAG	UNP Q9HVH5
F	335	GLU	-	EXPRESSION TAG	UNP Q9HVH5
F	336	ASN	-	EXPRESSION TAG	UNP Q9HVH5
F	337	LEU	-	EXPRESSION TAG	UNP Q9HVH5
F	338	TYR	-	EXPRESSION TAG	UNP Q9HVH5
F	339	PHE	-	EXPRESSION TAG	UNP Q9HVH5
F	340	GLN	-	EXPRESSION TAG	UNP Q9HVH5
G	334	ALA	-	EXPRESSION TAG	UNP Q9HVH5
G	335	GLU	-	EXPRESSION TAG	UNP Q9HVH5
G	336	ASN	-	EXPRESSION TAG	UNP Q9HVH5
G	337	LEU	-	EXPRESSION TAG	UNP Q9HVH5
G	338	TYR	-	EXPRESSION TAG	UNP Q9HVH5
G	339	PHE	-	EXPRESSION TAG	UNP Q9HVH5
G	340	GLN	-	EXPRESSION TAG	UNP Q9HVH5
H	334	ALA	-	EXPRESSION TAG	UNP Q9HVH5
H	335	GLU	-	EXPRESSION TAG	UNP Q9HVH5
H	336	ASN	-	EXPRESSION TAG	UNP Q9HVH5
H	337	LEU	-	EXPRESSION TAG	UNP Q9HVH5
H	338	TYR	-	EXPRESSION TAG	UNP Q9HVH5
H	339	PHE	-	EXPRESSION TAG	UNP Q9HVH5

Continued on next page...

Continued from previous page...

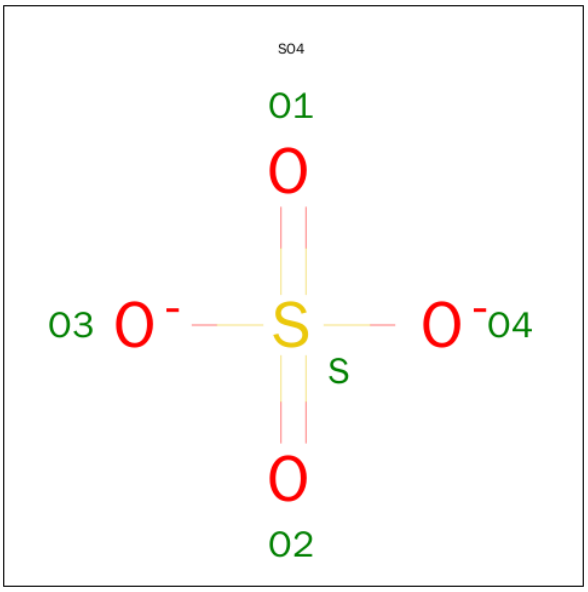
Chain	Residue	Modelled	Actual	Comment	Reference
H	340	GLN	-	EXPRESSION TAG	UNP Q9HVH5

- Molecule 2 is (2S)-2-HYDROXYBUTANEDIOIC ACID (three-letter code: LMR) (formula: $C_4H_6O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			9	4	5		
2	B	1	Total	C	O	0	0
			9	4	5		
2	C	1	Total	C	O	0	0
			9	4	5		
2	D	1	Total	C	O	0	0
			9	4	5		
2	F	1	Total	C	O	0	0
			9	4	5		
2	G	1	Total	C	O	0	0
			9	4	5		
2	H	1	Total	C	O	0	0
			9	4	5		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	F	1	Total O S 5 4 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	221	Total O 221 221	0	0
4	B	221	Total O 221 221	0	0
4	C	270	Total O 270 270	0	0
4	D	263	Total O 263 263	0	0
4	E	100	Total O 100 100	0	0
4	F	201	Total O 201 201	0	0

Continued on next page...

Continued from previous page...

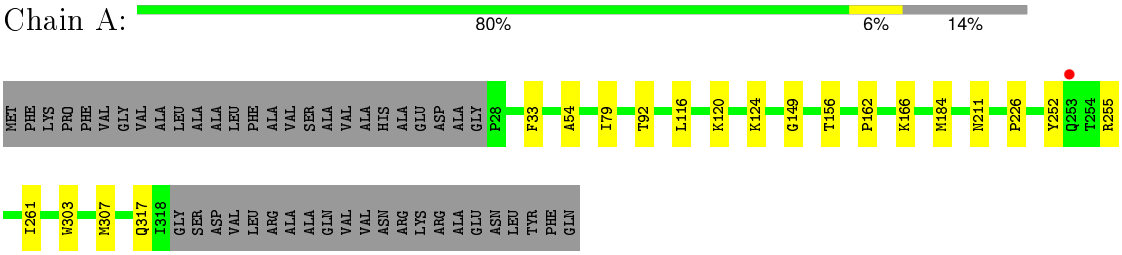
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	G	261	Total O 261 261	0	0
4	H	117	Total O 117 117	0	0

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.

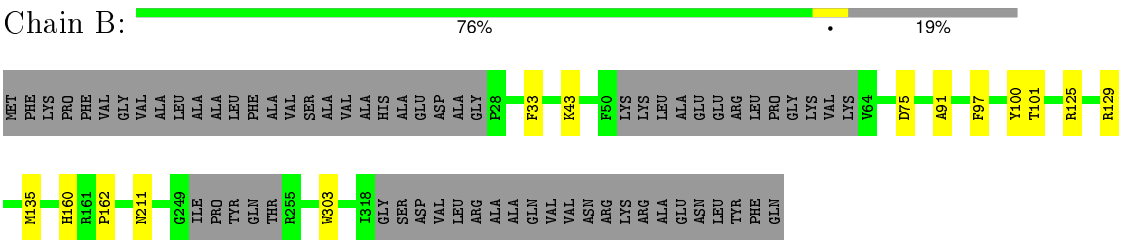
- Molecule 1: Probable c4-dicarboxylate-binding protein

Chain A:



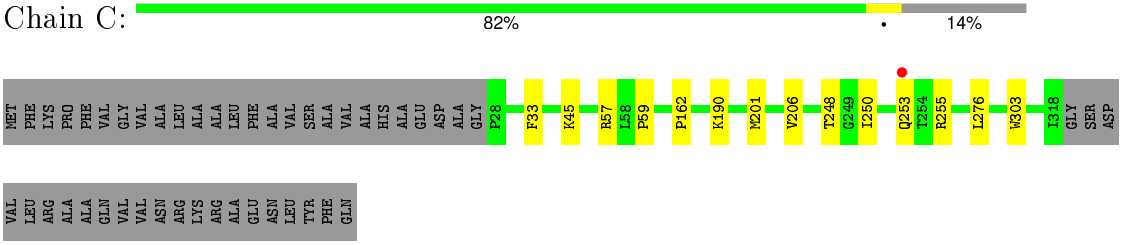
- Molecule 1: Probable c4-dicarboxylate-binding protein

Chain B:



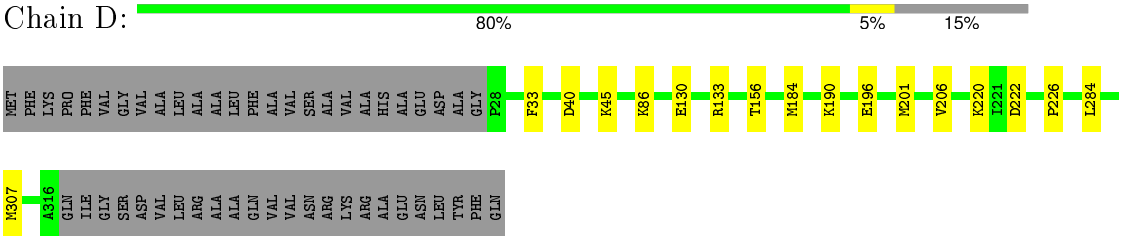
- Molecule 1: Probable c4-dicarboxylate-binding protein

Chain C:



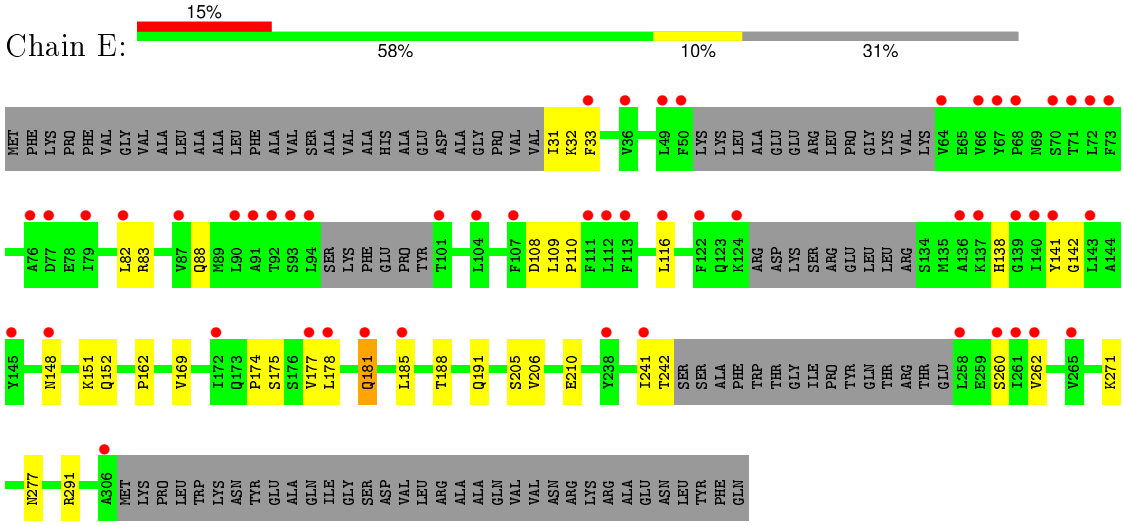
- Molecule 1: Probable c4-dicarboxylate-binding protein

Chain D:



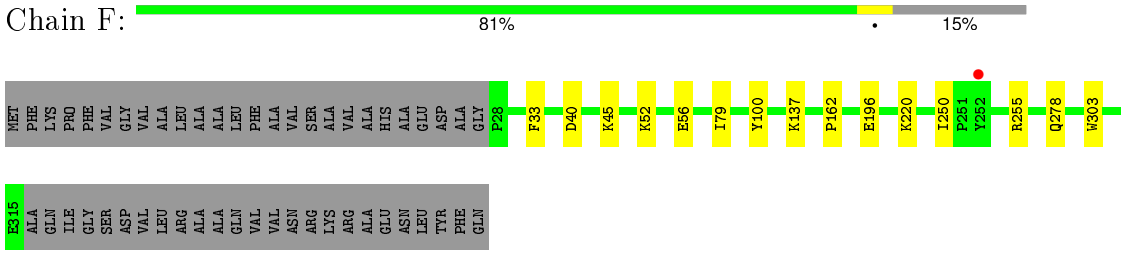
• Molecule 1: Probable c4-dicarboxylate-binding protein

Chain E:



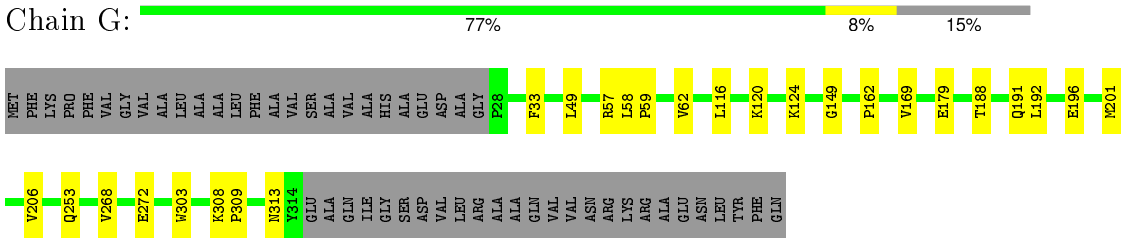
• Molecule 1: Probable c4-dicarboxylate-binding protein

Chain F:



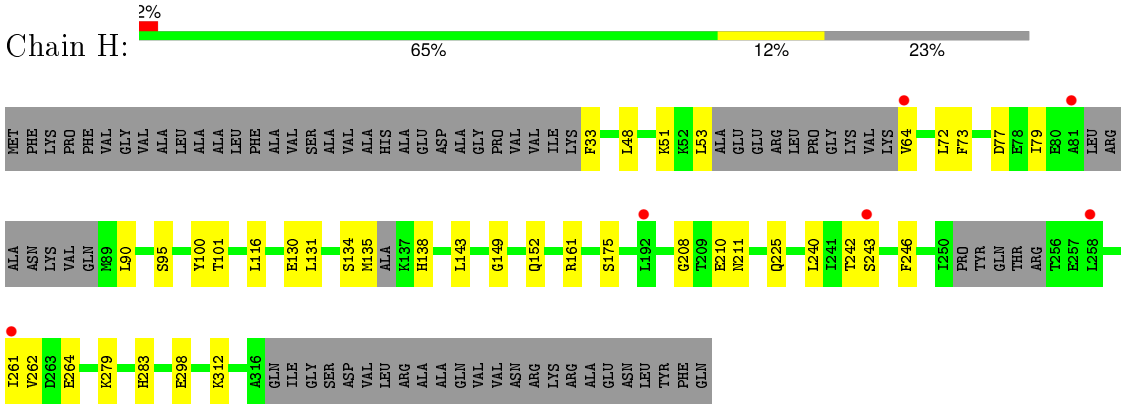
• Molecule 1: Probable c4-dicarboxylate-binding protein

Chain G:



• Molecule 1: Probable c4-dicarboxylate-binding protein

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	71.96Å 73.91Å 122.14Å 99.01° 91.59° 95.09°	Depositor
Resolution (Å)	33.56 – 1.85 120.52 – 1.85	Depositor EDS
% Data completeness (in resolution range)	96.1 (33.56-1.85) 91.5 (120.52-1.85)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	3.67 (at 1.84Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.195 , 0.239 0.197 , 0.237	Depositor DCC
R_{free} test set	10268 reflections (5.30%)	DCC
Wilson B-factor (Å^2)	23.1	Xtriage
Anisotropy	0.073	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 58.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 204100 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	19172	wwPDB-VP
Average B, all atoms (Å^2)	31.0	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 35.14 % 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 6.1104e-04.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: LMR, SO4

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	0.35	0/2345	0.47	0/3170
1	B	0.38	0/2197	0.51	0/2967
1	C	0.40	0/2343	0.51	0/3168
1	D	0.39	0/2326	0.51	0/3147
1	E	0.41	0/1808	0.54	0/2446
1	F	0.37	0/2327	0.51	0/3144
1	G	0.40	0/2322	0.51	0/3136
1	H	0.35	0/2094	0.50	0/2826
All	All	0.38	0/17762	0.51	0/24004

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	2299	0	2302	10	0
1	B	2156	0	2146	12	0
1	C	2297	0	2302	8	0
1	D	2280	0	2265	11	0
1	E	1780	0	1732	23	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2281	0	2289	9	0
1	G	2276	0	2294	18	0
1	H	2056	0	2023	23	1
2	A	9	0	4	0	0
2	B	9	0	4	0	0
2	C	9	0	4	0	0
2	D	9	0	4	0	0
2	F	9	0	4	0	0
2	G	9	0	4	0	0
2	H	9	0	4	0	0
3	B	10	0	0	0	0
3	C	5	0	0	0	0
3	D	10	0	0	0	0
3	F	5	0	0	0	0
4	A	221	0	0	2	0
4	B	221	0	0	2	0
4	C	270	0	0	0	0
4	D	263	0	0	3	1
4	E	100	0	0	2	0
4	F	201	0	0	1	0
4	G	261	0	0	7	0
4	H	117	0	0	1	0
All	All	19172	0	17381	114	1

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 3.

All (114) 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:B:97:PHE:HB3	1:B:135:MET:HE3	1.61	0.82
1:B:135:MET:SD	4:B:608:HOH:O	2.41	0.78
1:C:250:ILE:O	1:C:255:ARG:NH2	2.20	0.73
1:F:40:ASP:OD1	1:F:45:LYS:NZ	2.21	0.73
1:G:179:GLU:OE1	1:G:191:GLN:NE2	2.21	0.72
1:B:100:TYR:HB2	1:B:135:MET:CE	2.22	0.69
1:G:120:LYS:NZ	4:G:709:HOH:O	2.27	0.67
1:E:142:GLY:HA2	1:E:241:ILE:HD12	1.78	0.65
1:E:88:GLN:N	1:E:88:GLN:OE1	2.29	0.64
1:B:160:HIS:ND1	4:B:549:HOH:O	2.30	0.63
1:E:108:ASP:OD1	4:E:411:HOH:O	2.15	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:243:SER:OG	1:H:246:PHE:HB3	1.98	0.62
1:B:97:PHE:HB3	1:B:135:MET:CE	2.29	0.62
1:H:79:ILE:HA	1:H:90:LEU:HD11	1.82	0.61
1:D:190:LYS:NZ	4:D:661:HOH:O	2.32	0.61
1:A:116:LEU:HD11	1:A:149:GLY:HA2	1.83	0.59
1:E:174:PRO:HA	1:E:191:GLN:HB3	1.86	0.58
1:D:86:LYS:NZ	4:D:666:HOH:O	2.35	0.58
1:E:110:PRO:HG3	1:E:181:GLN:HG2	1.85	0.57
1:E:169:VAL:HG23	1:E:206:VAL:HA	1.86	0.57
1:G:253:GLN:CD	1:G:253:GLN:H	2.08	0.57
1:C:162:PRO:HG3	1:C:303:TRP:HA	1.86	0.55
1:G:57:ARG:NH2	4:G:692:HOH:O	2.27	0.55
1:B:100:TYR:HB2	1:B:135:MET:HE2	1.87	0.55
1:G:58:LEU:HB2	1:G:62:VAL:HG22	1.88	0.55
1:D:40:ASP:OD1	1:D:45:LYS:NZ	2.39	0.54
1:B:100:TYR:HB2	1:B:135:MET:HE1	1.89	0.54
1:E:32:LYS:NZ	1:E:88:GLN:HE22	2.06	0.53
1:G:162:PRO:HG3	1:G:303:TRP:HA	1.89	0.53
1:C:201:MET:HG2	1:C:206:VAL:HG23	1.90	0.53
1:C:201:MET:HG2	1:C:206:VAL:CG2	2.39	0.53
1:D:130:GLU:OE1	1:D:133:ARG:NH1	2.41	0.52
1:E:83:ARG:HE	1:E:138:HIS:HB3	1.73	0.52
1:F:196:GLU:OE2	4:F:699:HOH:O	2.19	0.52
1:B:101:THR:HG22	1:B:135:MET:CE	2.40	0.52
1:H:143:LEU:HD11	1:H:242:THR:HG22	1.92	0.52
1:H:53:LEU:HB3	1:H:261:ILE:HD13	1.92	0.52
1:A:162:PRO:HG3	1:A:303:TRP:HA	1.90	0.52
1:H:161:ARG:NH1	1:H:298:GLU:OE1	2.44	0.51
1:G:272:GLU:OE1	4:G:643:HOH:O	2.19	0.51
1:F:162:PRO:HG3	1:F:303:TRP:HA	1.93	0.51
1:G:201:MET:HG3	1:G:206:VAL:HG23	1.92	0.51
1:E:32:LYS:HB2	1:E:88:GLN:OE1	2.11	0.50
1:B:162:PRO:HG3	1:B:303:TRP:HA	1.93	0.50
1:B:101:THR:HG22	1:B:135:MET:HE3	1.93	0.50
1:C:248:THR:O	1:C:255:ARG:NH2	2.45	0.49
1:E:151:LYS:NZ	1:E:210:GLU:OE2	2.34	0.49
1:A:166:LYS:NZ	4:A:623:HOH:O	2.45	0.49
1:C:45:LYS:HZ2	1:C:276:LEU:HD21	1.77	0.49
1:H:261:ILE:HA	1:H:264:GLU:H	1.78	0.49
1:G:313:ASN:ND2	4:G:617:HOH:O	2.42	0.49
1:E:169:VAL:HG21	1:E:205:SER:O	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:116:LEU:HD11	1:G:149:GLY:HA2	1.93	0.48
1:D:196:GLU:OE1	4:D:621:HOH:O	2.19	0.48
1:H:135:MET:HB3	1:H:135:MET:HE2	1.58	0.48
1:H:48:LEU:O	1:H:51:LYS:HB3	2.14	0.47
1:H:131:LEU:O	1:H:134:SER:HB2	2.14	0.47
1:G:192:LEU:HB3	1:G:196:GLU:HG3	1.96	0.47
1:H:242:THR:OG1	1:H:243:SER:N	2.47	0.47
1:H:312:LYS:HA	1:H:312:LYS:HD3	1.66	0.47
1:H:279:LYS:HE2	1:H:283:HIS:HE1	1.80	0.46
1:E:178:LEU:HD13	4:E:408:HOH:O	2.14	0.46
1:G:49:LEU:CD2	1:G:268:VAL:HG11	2.46	0.46
1:G:169:VAL:HG22	1:G:188:THR:CG2	2.45	0.46
1:B:43:LYS:HD3	1:B:91:ALA:HB3	1.97	0.46
1:E:148:ASN:O	1:E:277:ASN:ND2	2.49	0.45
1:E:109:LEU:HA	1:E:110:PRO:HD2	1.83	0.45
1:A:156:THR:HA	1:A:226:PRO:HD2	1.98	0.45
1:D:220:LYS:HE2	1:D:220:LYS:HB2	1.76	0.45
1:B:125:ARG:O	1:B:129:ARG:HG2	2.16	0.44
1:E:162:PRO:HB3	1:E:185:LEU:HD21	1.98	0.44
1:E:169:VAL:CG2	1:E:206:VAL:HA	2.46	0.44
1:H:152:GLN:O	1:H:210:GLU:HA	2.17	0.44
1:H:51:LYS:HE3	1:H:64:VAL:HG13	1.98	0.44
1:D:184:MET:HE1	1:D:307:MET:HA	2.00	0.44
1:H:90:LEU:O	1:H:240:LEU:HD12	2.18	0.44
1:E:82:LEU:HD22	1:E:241:ILE:HG23	2.00	0.44
1:F:278:GLN:HG3	4:G:761:HOH:O	2.17	0.44
1:A:252:TYR:HD1	1:A:255:ARG:NH2	2.16	0.43
1:D:156:THR:HA	1:D:226:PRO:HD2	2.01	0.43
1:D:184:MET:CE	1:D:307:MET:HA	2.49	0.43
1:H:116:LEU:HD11	1:H:149:GLY:HA2	1.99	0.43
1:G:124:LYS:NZ	4:G:683:HOH:O	2.49	0.43
1:E:116:LEU:HA	1:E:116:LEU:HD12	1.83	0.43
1:F:137:LYS:HE3	1:F:137:LYS:HB3	1.80	0.43
1:H:143:LEU:HB3	1:H:262:VAL:HG11	2.01	0.43
1:F:250:ILE:O	1:F:255:ARG:NH2	2.52	0.43
1:G:308:LYS:HG2	1:G:309:PRO:HD3	2.01	0.43
1:A:184:MET:HE1	1:A:307:MET:O	2.19	0.42
1:E:141:TYR:HB3	1:E:242:THR:HG23	2.01	0.42
1:G:188:THR:HG22	4:G:760:HOH:O	2.20	0.42
1:A:54:ALA:HA	1:A:261:ILE:HD13	2.00	0.42
1:H:79:ILE:HD11	1:H:100:TYR:CZ	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:152:GLN:O	1:E:210:GLU:HA	2.19	0.42
1:E:271:LYS:HB3	1:E:271:LYS:HE3	1.65	0.42
1:G:201:MET:CG	1:G:206:VAL:HG23	2.50	0.42
1:G:57:ARG:C	1:G:59:PRO:HD3	2.40	0.42
1:C:190:LYS:HB2	1:C:190:LYS:HE3	1.80	0.42
1:A:317:GLN:HG3	4:A:688:HOH:O	2.20	0.41
1:F:79:ILE:HG21	1:F:100:TYR:CZ	2.55	0.41
1:E:291:ARG:HG2	1:E:291:ARG:HH11	1.85	0.41
1:F:220:LYS:HE3	1:F:220:LYS:HB2	1.86	0.41
1:H:72:LEU:HG	1:H:73:PHE:CD1	2.54	0.41
1:F:52:LYS:NZ	1:F:56:GLU:OE2	2.54	0.41
1:A:120:LYS:HG2	1:A:124:LYS:HE3	2.02	0.41
1:C:57:ARG:C	1:C:59:PRO:HD3	2.40	0.41
1:H:95:SER:O	1:H:175:SER:HB2	2.19	0.41
1:H:101:THR:HG22	1:H:135:MET:HE3	2.03	0.41
1:H:208:GLY:HA2	1:H:225:GLN:OE1	2.21	0.41
1:H:138:HIS:HA	4:H:567:HOH:O	2.20	0.41
1:E:175:SER:HB3	1:E:178:LEU:HD12	2.03	0.41
1:A:79:ILE:HD11	1:A:92:THR:HG21	2.01	0.41
1:D:222:ASP:HB3	1:D:284:LEU:HD11	2.02	0.41
1:D:201:MET:HG3	1:D:206:VAL:HG23	2.02	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:130:GLU:OE2	4:D:678:HOH:O[1_544]	2.02	0.18

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	289/339 (85%)	283 (98%)	6 (2%)	0	100	100
1	B	267/339 (79%)	262 (98%)	5 (2%)	0	100	100
1	C	290/339 (86%)	284 (98%)	6 (2%)	0	100	100
1	D	288/339 (85%)	284 (99%)	4 (1%)	0	100	100
1	E	223/339 (66%)	216 (97%)	7 (3%)	0	100	100
1	F	286/339 (84%)	281 (98%)	5 (2%)	0	100	100
1	G	285/339 (84%)	277 (97%)	8 (3%)	0	100	100
1	H	251/339 (74%)	241 (96%)	9 (4%)	1 (0%)	39	22
All	All	2179/2712 (80%)	2128 (98%)	50 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	77	ASP

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	245/281 (87%)	243 (99%)	2 (1%)	86	82
1	B	230/281 (82%)	227 (99%)	3 (1%)	76	65
1	C	244/281 (87%)	242 (99%)	2 (1%)	86	82
1	D	242/281 (86%)	241 (100%)	1 (0%)	93	92
1	E	185/281 (66%)	178 (96%)	7 (4%)	40	19
1	F	244/281 (87%)	243 (100%)	1 (0%)	93	92
1	G	244/281 (87%)	243 (100%)	1 (0%)	93	92
1	H	217/281 (77%)	215 (99%)	2 (1%)	84	79
All	All	1851/2248 (82%)	1832 (99%)	19 (1%)	82	76

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	PHE
1	A	211	ASN
1	B	33	PHE
1	B	75	ASP
1	B	211	ASN
1	C	33	PHE
1	C	253	GLN
1	D	33	PHE
1	E	31	ILE
1	E	33	PHE
1	E	177	VAL
1	E	181	GLN
1	E	188	THR
1	E	260	SER
1	E	262	VAL
1	F	33	PHE
1	G	33	PHE
1	H	33	PHE
1	H	211	ASN

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

Mol	Chain	Res	Type
1	G	105	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

13 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	$\#\|Z\| > 2$
2	LMR	A	401	-	1,8,8	0.47	0	2,10,10	1.12	0
2	LMR	B	401	-	1,8,8	0.88	0	2,10,10	2.02	1 (50%)
3	SO4	B	402	-	4,4,4	0.11	0	6,6,6	0.09	0
3	SO4	B	403	-	4,4,4	0.13	0	6,6,6	0.29	0
2	LMR	C	401	-	1,8,8	1.24	0	2,10,10	1.20	0
3	SO4	C	402	-	4,4,4	0.15	0	6,6,6	0.14	0
2	LMR	D	401	-	1,8,8	0.63	0	2,10,10	2.03	1 (50%)
3	SO4	D	402	-	4,4,4	0.25	0	6,6,6	0.16	0
3	SO4	D	403	-	4,4,4	0.22	0	6,6,6	0.10	0
2	LMR	F	401	-	1,8,8	0.02	0	2,10,10	0.66	0
3	SO4	F	402	-	4,4,4	0.18	0	6,6,6	0.11	0
2	LMR	G	401	-	1,8,8	0.68	0	2,10,10	1.32	0
2	LMR	H	401	-	1,8,8	0.89	0	2,10,10	1.09	0

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
2	LMR	A	401	-	-	0/2/8/8	0/0/0/0
2	LMR	B	401	-	-	0/2/8/8	0/0/0/0
3	SO4	B	402	-	-	0/0/0/0	0/0/0/0
3	SO4	B	403	-	-	0/0/0/0	0/0/0/0
2	LMR	C	401	-	-	0/2/8/8	0/0/0/0
3	SO4	C	402	-	-	0/0/0/0	0/0/0/0
2	LMR	D	401	-	-	0/2/8/8	0/0/0/0
3	SO4	D	402	-	-	0/0/0/0	0/0/0/0
3	SO4	D	403	-	-	0/0/0/0	0/0/0/0
2	LMR	F	401	-	-	0/2/8/8	0/0/0/0
3	SO4	F	402	-	-	0/0/0/0	0/0/0/0
2	LMR	G	401	-	-	0/2/8/8	0/0/0/0
2	LMR	H	401	-	-	0/2/8/8	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})
2	B	401	LMR	C3-C2-C1	-2.85	107.10	111.19
2	D	401	LMR	C3-C2-C1	-2.70	107.31	111.19

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	291/339 (85%)	-0.28	1 (0%) 94 93	16, 28, 48, 61	0
1	B	273/339 (80%)	-0.24	0 100 100	13, 26, 48, 60	0
1	C	291/339 (85%)	-0.33	1 (0%) 94 93	12, 24, 43, 71	0
1	D	289/339 (85%)	-0.36	0 100 100	12, 22, 41, 53	0
1	E	233/339 (68%)	1.05	52 (22%) 1 1	23, 52, 75, 90	0
1	F	288/339 (84%)	-0.24	1 (0%) 94 93	15, 28, 48, 61	0
1	G	287/339 (84%)	-0.32	0 100 100	12, 24, 40, 52	0
1	H	261/339 (76%)	0.08	6 (2%) 64 62	18, 38, 60, 79	0
All	All	2213/2712 (81%)	-0.11	61 (2%) 56 54	12, 28, 58, 90	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	258	LEU	8.4
1	E	104	LEU	4.8
1	E	124	LYS	4.4
1	H	64	VAL	4.3
1	E	90	LEU	4.1
1	E	113	PHE	3.8
1	E	82	LEU	3.6
1	H	261	ILE	3.6
1	E	36	VAL	3.6
1	E	50	PHE	3.5
1	E	262	VAL	3.5
1	E	265	VAL	3.5
1	E	66	VAL	3.3
1	E	68	PRO	3.3
1	E	141	TYR	3.2
1	E	143	LEU	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	107	PHE	3.1
1	E	93	SER	3.1
1	E	261	ILE	3.0
1	E	72	LEU	3.0
1	C	253	GLN	2.9
1	E	136	ALA	2.8
1	E	241	ILE	2.8
1	E	140	ILE	2.8
1	E	177	VAL	2.7
1	E	238	TYR	2.7
1	E	178	LEU	2.7
1	E	79	ILE	2.7
1	E	76	ALA	2.7
1	E	67	TYR	2.6
1	E	172	ILE	2.6
1	H	243	SER	2.5
1	E	181	GLN	2.5
1	E	49	LEU	2.5
1	H	258	LEU	2.5
1	E	92	THR	2.5
1	H	81	ALA	2.5
1	E	111	PHE	2.4
1	A	253	GLN	2.4
1	E	94	LEU	2.4
1	E	306	ALA	2.4
1	E	112	LEU	2.4
1	H	192	LEU	2.4
1	E	91	ALA	2.4
1	E	260	SER	2.3
1	E	33	PHE	2.3
1	E	185	LEU	2.3
1	E	70	SER	2.3
1	E	71	THR	2.3
1	E	64	VAL	2.2
1	E	145	TYR	2.2
1	E	116	LEU	2.2
1	E	139	GLY	2.2
1	E	73	PHE	2.2
1	E	148	ASN	2.2
1	E	87	VAL	2.2
1	E	77	ASP	2.1
1	E	101	THR	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	137	LYS	2.1
1	E	122	PHE	2.1
1	F	252	TYR	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)

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	LMR	H	401	9/9	0.78	0.15	3.09	25,26,30,31	0
3	SO4	C	402	5/5	0.90	0.15	2.30	45,50,57,64	0
3	SO4	D	403	5/5	0.95	0.10	0.66	50,52,53,54	0
3	SO4	D	402	5/5	0.97	0.10	0.50	35,36,40,41	0
2	LMR	A	401	9/9	0.97	0.09	0.23	19,21,25,26	0
2	LMR	B	401	9/9	0.97	0.09	0.06	13,17,18,19	0
3	SO4	B	402	5/5	0.96	0.11	-0.01	37,40,48,57	0
2	LMR	F	401	9/9	0.97	0.08	-0.20	14,18,19,21	0
2	LMR	G	401	9/9	0.98	0.07	-1.13	14,16,17,19	0
3	SO4	B	403	5/5	0.95	0.07	-1.31	42,51,55,55	0
2	LMR	D	401	9/9	0.98	0.07	-1.69	10,12,15,15	0
2	LMR	C	401	9/9	0.97	0.07	-2.04	13,16,19,20	0
3	SO4	F	402	5/5	0.96	0.07	-2.22	59,60,66,69	0

6.5 Other polymers (i)

There are no such residues in this entry.