Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 10:46 pm BST

PDB ID	:	5V7X
Title	:	Crystal Structure of Myosin 1b residues 1-728 with bound sulfate and Calmodulin
Authors	:	Zwolak, A.; Shuman, H.; Dominguez, R.; Ostap, E.M.
Deposited on	:	2017-03-20
Resolution	:	3.14 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
https://www.wwpdb.org/validation/2017/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:

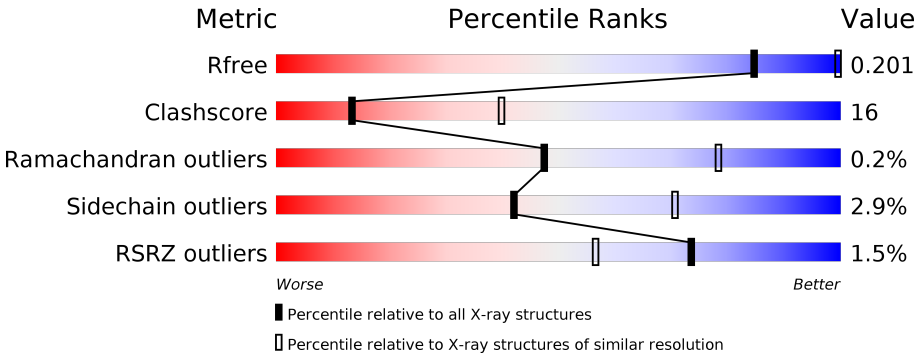
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance

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

The reported resolution of this entry is 3.14 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}	130704	1626 (3.18-3.10)
Clashscore	141614	1735 (3.18-3.10)
Ramachandran outliers	138981	1677 (3.18-3.10)
Sidechain outliers	138945	1677 (3.18-3.10)
RSRZ outliers	127900	1588 (3.18-3.10)

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 respectively. 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	752	63% 32%
2	B	149	7% 58% 36%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7008 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 Unconventional myosin-Ib.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	721	Total	C	N	O	S	0	0	0
			5858	3726	1012	1096	24			

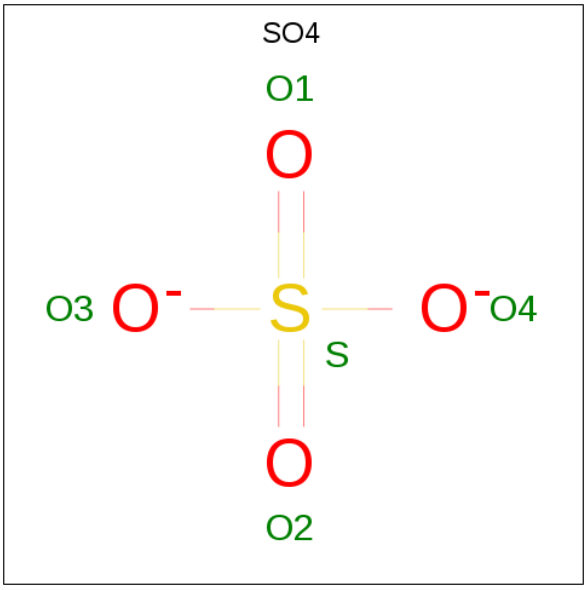
There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	729	GLY	-	expression tag	UNP Q05096
A	730	LEU	-	expression tag	UNP Q05096
A	731	ASN	-	expression tag	UNP Q05096
A	732	ASP	-	expression tag	UNP Q05096
A	733	ILE	-	expression tag	UNP Q05096
A	734	PHE	-	expression tag	UNP Q05096
A	735	GLU	-	expression tag	UNP Q05096
A	736	ALA	-	expression tag	UNP Q05096
A	737	GLN	-	expression tag	UNP Q05096
A	738	LYS	-	expression tag	UNP Q05096
A	739	ALA	-	expression tag	UNP Q05096
A	740	ILE	-	expression tag	UNP Q05096
A	741	GLU	-	expression tag	UNP Q05096
A	742	TRP	-	expression tag	UNP Q05096
A	743	HIS	-	expression tag	UNP Q05096
A	744	GLU	-	expression tag	UNP Q05096
A	745	ASP	-	expression tag	UNP Q05096
A	746	TYR	-	expression tag	UNP Q05096
A	747	LYS	-	expression tag	UNP Q05096
A	748	ASP	-	expression tag	UNP Q05096
A	749	ASP	-	expression tag	UNP Q05096
A	750	ASP	-	expression tag	UNP Q05096
A	751	ASP	-	expression tag	UNP Q05096
A	752	LYS	-	expression tag	UNP Q05096

- Molecule 2 is a protein called Calmodulin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	145	Total	C	N	O	S	0	0	0
			1145	702	185	249	9			

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



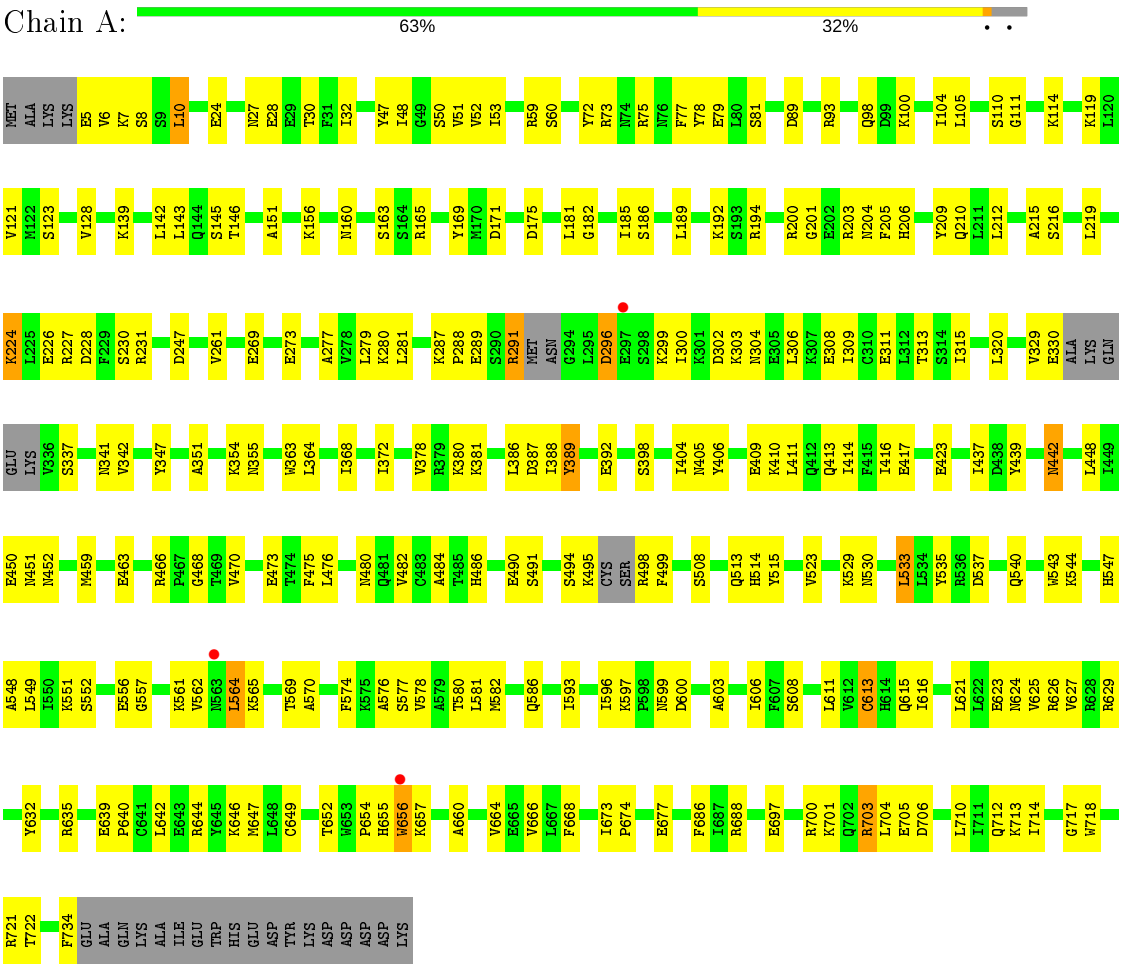
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	O	S		0	0
			5	4	1			

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 the various outlier classes 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.

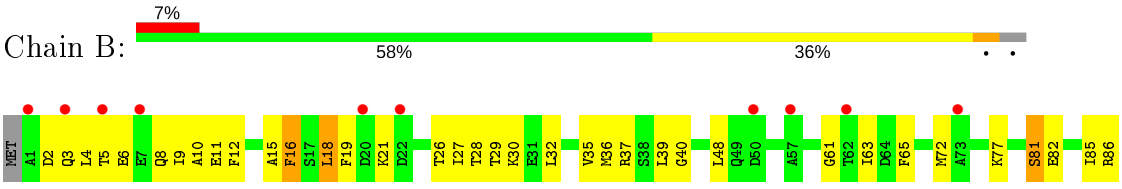
- Molecule 1: Unconventional myosin-Ib

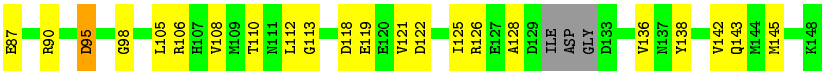
Chain A:



- Molecule 2: Calmodulin-1

Chain B:




E87
R90
D95
G98
L105
R106
H107
V108
M109
T110
N111
L112
G113
D118
E119
E120
V121
D122
I125
R126
E127
A128
D129
ILE
ASP
GLY
D133
V136
N137
Y138
V142
Q143
M144
M145
K148

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	109.77Å 48.73Å 118.51Å 90.00° 89.95° 90.00°	Depositor
Resolution (Å)	39.50 – 3.14 39.50 – 3.14	Depositor EDS
% Data completeness (in resolution range)	98.7 (39.50-3.14) 98.7 (39.50-3.14)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	101.23 (at 3.12Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.188 , 0.202 0.187 , 0.201	Depositor DCC
R_{free} test set	1094 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	41.1	Xtriage
Anisotropy	0.118	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , -1.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.38$, $< L^2 > = 0.21$	Xtriage
Estimated twinning fraction	0.349 for h,-k,-l	Xtriage
Reported twinning fraction	0.390 for h,-k,-l	Depositor
Outliers	0 of 22155 reflections	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	7008	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.51% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.60	0/5971	0.54	1/8052 (0.0%)
2	B	0.39	0/1156	0.51	0/1550
All	All	0.57	0/7127	0.54	1/9602 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	10	LEU	CA-CB-CG	6.55	130.36	115.30

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	5858	0	5837	181	0
2	B	1145	0	1077	52	0
3	A	5	0	0	1	0
All	All	7008	0	6914	224	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 16.

All (224) 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:389:TYR:CD1	1:A:404:ILE:HG23	1.79	1.17
1:A:388:ILE:HD13	1:A:411:LEU:CD1	1.91	1.01
1:A:495:LYS:NZ	1:A:498:ARG:O	1.93	1.01
2:B:82:GLU:OE2	2:B:86:ARG:NH1	1.93	1.00
1:A:389:TYR:HE1	1:A:404:ILE:HA	1.25	1.00
1:A:623:GLU:OE2	1:A:626:ARG:NH2	2.01	0.94
1:A:389:TYR:HD1	1:A:404:ILE:HG23	1.27	0.94
1:A:388:ILE:HD13	1:A:411:LEU:HD11	1.49	0.92
1:A:111:GLY:N	3:A:800:SO4:O1	2.02	0.92
1:A:156:LYS:NZ	1:A:201:GLY:O	2.03	0.90
2:B:87:GLU:OE2	2:B:90:ARG:NH1	2.06	0.89
1:A:459:MET:SD	1:A:482:VAL:HG21	2.15	0.86
1:A:389:TYR:CE1	1:A:404:ILE:HA	2.12	0.84
1:A:347:TYR:HB3	1:A:533:LEU:HD21	1.59	0.82
1:A:466:ARG:HG2	1:A:468:GLY:H	1.44	0.82
1:A:28:GLU:OE2	1:A:613:CYS:SG	2.37	0.80
1:A:24:GLU:OE1	1:A:629:ARG:NH2	2.13	0.80
2:B:36:MET:HA	2:B:72:MET:HE1	1.64	0.79
1:A:473:GLU:OE2	1:A:508:SER:OG	2.00	0.79
1:A:644:ARG:NE	1:A:697:GLU:OE2	2.13	0.79
1:A:273:GLU:OE1	1:A:547:HIS:NE2	2.14	0.78
2:B:39:LEU:O	2:B:39:LEU:HD12	1.82	0.78
1:A:674:PRO:HG2	1:A:677:GLU:HG3	1.66	0.77
1:A:389:TYR:CE1	1:A:404:ILE:HG23	2.19	0.77
1:A:398:SER:OG	1:A:529:LYS:NZ	2.17	0.77
1:A:388:ILE:CD1	1:A:411:LEU:CD1	2.64	0.76
1:A:490:GLU:OE1	1:A:498:ARG:N	2.20	0.74
2:B:106:ARG:NH1	2:B:122:ASP:OD1	2.22	0.73
2:B:26:THR:HG1	2:B:63:ILE:H	1.34	0.73
1:A:406:TYR:OH	1:A:450:GLU:OE1	2.07	0.72
1:A:8:SER:OG	1:A:79:GLU:O	2.06	0.72
1:A:616:ILE:HD12	1:A:621:LEU:HD12	1.71	0.71
1:A:564:LEU:HG	1:A:565:LYS:H	1.54	0.71
1:A:215:ALA:O	1:A:227:ARG:NH2	2.24	0.70
1:A:210:GLN:HA	1:A:247:ASP:HB3	1.73	0.70
2:B:4:LEU:HD11	2:B:8:GLN:HG2	1.73	0.70
1:A:104:ILE:HD12	1:A:121:VAL:HG11	1.75	0.69
1:A:224:LYS:NZ	1:A:311:GLU:OE1	2.27	0.67
2:B:26:THR:OG1	2:B:63:ILE:N	2.19	0.67
1:A:632:TYR:HA	1:A:688:ARG:HA	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:PRO:HB2	1:A:291:ARG:HB3	1.78	0.66
1:A:309:ILE:O	1:A:313:THR:OG1	2.12	0.66
1:A:119:LYS:O	1:A:123:SER:OG	2.05	0.65
1:A:388:ILE:CD1	1:A:411:LEU:HD12	2.26	0.65
1:A:721:ARG:HH11	2:B:40:GLY:HA2	1.61	0.64
1:A:513:GLN:NE2	1:A:514:HIS:O	2.28	0.64
1:A:59:ARG:HD3	1:A:60:SER:H	1.63	0.64
1:A:302:ASP:OD1	1:A:303:LYS:N	2.31	0.64
1:A:388:ILE:HD13	1:A:411:LEU:HD12	1.78	0.64
1:A:710:LEU:HD21	2:B:85:ILE:HG12	1.79	0.63
1:A:98:GLN:N	1:A:98:GLN:OE1	2.32	0.63
1:A:466:ARG:HG2	1:A:468:GLY:N	2.12	0.63
1:A:721:ARG:HD2	2:B:40:GLY:H	1.64	0.63
1:A:75:ARG:HD2	1:A:79:GLU:OE1	1.99	0.62
1:A:280:LYS:NZ	1:A:280:LYS:HB3	2.15	0.62
2:B:16:PHE:HE2	2:B:65:PHE:HA	1.64	0.62
1:A:703:ARG:NH1	1:A:706:ASP:OD2	2.32	0.62
1:A:717:GLY:HA2	2:B:37:ARG:HB3	1.82	0.62
1:A:657:LYS:HD2	1:A:666:VAL:HG21	1.81	0.61
1:A:143:LEU:O	1:A:146:THR:OG1	2.18	0.61
1:A:437:ILE:O	1:A:439:TYR:HD1	1.84	0.61
1:A:655:HIS:HB3	1:A:656:TRP:CD1	2.36	0.61
1:A:721:ARG:NH1	2:B:40:GLY:HA2	2.15	0.61
2:B:87:GLU:OE2	2:B:90:ARG:HD2	2.01	0.61
1:A:50:SER:HA	1:A:77:PHE:CE2	2.36	0.61
1:A:50:SER:HA	1:A:77:PHE:HE2	1.66	0.60
2:B:81:SER:OG	2:B:82:GLU:N	2.34	0.60
1:A:389:TYR:CE1	1:A:404:ILE:HG12	2.37	0.60
1:A:315:ILE:CD1	1:A:320:LEU:HD11	2.32	0.59
1:A:700:ARG:O	1:A:704:LEU:HG	2.01	0.59
1:A:549:LEU:O	1:A:552:SER:OG	2.19	0.59
1:A:204:ASN:OD1	1:A:205:PHE:N	2.33	0.58
1:A:151:ALA:HA	1:A:206:HIS:HB2	1.84	0.58
1:A:5:GLU:O	1:A:6:VAL:HG23	2.04	0.58
1:A:498:ARG:HH21	1:A:499:PHE:H	1.51	0.58
2:B:106:ARG:O	2:B:110:THR:OG1	2.10	0.58
1:A:718:TRP:O	1:A:722:THR:OG1	2.11	0.57
1:A:139:LYS:HB3	1:A:139:LYS:NZ	2.18	0.57
1:A:48:ILE:HD11	1:A:53:ILE:HD11	1.85	0.57
1:A:576:ALA:O	1:A:580:THR:HG23	2.06	0.56
1:A:459:MET:SD	1:A:482:VAL:CG2	2.93	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:655:HIS:HB3	1:A:656:TRP:CG	2.41	0.56
1:A:556:GLU:HA	1:A:561:LYS:HD3	1.89	0.55
1:A:182:GLY:HA2	1:A:372:ILE:HG22	1.88	0.55
1:A:165:ARG:NH2	1:A:392:GLU:OE2	2.21	0.55
1:A:600:ASP:N	1:A:600:ASP:OD1	2.39	0.55
1:A:315:ILE:HD12	1:A:320:LEU:HD11	1.89	0.55
2:B:106:ARG:HA	2:B:121:VAL:HG21	1.89	0.55
2:B:16:PHE:CD2	2:B:65:PHE:HD1	2.25	0.55
1:A:142:LEU:HG	1:A:185:ILE:HD11	1.90	0.54
1:A:530:ASN:HA	1:A:570:ALA:HB3	1.90	0.54
1:A:5:GLU:N	1:A:5:GLU:OE1	2.41	0.54
1:A:145:SER:HB2	1:A:368:ILE:HD13	1.88	0.54
2:B:2:ASP:N	2:B:3:GLN:HA	2.23	0.53
2:B:5:THR:O	2:B:9:ILE:HG13	2.08	0.53
1:A:156:LYS:HB3	1:A:203:ARG:HB3	1.90	0.53
1:A:160:ASN:HB2	1:A:163:SER:HB2	1.90	0.53
1:A:228:ASP:HB3	1:A:231:ARG:HG3	1.90	0.53
1:A:578:VAL:O	1:A:582:MET:HG2	2.08	0.53
2:B:15:ALA:O	2:B:19:PHE:HD2	1.92	0.53
2:B:29:THR:OG1	2:B:30:LYS:N	2.42	0.53
1:A:416:ILE:HG23	1:A:627:VAL:HG21	1.91	0.53
1:A:337:SER:O	1:A:337:SER:OG	2.25	0.53
1:A:10:LEU:N	1:A:78:TYR:O	2.42	0.53
2:B:6:GLU:O	2:B:10:ALA:N	2.38	0.52
1:A:341:ASN:OD1	1:A:342:VAL:N	2.42	0.52
1:A:608:SER:OG	1:A:611:LEU:HB3	2.09	0.52
1:A:261:VAL:HG11	1:A:368:ILE:HG12	1.91	0.52
1:A:181:LEU:HD12	1:A:380:LYS:HD3	1.90	0.52
1:A:287:LYS:HE3	1:A:299:LYS:NZ	2.25	0.52
1:A:6:VAL:CG2	1:A:75:ARG:HH21	2.22	0.52
2:B:8:GLN:O	2:B:11:GLU:N	2.43	0.52
1:A:224:LYS:HG2	1:A:308:GLU:HB3	1.92	0.51
1:A:654:PRO:O	1:A:655:HIS:ND1	2.44	0.51
1:A:189:LEU:HD23	1:A:574:PHE:HD1	1.75	0.50
1:A:491:SER:N	1:A:494:SER:O	2.22	0.50
1:A:599:ASN:OD1	1:A:603:ALA:N	2.40	0.50
1:A:599:ASN:ND2	1:A:606:ILE:O	2.44	0.50
1:A:169:TYR:OH	1:A:171:ASP:OD2	2.16	0.50
1:A:569:THR:HG22	1:A:570:ALA:H	1.77	0.50
1:A:463:GLU:HB3	1:A:470:VAL:HG21	1.93	0.50
2:B:2:ASP:HB3	2:B:4:LEU:N	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:LYS:HB3	1:A:354:LYS:HB2	1.94	0.50
1:A:409:GLU:OE1	1:A:442:ASN:ND2	2.40	0.49
1:A:409:GLU:OE2	1:A:515:TYR:HD1	1.95	0.49
1:A:28:GLU:O	1:A:32:ILE:HG12	2.13	0.49
1:A:277:ALA:O	1:A:281:LEU:HB2	2.13	0.49
2:B:108:VAL:HA	2:B:112:LEU:HD13	1.94	0.49
2:B:18:LEU:H	2:B:18:LEU:HD23	1.77	0.48
1:A:6:VAL:HG23	1:A:75:ARG:HH21	1.78	0.48
1:A:411:LEU:HA	1:A:582:MET:HE1	1.96	0.48
1:A:535:TYR:CE1	1:A:537:ASP:HB2	2.48	0.48
1:A:714:ILE:HG22	2:B:145:MET:HE2	1.96	0.48
1:A:216:SER:O	1:A:219:LEU:N	2.46	0.47
1:A:548:ALA:HA	1:A:551:LYS:HE2	1.96	0.47
1:A:712:GLN:NE2	2:B:112:LEU:O	2.34	0.47
2:B:28:THR:HA	2:B:61:GLY:O	2.13	0.47
1:A:300:ILE:HD12	1:A:300:ILE:O	2.14	0.47
1:A:596:ILE:HG23	1:A:615:GLN:OE1	2.15	0.47
2:B:118:ASP:OD1	2:B:119:GLU:N	2.47	0.47
1:A:114:LYS:HE2	1:A:387:ASP:OD1	2.13	0.47
1:A:52:VAL:HG13	1:A:593:ILE:HG23	1.97	0.47
1:A:540:GLN:O	1:A:544:LYS:HG3	2.15	0.47
1:A:451:ASN:OD1	1:A:452:ASN:N	2.48	0.47
1:A:414:ILE:HG12	1:A:582:MET:HE2	1.97	0.46
1:A:386:LEU:HD21	1:A:581:LEU:HD11	1.98	0.46
1:A:480:ASN:O	1:A:484:ALA:HB2	2.16	0.46
1:A:299:LYS:HE2	1:A:300:ILE:HD12	1.96	0.46
1:A:639:GLU:HB2	1:A:640:PRO:HD3	1.98	0.46
1:A:562:VAL:HG12	1:A:564:LEU:H	1.80	0.46
1:A:291:ARG:HB2	1:A:296:ASP:HB2	1.98	0.46
2:B:98:GLY:HA2	2:B:138:TYR:CZ	2.51	0.46
1:A:705:GLU:OE1	2:B:113:GLY:N	2.47	0.46
1:A:89:ASP:OD2	1:A:93:ARG:NH1	2.38	0.46
2:B:8:GLN:HG3	2:B:12:PHE:CZ	2.51	0.46
1:A:448:LEU:HD13	1:A:486:HIS:CG	2.50	0.45
1:A:442:ASN:O	1:A:442:ASN:ND2	2.44	0.45
1:A:304:ASN:O	1:A:308:GLU:HG3	2.16	0.45
1:A:105:LEU:HD13	1:A:386:LEU:HD23	1.98	0.45
2:B:6:GLU:O	2:B:9:ILE:N	2.50	0.44
1:A:410:LYS:O	1:A:414:ILE:HD13	2.17	0.44
1:A:632:TYR:OH	1:A:688:ARG:NH2	2.50	0.44
1:A:655:HIS:HA	1:A:656:TRP:HA	1.60	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:82:GLU:CD	2:B:86:ARG:HH11	2.21	0.44
1:A:228:ASP:OD1	1:A:230:SER:OG	2.35	0.44
1:A:73:ARG:NH2	1:A:128:VAL:HG12	2.33	0.44
1:A:389:TYR:CE1	1:A:404:ILE:CA	2.95	0.44
1:A:625:VAL:O	1:A:629:ARG:HB2	2.18	0.44
1:A:632:TYR:CD2	1:A:686:PHE:HB3	2.53	0.44
2:B:95:ASP:OD1	2:B:95:ASP:N	2.51	0.44
1:A:226:GLU:OE1	1:A:231:ARG:NH1	2.51	0.44
1:A:543:TRP:HB2	1:A:557:GLY:HA3	1.98	0.44
1:A:169:TYR:CE2	1:A:171:ASP:OD2	2.71	0.44
2:B:138:TYR:O	2:B:142:VAL:HG13	2.18	0.44
2:B:32:LEU:HG	2:B:48:LEU:HD11	1.99	0.44
1:A:280:LYS:HZ1	1:A:280:LYS:HB3	1.83	0.43
1:A:646:LYS:O	1:A:652:THR:OG1	2.22	0.43
2:B:126:ARG:HA	2:B:126:ARG:HD2	1.68	0.43
1:A:463:GLU:CD	1:A:466:ARG:HH22	2.21	0.43
1:A:476:LEU:HB2	1:A:523:VAL:HG11	2.00	0.43
1:A:574:PHE:O	1:A:577:SER:N	2.52	0.43
1:A:204:ASN:HB3	1:A:209:TYR:HE1	1.84	0.43
1:A:649:CYS:SG	1:A:652:THR:OG1	2.73	0.43
1:A:226:GLU:CD	1:A:231:ARG:HH11	2.21	0.43
1:A:306:LEU:HD11	1:A:320:LEU:HD12	2.00	0.43
1:A:660:ALA:O	1:A:664:VAL:HG23	2.18	0.43
2:B:16:PHE:HD2	2:B:65:PHE:HD1	1.64	0.43
1:A:72:TYR:OH	1:A:81:SER:O	2.20	0.43
1:A:535:TYR:HE1	1:A:537:ASP:HB2	1.84	0.42
1:A:378:VAL:O	1:A:380:LYS:HG3	2.19	0.42
1:A:27:ASN:OD1	1:A:30:THR:HG23	2.19	0.42
1:A:703:ARG:CZ	1:A:706:ASP:OD2	2.67	0.42
2:B:16:PHE:CE1	2:B:27:ILE:HG23	2.54	0.42
2:B:32:LEU:HA	2:B:35:VAL:HG12	2.01	0.42
2:B:128:ALA:O	2:B:136:VAL:HG22	2.19	0.42
2:B:143:GLN:HG3	2:B:143:GLN:H	1.64	0.42
1:A:498:ARG:HD2	1:A:499:PHE:H	1.85	0.42
1:A:668:PHE:CG	1:A:673:ILE:HD11	2.55	0.42
1:A:98:GLN:HB3	1:A:100:LYS:HD3	2.01	0.42
1:A:351:ALA:O	1:A:355:ASN:ND2	2.45	0.41
1:A:269:GLU:O	1:A:273:GLU:HG3	2.20	0.41
1:A:315:ILE:HD12	1:A:320:LEU:HD21	2.00	0.41
1:A:388:ILE:HD11	1:A:411:LEU:HD12	2.00	0.41
1:A:413:GLN:O	1:A:417:GLU:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:106:ARG:HG2	2:B:121:VAL:HG22	2.03	0.41
1:A:194:ARG:NH1	1:A:203:ARG:O	2.51	0.41
1:A:47:TYR:HA	1:A:51:VAL:O	2.20	0.41
2:B:77:LYS:HE3	2:B:77:LYS:HB3	1.90	0.41
2:B:6:GLU:HA	2:B:9:ILE:HB	2.03	0.41
1:A:423:GLU:CD	1:A:635:ARG:HH12	2.23	0.41
1:A:169:TYR:HB3	1:A:186:SER:HB3	2.02	0.41
1:A:405:ASN:OD1	1:A:405:ASN:N	2.54	0.41
1:A:642:LEU:HD12	1:A:642:LEU:HA	1.86	0.41
1:A:7:LYS:NZ	2:B:90:ARG:O	2.41	0.41
1:A:315:ILE:HD12	1:A:320:LEU:CD1	2.50	0.41
1:A:313:THR:OG1	1:A:315:ILE:HG12	2.21	0.40
2:B:105:LEU:HD23	2:B:125:ILE:HD11	2.03	0.40
1:A:713:LYS:HG3	1:A:714:ILE:HG12	2.03	0.40
2:B:21:LYS:HB3	2:B:21:LYS:HE3	1.85	0.40
1:A:363:TRP:CE3	1:A:364:LEU:HD23	2.56	0.40
1:A:110:SER:O	1:A:597:LYS:HD3	2.21	0.40
1:A:175:ASP:O	1:A:381:LYS:HE2	2.22	0.40
1:A:212:LEU:HD11	1:A:279:LEU:HD21	2.03	0.40
1:A:409:GLU:OE2	1:A:514:HIS:HB3	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	713/752 (95%)	665 (93%)	46 (6%)	2 (0%)	41 72
2	B	141/149 (95%)	131 (93%)	10 (7%)	0	100 100
All	All	854/901 (95%)	796 (93%)	56 (7%)	2 (0%)	47 78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	564	LEU
1	A	329	VAL

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	644/671 (96%)	626 (97%)	18 (3%)	43 71
2	B	124/127 (98%)	120 (97%)	4 (3%)	39 68
All	All	768/798 (96%)	746 (97%)	22 (3%)	42 70

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	200	ARG
1	A	224	LYS
1	A	289	GLU
1	A	291	ARG
1	A	296	ASP
1	A	330	GLU
1	A	389	TYR
1	A	442	ASN
1	A	475	PHE
1	A	533	LEU
1	A	586	GLN
1	A	613	CYS
1	A	624	ASN
1	A	647	MET
1	A	656	TRP
1	A	701	LYS
1	A	703	ARG
1	A	734	PHE
2	B	16	PHE
2	B	18	LEU
2	B	81	SER
2	B	95	ASP

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

Mol	Chain	Res	Type
1	A	408	ASN
1	A	573	GLN
1	A	589	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	SO4	A	800	-	4,4,4	0.34	0	6,6,6	0.17	0

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	800	SO4	1	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	721/752 (95%)	-0.15	3 (0%) 92 86	12, 32, 58, 85	0
2	B	145/149 (97%)	0.56	10 (6%) 16 7	42, 70, 99, 117	0
All	All	866/901 (96%)	-0.03	13 (1%) 73 56	12, 35, 86, 117	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	563	ASN	4.2
2	B	3	GLN	4.1
2	B	73	ALA	3.2
2	B	1	ALA	3.1
2	B	7	GLU	2.8
2	B	57	ALA	2.8
2	B	62	THR	2.7
2	B	5	THR	2.6
2	B	20	ASP	2.6
2	B	50	ASP	2.5
2	B	22	ASP	2.3
1	A	297	GLU	2.3
1	A	656	TRP	2.3

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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. 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	B-factors(Å^2)	Q<0.9
3	SO4	A	800	5/5	0.97	0.14	20,21,24,27	0

6.5 Other polymers

There are no such residues in this entry.