Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 10:08 AM GMT

PDB ID	:	3L0M
Title	:	Crystal structure of Rab1-activation domain and P4M domain of SidM/DrrA from legionella
Authors	:	Zhu, Y.; Shao, F.
Deposited on	:	2009-12-10
Resolution	:	3.45 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:

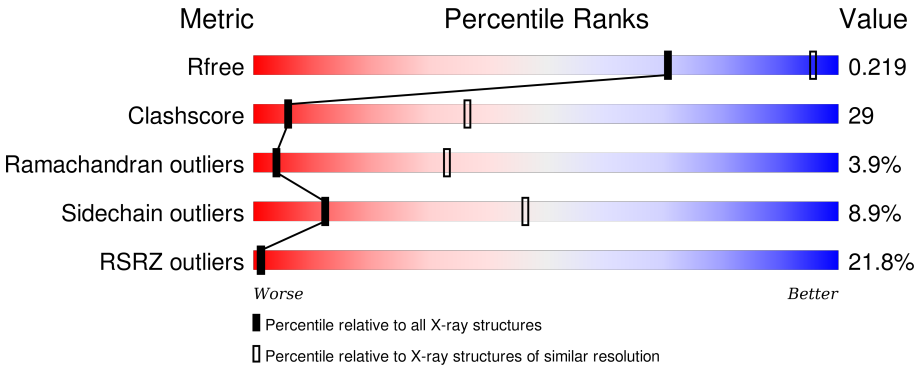
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.45 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	1000 (3.56-3.36)
Clashscore	102246	1090 (3.56-3.36)
Ramachandran outliers	100387	1057 (3.56-3.36)
Sidechain outliers	100360	1058 (3.56-3.36)
RSRZ outliers	91569	1005 (3.56-3.36)

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	336	18% 49% 42% 6%
1	B	336	22% 49% 40% 7%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 5119 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.

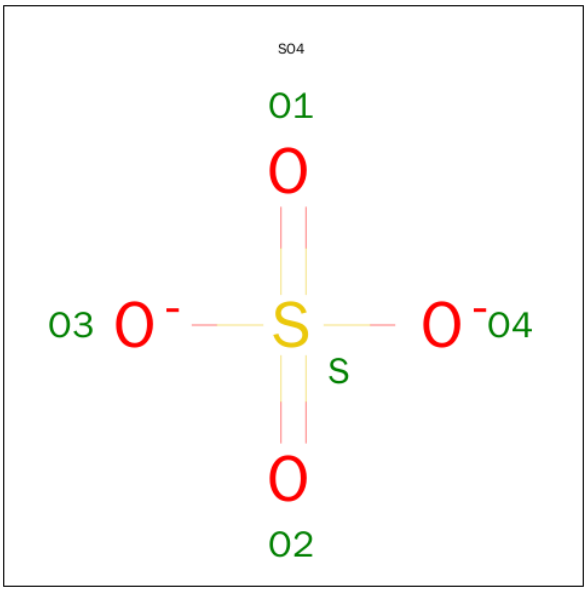
- Molecule 1 is a protein called DrrA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	328	Total	C	N	O	S	Se	0	0	0
			2578	1613	441	512	1	11			
1	B	323	Total	C	N	O	S	Se	0	0	0
			2531	1584	433	502	1	11			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	312	GLY	-	EXPRESSION TAG	UNP Q29ST3
A	313	PRO	-	EXPRESSION TAG	UNP Q29ST3
A	314	LEU	-	EXPRESSION TAG	UNP Q29ST3
A	315	GLY	-	EXPRESSION TAG	UNP Q29ST3
A	316	SER	-	EXPRESSION TAG	UNP Q29ST3
B	312	GLY	-	EXPRESSION TAG	UNP Q29ST3
B	313	PRO	-	EXPRESSION TAG	UNP Q29ST3
B	314	LEU	-	EXPRESSION TAG	UNP Q29ST3
B	315	GLY	-	EXPRESSION TAG	UNP Q29ST3
B	316	SER	-	EXPRESSION TAG	UNP Q29ST3

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



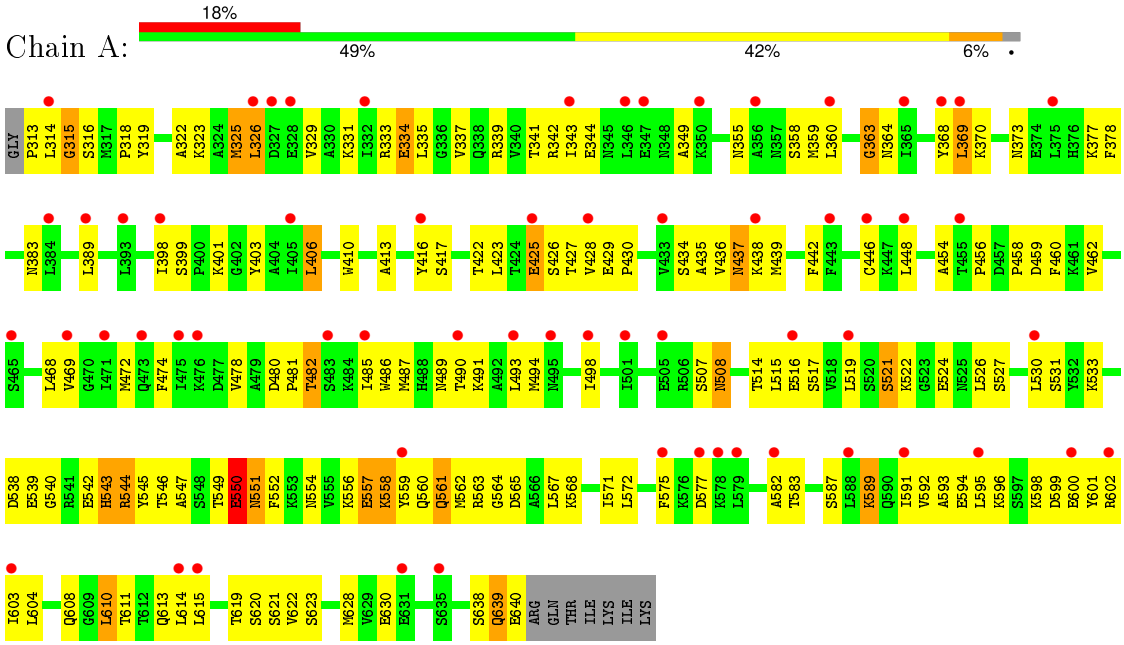
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0

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.

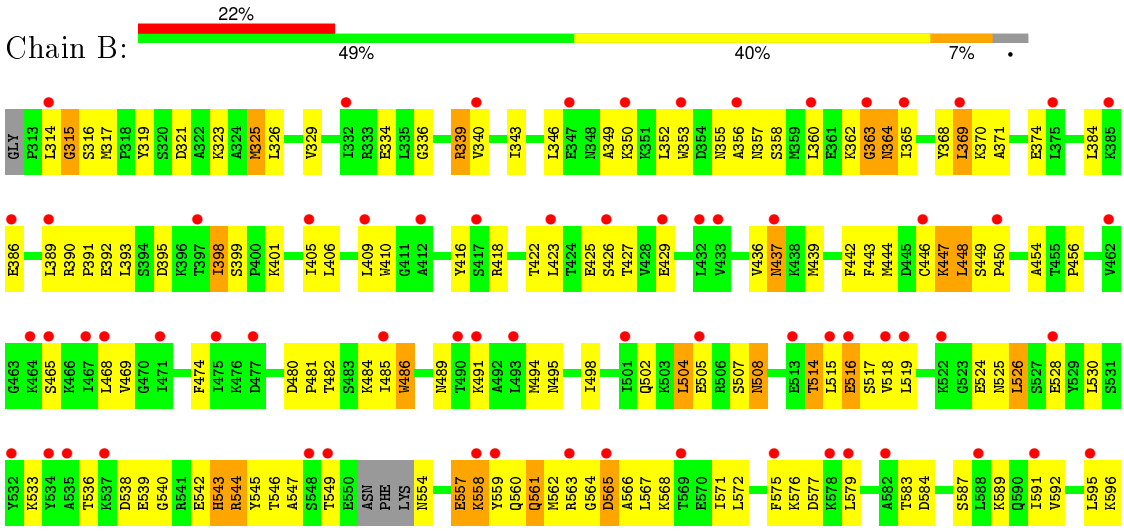
- Molecule 1: DrrA

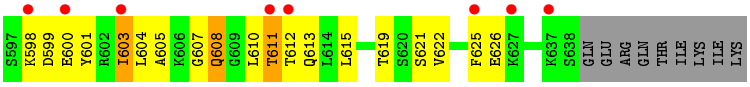
Chain A:



- Molecule 1: DrrA

Chain B:




S597
K598
D599
E600
Y601
R602
I603
L604
A605
K606
G607
Q608
G609
L610
T611
T612
Q613
L614
L615
T619
S620
S621
V622
F625
E626
K627
K637
S638
GLN
GLU
ARG
GLN
THR
ILE
LYS
ILE
LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α, β, γ	144.34Å 144.34Å 102.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.45 19.83 – 3.45	Depositor EDS
% Data completeness (in resolution range)	98.8 (20.00-3.45) 98.8 (19.83-3.45)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.02 (at 3.44Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.214 , 0.241 0.217 , 0.219	Depositor DCC
R_{free} test set	2728 reflections (11.07%)	DCC
Wilson B-factor (Å^2)	127.1	Xtriage
Anisotropy	0.567	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 105.7	EDS
Estimated twinning fraction	0.117 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Outliers	0 of 27365 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5119	wwPDB-VP
Average B, all atoms (Å^2)	145.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.74% 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: 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	0.37	0/2603	0.68	4/3476 (0.1%)
1	B	0.35	0/2554	0.64	3/3410 (0.1%)
All	All	0.37	0/5157	0.66	7/6886 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	437	ASN	CB-CA-C	6.02	122.44	110.40
1	A	521	SER	N-CA-C	5.47	125.78	111.00
1	A	521	SER	N-CA-CB	-5.22	102.67	110.50
1	B	363	GLY	N-CA-C	5.21	126.13	113.10
1	B	448	LEU	CA-CB-CG	5.17	127.19	115.30
1	A	363	GLY	N-CA-C	5.14	125.96	113.10
1	A	448	LEU	CA-CB-CG	5.10	127.04	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	2578	0	2609	138	0
1	B	2531	0	2563	160	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	5	0	0	1	0
2	B	5	0	0	0	0
All	All	5119	0	5172	294	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 29.

All (294) 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:544:ARG:HD2	1:B:610:LEU:HG	1.31	1.10
1:A:526:LEU:HD13	1:A:530:LEU:HD11	1.49	0.93
1:A:539:GLU:HG3	1:A:540:GLY:H	1.35	0.91
1:B:468:LEU:HD13	1:B:519:LEU:HD21	1.56	0.86
1:B:604:LEU:HD22	1:B:621:SER:HB3	1.58	0.85
1:A:572:LEU:HG	1:A:628:MSE:HE1	1.60	0.84
1:A:568:LYS:HD2	1:A:608:GLN:HE21	1.41	0.84
1:A:468:LEU:HD13	1:A:519:LEU:HD21	1.60	0.83
1:A:568:LYS:HD2	1:A:608:GLN:NE2	1.94	0.82
1:A:562:MSE:O	1:A:567:LEU:HD12	1.81	0.80
1:B:339:ARG:HG2	1:B:339:ARG:HH11	1.45	0.80
1:B:399:SER:C	1:B:401:LYS:H	1.87	0.78
1:A:561:GLN:HE21	1:A:561:GLN:H	1.31	0.77
1:A:559:TYR:HA	1:A:562:MSE:HG3	1.66	0.76
1:B:339:ARG:HE	1:B:343:ILE:HD11	1.50	0.76
1:A:544:ARG:HD2	1:A:610:LEU:HG	1.68	0.76
1:B:339:ARG:HD3	1:B:339:ARG:O	1.85	0.76
1:B:369:LEU:HD21	1:B:409:LEU:HD11	1.67	0.76
1:A:587:SER:O	1:A:591:ILE:HG13	1.85	0.76
1:A:596:LYS:HD3	1:A:601:TYR:CE2	2.22	0.74
1:A:333:ARG:O	1:A:337:VAL:HG13	1.87	0.74
1:B:465:SER:O	1:B:469:VAL:HG23	1.85	0.74
1:A:526:LEU:CD1	1:A:530:LEU:HD11	2.18	0.74
1:A:604:LEU:O	1:A:619:THR:HG21	1.87	0.73
1:A:429:GLU:HB2	1:A:485:ILE:HD13	1.70	0.73
1:A:425:GLU:HG3	1:A:522:LYS:NZ	2.03	0.73
1:B:422:THR:HG22	1:B:423:LEU:H	1.53	0.73
1:A:539:GLU:HG3	1:A:540:GLY:N	2.03	0.72
1:B:369:LEU:HD13	1:B:439:MSE:HE3	1.71	0.72
1:A:547:ALA:HB3	1:A:564:GLY:HA2	1.72	0.72
1:A:560:GLN:C	1:A:562:MSE:H	1.94	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:439:MSE:HE1	1:B:474:PHE:CZ	2.25	0.70
1:B:439:MSE:HE1	1:B:474:PHE:CE2	2.27	0.69
1:B:544:ARG:HD2	1:B:610:LEU:CG	2.17	0.69
1:A:494:MSE:O	1:A:498:ILE:HG13	1.92	0.69
1:B:567:LEU:HD23	1:B:567:LEU:C	2.14	0.69
1:A:589:LYS:O	1:A:592:VAL:HG12	1.93	0.68
1:B:409:LEU:HD23	1:B:409:LEU:O	1.94	0.68
1:B:494:MSE:O	1:B:498:ILE:HG13	1.93	0.68
1:B:315:GLY:O	1:B:316:SER:HB3	1.93	0.68
1:B:530:LEU:HD12	1:B:530:LEU:H	1.58	0.68
1:B:526:LEU:HD13	1:B:530:LEU:HD11	1.75	0.67
1:A:604:LEU:HD22	1:A:621:SER:HB3	1.78	0.66
1:B:604:LEU:O	1:B:619:THR:HG21	1.95	0.66
1:A:426:SER:O	1:B:418:ARG:NH1	2.28	0.66
1:A:416:TYR:CD1	1:A:519:LEU:HD22	2.31	0.66
1:B:544:ARG:HG2	1:B:545:TYR:CD2	2.29	0.66
1:B:557:GLU:O	1:B:560:GLN:HG2	1.97	0.65
1:B:339:ARG:NE	1:B:343:ILE:HD11	2.12	0.65
1:B:568:LYS:HD2	1:B:608:GLN:NE2	2.13	0.64
1:A:619:THR:HG23	1:A:622:VAL:H	1.61	0.64
1:B:336:GLY:O	1:B:340:VAL:HG23	1.98	0.64
1:B:571:ILE:HD12	1:B:603:ILE:HG21	1.80	0.64
1:B:325:MSE:O	1:B:329:VAL:HG23	1.97	0.64
1:B:399:SER:C	1:B:401:LYS:N	2.51	0.64
1:A:539:GLU:CG	1:A:540:GLY:H	2.08	0.64
1:B:469:VAL:HG13	1:B:498:ILE:HG23	1.80	0.64
1:B:369:LEU:HD11	1:B:436:VAL:HG13	1.81	0.63
1:A:549:THR:HG21	1:A:560:GLN:HA	1.81	0.62
1:A:544:ARG:CD	1:A:610:LEU:HG	2.28	0.62
1:A:369:LEU:HD11	1:A:436:VAL:HG13	1.80	0.62
1:B:543:HIS:CD2	1:B:546:THR:H	2.18	0.62
1:A:425:GLU:HG3	1:A:522:LYS:HZ2	1.65	0.62
1:A:560:GLN:HA	1:A:560:GLN:NE2	2.15	0.61
1:B:549:THR:HG21	1:B:560:GLN:HA	1.83	0.61
1:B:571:ILE:CD1	1:B:603:ILE:HG21	2.31	0.61
1:B:530:LEU:N	1:B:530:LEU:HD12	2.15	0.60
1:B:554:ASN:HB2	1:B:599:ASP:OD2	2.00	0.60
1:A:639:GLN:HE21	1:A:639:GLN:HA	1.66	0.60
1:B:568:LYS:HD2	1:B:608:GLN:HE21	1.67	0.60
1:B:339:ARG:HG2	1:B:339:ARG:NH1	2.10	0.60
1:B:357:ASN:OD1	1:B:398:ILE:HG23	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:582:ALA:HB2	1:A:591:ILE:HD12	1.85	0.59
1:B:389:LEU:O	1:B:389:LEU:HG	2.03	0.58
1:B:544:ARG:HG2	1:B:545:TYR:CE2	2.39	0.58
1:B:525:ASN:OD1	1:B:528:GLU:HB3	2.03	0.58
1:B:406:LEU:HD23	1:B:444:MSE:SE	2.54	0.57
1:A:561:GLN:HE21	1:A:561:GLN:N	2.02	0.57
1:B:595:LEU:O	1:B:598:LYS:HB2	2.05	0.57
1:B:544:ARG:NH1	1:B:544:ARG:HB2	2.20	0.57
1:B:605:ALA:HA	1:B:619:THR:HG21	1.85	0.57
1:B:575:PHE:CD1	1:B:595:LEU:HD13	2.39	0.57
1:B:622:VAL:O	1:B:626:GLU:HG3	2.04	0.56
1:B:543:HIS:CG	1:B:544:ARG:N	2.71	0.56
1:B:314:LEU:HD12	1:B:317:MSE:SE	2.55	0.56
1:B:349:ALA:HB3	1:B:389:LEU:HD13	1.87	0.56
1:A:456:PRO:O	1:A:458:PRO:HD3	2.05	0.56
1:A:568:LYS:CE	1:A:604:LEU:HA	2.36	0.56
1:A:560:GLN:HA	1:A:560:GLN:HE21	1.71	0.56
1:A:521:SER:O	1:A:522:LYS:HD3	2.07	0.55
1:A:326:LEU:HD22	1:B:611:THR:HG23	1.89	0.55
1:A:514:THR:O	1:A:517:SER:HB3	2.07	0.55
1:A:544:ARG:HG2	1:A:545:TYR:CD2	2.42	0.55
1:B:584:ASP:OD1	1:B:587:SER:HB2	2.06	0.55
1:B:346:LEU:HD23	1:B:384:LEU:HD13	1.88	0.55
1:A:561:GLN:NE2	1:A:561:GLN:H	2.02	0.55
1:B:562:MSE:HE2	1:B:562:MSE:HA	1.89	0.55
1:B:489:ASN:HB2	1:B:577:ASP:OD2	2.06	0.55
1:A:325:MSE:HG2	1:A:325:MSE:O	2.07	0.55
1:A:373:ASN:ND2	1:A:377:LYS:HE2	2.21	0.55
1:B:568:LYS:CE	1:B:604:LEU:HA	2.37	0.54
1:B:393:LEU:HD12	1:B:446:CYS:O	2.07	0.54
1:A:507:SER:O	1:A:508:ASN:C	2.45	0.54
1:A:575:PHE:CE1	1:A:595:LEU:HD22	2.43	0.54
1:B:568:LYS:O	1:B:572:LEU:HB2	2.08	0.54
1:A:557:GLU:HG3	1:A:558:LYS:H	1.72	0.54
1:A:560:GLN:C	1:A:562:MSE:N	2.61	0.54
1:B:422:THR:HG22	1:B:423:LEU:N	2.23	0.54
1:A:568:LYS:O	1:A:572:LEU:HB2	2.08	0.53
1:A:600:GLU:HA	1:A:603:ILE:HD12	1.90	0.53
1:A:550:GLU:C	1:A:552:PHE:H	2.11	0.53
1:B:613:GLN:C	1:B:615:LEU:H	2.10	0.53
1:B:539:GLU:HG3	1:B:540:GLY:N	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:557:GLU:HG3	1:B:558:LYS:H	1.73	0.53
1:A:315:GLY:O	1:A:316:SER:HB3	2.08	0.53
1:B:454:ALA:O	1:B:456:PRO:HD3	2.09	0.53
1:B:560:GLN:C	1:B:562:MSE:H	2.11	0.53
1:B:365:ILE:HD11	1:B:405:ILE:CG2	2.39	0.53
1:B:416:TYR:CD1	1:B:416:TYR:O	2.63	0.52
1:A:322:ALA:O	1:A:326:LEU:HB2	2.09	0.52
1:A:410:TRP:HD1	1:A:437:ASN:HD21	1.58	0.51
1:B:504:LEU:CD1	1:B:514:THR:HB	2.41	0.51
1:A:571:ILE:HD13	1:A:600:GLU:HB2	1.92	0.51
1:B:410:TRP:CD1	1:B:437:ASN:OD1	2.63	0.51
1:A:429:GLU:HB3	1:A:430:PRO:HD3	1.91	0.51
1:B:369:LEU:CD1	1:B:439:MSE:HE3	2.38	0.51
1:A:638:SER:C	1:A:640:GLU:N	2.63	0.51
1:B:362:LYS:O	1:B:364:ASN:N	2.43	0.51
1:B:547:ALA:HB3	1:B:564:GLY:HA2	1.91	0.51
1:A:610:LEU:HD22	1:A:614:LEU:HD11	1.92	0.51
1:B:319:TYR:CE2	1:B:323:LYS:HD2	2.46	0.51
1:A:398:ILE:HB	1:A:403:TYR:CE2	2.45	0.51
1:B:465:SER:HB2	1:B:505:GLU:OE1	2.11	0.51
1:A:638:SER:C	1:A:640:GLU:H	2.14	0.51
1:B:356:ALA:HB3	1:B:443:PHE:CE2	2.46	0.50
1:A:572:LEU:HG	1:A:628:MSE:CE	2.36	0.50
1:A:557:GLU:O	1:A:559:TYR:N	2.44	0.50
1:B:447:LYS:HD3	1:B:447:LYS:C	2.32	0.50
1:A:539:GLU:CG	1:A:540:GLY:N	2.71	0.50
1:B:546:THR:CG2	1:B:547:ALA:N	2.74	0.50
1:B:561:GLN:NE2	1:B:561:GLN:H	2.10	0.50
1:A:469:VAL:HG13	1:A:498:ILE:HG23	1.94	0.49
1:A:435:ALA:HB1	1:B:423:LEU:HG	1.93	0.49
1:B:486:TRP:CZ3	1:B:524:GLU:HA	2.46	0.49
1:B:539:GLU:HG3	1:B:540:GLY:H	1.77	0.49
1:B:399:SER:O	1:B:401:LYS:N	2.46	0.49
1:B:314:LEU:O	1:B:315:GLY:O	2.31	0.49
1:B:429:GLU:HG3	1:B:485:ILE:HD13	1.94	0.49
1:B:334:GLU:C	1:B:336:GLY:N	2.65	0.49
1:A:334:GLU:HG2	1:A:335:LEU:N	2.28	0.49
1:B:410:TRP:HD1	1:B:437:ASN:OD1	1.95	0.49
1:B:334:GLU:C	1:B:336:GLY:H	2.16	0.48
1:A:550:GLU:OE2	1:A:551:ASN:HB2	2.13	0.48
1:A:480:ASP:OD2	1:A:481:PRO:N	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:605:ALA:HA	1:B:619:THR:CG2	2.43	0.48
1:B:436:VAL:O	1:B:437:ASN:C	2.50	0.48
1:A:478:VAL:HG21	1:B:423:LEU:HD22	1.94	0.48
1:B:449:SER:HB2	1:B:450:PRO:HD2	1.96	0.48
1:B:371:ALA:O	1:B:374:GLU:HB2	2.13	0.48
1:A:599:ASP:O	1:A:603:ILE:HG13	2.14	0.48
1:B:596:LYS:HD3	1:B:601:TYR:CE2	2.48	0.48
1:A:600:GLU:HA	1:A:603:ILE:CD1	2.44	0.48
1:B:353:TRP:CE3	1:B:353:TRP:O	2.67	0.48
1:B:390:ARG:HB3	1:B:391:PRO:HD3	1.96	0.48
1:A:355:ASN:O	1:A:358:SER:HB3	2.13	0.48
1:B:561:GLN:HE21	1:B:561:GLN:H	1.61	0.47
1:B:564:GLY:O	1:B:567:LEU:HB3	2.14	0.47
1:A:567:LEU:O	1:A:567:LEU:HD23	2.13	0.47
1:A:552:PHE:CE2	1:A:602:ARG:NH1	2.82	0.47
1:A:568:LYS:HE2	1:A:604:LEU:HA	1.96	0.47
1:B:575:PHE:O	1:B:579:LEU:HB2	2.14	0.47
1:B:543:HIS:HD2	1:B:546:THR:H	1.59	0.47
1:A:489:ASN:OD1	1:A:491:LYS:HB2	2.15	0.47
1:B:355:ASN:O	1:B:358:SER:HB3	2.14	0.47
1:B:567:LEU:C	1:B:567:LEU:CD2	2.83	0.46
1:A:575:PHE:CD1	1:A:595:LEU:HD13	2.51	0.46
1:A:349:ALA:HB2	1:A:378:PHE:HE2	1.79	0.46
1:B:567:LEU:HD21	1:B:571:ILE:CD1	2.45	0.46
1:A:416:TYR:CZ	1:A:472:MSE:HE3	2.50	0.46
1:B:560:GLN:NE2	1:B:560:GLN:HA	2.31	0.46
1:A:442:PHE:CD1	1:A:442:PHE:C	2.89	0.46
1:A:515:LEU:C	1:A:517:SER:H	2.18	0.46
1:A:575:PHE:CZ	1:A:595:LEU:HD22	2.50	0.46
1:A:546:THR:CG2	1:A:547:ALA:N	2.79	0.46
1:B:543:HIS:CD2	1:B:544:ARG:N	2.84	0.46
1:A:339:ARG:O	1:A:343:ILE:HG13	2.16	0.46
1:A:413:ALA:O	1:A:417:SER:HB2	2.16	0.45
1:A:561:GLN:NE2	1:A:561:GLN:N	2.61	0.45
1:B:447:LYS:HD3	1:B:447:LYS:O	2.16	0.45
1:A:515:LEU:C	1:A:517:SER:N	2.68	0.45
1:B:350:LYS:HE2	1:B:392:GLU:O	2.17	0.45
1:A:460:PHE:CE2	1:A:462:VAL:HG22	2.51	0.45
1:B:339:ARG:HD3	1:B:339:ARG:C	2.36	0.45
1:A:425:GLU:HG3	1:A:522:LYS:HZ3	1.78	0.45
1:A:486:TRP:CG	1:A:487:MSE:N	2.83	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:561:GLN:N	1:B:561:GLN:NE2	2.65	0.45
1:B:448:LEU:HD13	1:B:449:SER:O	2.14	0.45
1:A:542:GLU:OE2	1:A:542:GLU:HA	2.16	0.45
1:A:369:LEU:HD12	1:A:474:PHE:CD2	2.52	0.45
1:B:536:THR:O	1:B:566:ALA:HA	2.17	0.45
1:B:502:GLN:O	1:B:505:GLU:N	2.50	0.45
1:A:315:GLY:O	1:A:316:SER:CB	2.64	0.45
1:A:460:PHE:HE2	1:A:462:VAL:HG22	1.81	0.45
1:A:567:LEU:HD23	1:A:571:ILE:HG13	1.99	0.45
1:A:326:LEU:O	1:A:329:VAL:HG12	2.17	0.44
1:A:594:GLU:O	1:A:598:LYS:HD2	2.17	0.44
1:B:468:LEU:CD1	1:B:519:LEU:HD21	2.37	0.44
1:B:575:PHE:HD1	1:B:625:PHE:CE1	2.36	0.44
1:A:434:SER:O	1:A:435:ALA:C	2.55	0.44
1:B:416:TYR:CD1	1:B:519:LEU:HD22	2.52	0.44
1:B:515:LEU:O	1:B:517:SER:N	2.51	0.44
1:A:613:GLN:C	1:A:615:LEU:H	2.21	0.44
1:A:619:THR:CG2	1:A:622:VAL:HG23	2.47	0.44
1:A:601:TYR:CD1	1:A:601:TYR:C	2.90	0.44
1:B:544:ARG:HH11	1:B:544:ARG:HB2	1.83	0.44
1:B:514:THR:O	1:B:518:VAL:HG23	2.18	0.44
1:B:362:LYS:HG3	1:B:362:LYS:O	2.17	0.44
1:A:493:LEU:HG	1:A:493:LEU:O	2.17	0.44
1:A:521:SER:C	1:A:522:LYS:HD3	2.38	0.43
1:B:515:LEU:C	1:B:517:SER:N	2.71	0.43
1:B:480:ASP:C	1:B:482:THR:H	2.21	0.43
1:B:360:LEU:HB2	1:B:368:TYR:CD1	2.53	0.43
1:B:349:ALA:CB	1:B:389:LEU:HD13	2.48	0.43
1:A:480:ASP:C	1:A:482:THR:H	2.21	0.43
1:B:393:LEU:C	1:B:395:ASP:H	2.22	0.43
1:A:370:LYS:NZ	1:A:373:ASN:HD22	2.17	0.43
1:B:346:LEU:CD2	1:B:384:LEU:HD13	2.48	0.43
1:B:489:ASN:OD1	1:B:491:LYS:HB2	2.17	0.43
1:A:422:THR:HG22	1:A:423:LEU:N	2.33	0.43
1:A:530:LEU:HD12	1:A:530:LEU:N	2.33	0.43
1:B:416:TYR:OH	1:B:494:MSE:HE1	2.17	0.43
1:A:360:LEU:HD21	1:A:406:LEU:HD13	2.00	0.43
1:A:526:LEU:O	1:A:527:SER:C	2.57	0.43
1:B:587:SER:O	1:B:591:ILE:HG13	2.18	0.43
1:B:543:HIS:CG	1:B:546:THR:OG1	2.72	0.43
1:B:539:GLU:CG	1:B:540:GLY:H	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:314:LEU:O	1:B:315:GLY:C	2.56	0.43
1:B:317:MSE:HE2	1:B:321:ASP:HB3	2.01	0.42
1:B:539:GLU:CG	1:B:540:GLY:N	2.82	0.42
1:B:406:LEU:HD21	1:B:444:MSE:HB2	2.01	0.42
1:B:352:LEU:O	1:B:355:ASN:HB2	2.19	0.42
1:B:576:LYS:HD2	1:B:576:LYS:O	2.19	0.42
1:B:562:MSE:O	1:B:567:LEU:HD12	2.20	0.42
1:B:575:PHE:O	1:B:579:LEU:CB	2.68	0.42
1:A:480:ASP:OD2	1:A:481:PRO:HD2	2.20	0.42
1:B:480:ASP:OD2	1:B:481:PRO:N	2.53	0.42
1:A:349:ALA:HB2	1:A:378:PHE:CE2	2.54	0.42
1:A:341:THR:HA	1:A:344:GLU:HB2	2.02	0.42
1:A:313:PRO:HB2	1:A:314:LEU:H	1.53	0.42
1:B:571:ILE:HG21	1:B:600:GLU:O	2.20	0.42
1:A:543:HIS:CG	1:A:544:ARG:N	2.86	0.42
1:A:437:ASN:C	1:A:437:ASN:HD22	2.22	0.42
1:B:436:VAL:HA	1:B:439:MSE:HE2	2.01	0.42
1:B:386:GLU:HG3	1:B:442:PHE:CE2	2.55	0.42
1:B:546:THR:HG23	1:B:564:GLY:CA	2.50	0.41
1:A:530:LEU:O	1:A:531:SER:HB2	2.20	0.41
1:B:355:ASN:HA	1:B:355:ASN:HD22	1.62	0.41
1:A:572:LEU:HD12	1:A:572:LEU:HA	1.88	0.41
1:A:326:LEU:C	1:A:329:VAL:HG12	2.40	0.41
1:B:326:LEU:O	1:B:329:VAL:HB	2.20	0.41
1:A:567:LEU:HD21	1:A:571:ILE:HD11	2.02	0.41
1:B:557:GLU:O	1:B:559:TYR:N	2.53	0.41
1:B:484:LYS:HB3	1:B:484:LYS:HE2	1.86	0.41
1:A:630:GLU:HA	1:A:630:GLU:OE2	2.20	0.41
1:A:389:LEU:HD23	1:A:446:CYS:HB3	2.02	0.41
1:B:486:TRP:HZ3	1:B:524:GLU:HA	1.85	0.41
1:B:370:LYS:HD2	1:B:370:LYS:HA	1.93	0.41
1:B:507:SER:O	1:B:508:ASN:C	2.58	0.41
1:A:399:SER:C	1:A:401:LYS:N	2.74	0.41
1:B:560:GLN:HB2	1:B:561:GLN:NE2	2.36	0.41
1:B:544:ARG:HG3	1:B:544:ARG:O	2.21	0.41
1:A:619:THR:OG1	2:A:1:SO4:S	2.79	0.41
1:A:568:LYS:HE2	1:A:604:LEU:HD23	2.03	0.41
1:A:425:GLU:O	1:A:425:GLU:HG3	2.19	0.41
1:A:620:SER:O	1:A:623:SER:HB3	2.20	0.41
1:A:427:THR:OG1	1:A:428:VAL:N	2.54	0.41
1:B:549:THR:HG21	1:B:560:GLN:CA	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:389:LEU:HD23	1:B:446:CYS:HB3	2.02	0.41
1:A:489:ASN:O	1:A:490:THR:C	2.60	0.41
1:A:359:MSE:HB2	1:A:368:TYR:HA	2.03	0.41
1:B:603:ILE:HG22	1:B:604:LEU:N	2.36	0.40
1:A:468:LEU:HA	1:A:468:LEU:HD23	1.93	0.40
1:A:592:VAL:HG13	1:A:593:ALA:N	2.36	0.40
1:B:365:ILE:HD11	1:B:405:ILE:HG23	2.04	0.40
1:B:592:VAL:O	1:B:596:LYS:HG2	2.21	0.40
1:A:319:TYR:CZ	1:A:323:LYS:HE2	2.56	0.40
1:A:438:LYS:HE2	1:A:438:LYS:HB3	1.89	0.40
1:A:554:ASN:HB2	1:A:599:ASP:OD2	2.21	0.40
1:B:422:THR:O	1:B:426:SER:HB3	2.21	0.40
1:A:546:THR:HG23	1:A:564:GLY:HA3	2.02	0.40
1:A:454:ALA:O	1:A:456:PRO:HD3	2.22	0.40
1:B:369:LEU:HD11	1:B:436:VAL:CG1	2.50	0.40
1:A:425:GLU:CG	1:A:522:LYS:HZ3	2.35	0.40
1:B:364:ASN:C	1:B:364:ASN:HD22	2.24	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	326/336 (97%)	272 (83%)	42 (13%)	12 (4%)	4 35
1	B	319/336 (95%)	263 (82%)	43 (14%)	13 (4%)	3 32
All	All	645/672 (96%)	535 (83%)	85 (13%)	25 (4%)	4 33

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	363	GLY

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Mol	Chain	Res	Type
1	A	544	ARG
1	A	550	GLU
1	A	557	GLU
1	A	558	LYS
1	B	363	GLY
1	B	544	ARG
1	B	557	GLU
1	B	558	LYS
1	A	315	GLY
1	A	508	ASN
1	B	315	GLY
1	B	533	LYS
1	B	565	ASP
1	B	508	ASN
1	B	543	HIS
1	A	533	LYS
1	B	542	GLU
1	A	543	HIS
1	A	610	LEU
1	B	486	TRP
1	B	516	GLU
1	A	556	LYS
1	B	607	GLY
1	A	318	PRO

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	284/281 (101%)	257 (90%)	27 (10%)	11	42
1	B	278/281 (99%)	255 (92%)	23 (8%)	14	49
All	All	562/562 (100%)	512 (91%)	50 (9%)	12	46

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	325	MSE
1	A	326	LEU
1	A	331	LYS
1	A	334	GLU
1	A	342	ARG
1	A	364	ASN
1	A	369	LEU
1	A	383	ASN
1	A	406	LEU
1	A	425	GLU
1	A	437	ASN
1	A	439	MSE
1	A	459	ASP
1	A	482	THR
1	A	516	GLU
1	A	524	GLU
1	A	538	ASP
1	A	550	GLU
1	A	551	ASN
1	A	561	GLN
1	A	563	ARG
1	A	565	ASP
1	A	577	ASP
1	A	583	THR
1	A	589	LYS
1	A	611	THR
1	A	639	GLN
1	B	325	MSE
1	B	339	ARG
1	B	364	ASN
1	B	369	LEU
1	B	398	ILE
1	B	425	GLU
1	B	427	THR
1	B	447	LYS
1	B	495	ASN
1	B	504	LEU
1	B	514	THR
1	B	516	GLU
1	B	526	LEU
1	B	538	ASP
1	B	561	GLN
1	B	563	ARG

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Mol	Chain	Res	Type
1	B	565	ASP
1	B	583	THR
1	B	589	LYS
1	B	603	ILE
1	B	608	GLN
1	B	611	THR
1	B	612	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	355	ASN
1	A	364	ASN
1	A	373	ASN
1	A	437	ASN
1	A	508	ASN
1	A	509	ASN
1	A	525	ASN
1	A	543	HIS
1	A	551	ASN
1	A	560	GLN
1	A	561	GLN
1	A	608	GLN
1	A	639	GLN
1	B	345	ASN
1	B	355	ASN
1	B	364	ASN
1	B	509	ASN
1	B	543	HIS
1	B	560	GLN
1	B	561	GLN
1	B	608	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 (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

2 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	SO4	A	1	-	4,4,4	0.23	0	6,6,6	0.23	0
2	SO4	B	2	-	4,4,4	0.15	0	6,6,6	0.12	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	SO4	A	1	-	-	0/0/0/0	0/0/0/0
2	SO4	B	2	-	-	0/0/0/0	0/0/0/0

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
2	A	1	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	317/336 (94%)	1.24	62 (19%) 1 2	69, 134, 189, 200	0
1	B	312/336 (92%)	1.26	75 (24%) 1 1	75, 151, 197, 200	0
All	All	629/672 (93%)	1.25	137 (21%) 1 1	69, 142, 193, 200	0

All (137) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	548	SER	8.2
1	B	559	TYR	6.0
1	B	603	ILE	5.3
1	B	365	ILE	3.9
1	B	363	GLY	3.8
1	B	516	GLU	3.7
1	A	332	ILE	3.7
1	B	491	LYS	3.6
1	B	501	ILE	3.6
1	B	595	LEU	3.5
1	B	588	LEU	3.5
1	A	600	GLU	3.4
1	B	579	LEU	3.4
1	B	360	LEU	3.3
1	B	340	VAL	3.3
1	B	600	GLU	3.3
1	A	328	GLU	3.2
1	B	405	ILE	3.2
1	B	464	LYS	3.1
1	B	582	ALA	3.1
1	B	437	ASN	3.1
1	A	505	GLU	3.0
1	B	591	ILE	3.0
1	A	614	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	365	ILE	3.0
1	A	314	LEU	3.0
1	A	631	GLU	3.0
1	A	360	LEU	2.9
1	B	475	ILE	2.9
1	A	476	LYS	2.9
1	A	350	LYS	2.9
1	A	375	LEU	2.9
1	A	603	ILE	2.8
1	A	346	LEU	2.8
1	B	485	ILE	2.8
1	B	353	TRP	2.8
1	A	615	LEU	2.7
1	A	485	ILE	2.7
1	B	575	PHE	2.7
1	B	611	THR	2.7
1	A	428	VAL	2.7
1	B	462	VAL	2.7
1	A	595	LEU	2.7
1	A	516	GLU	2.7
1	A	384	LEU	2.7
1	B	549	THR	2.7
1	A	465	SER	2.6
1	A	446	CYS	2.6
1	A	582	ALA	2.6
1	A	369	LEU	2.6
1	B	432	LEU	2.6
1	B	386	GLU	2.6
1	B	493	LEU	2.5
1	B	347	GLU	2.5
1	B	426	SER	2.5
1	A	393	LEU	2.5
1	A	498	ILE	2.5
1	B	513	GLU	2.5
1	B	423	LEU	2.5
1	B	563	ARG	2.5
1	B	409	LEU	2.5
1	A	443	PHE	2.5
1	B	446	CYS	2.5
1	B	505	GLU	2.4
1	B	375	LEU	2.4
1	B	578	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	356	ALA	2.4
1	A	416	TYR	2.4
1	A	425	GLU	2.4
1	A	575	PHE	2.4
1	A	578	LYS	2.4
1	A	495	ASN	2.4
1	B	412	ALA	2.4
1	A	475	ILE	2.4
1	B	637	LYS	2.3
1	A	519	LEU	2.3
1	A	591	ILE	2.3
1	A	579	LEU	2.3
1	B	532	TYR	2.3
1	B	350	LYS	2.3
1	B	490	THR	2.3
1	A	389	LEU	2.3
1	B	397	THR	2.3
1	A	635	SER	2.3
1	B	389	LEU	2.3
1	B	518	VAL	2.3
1	A	327	ASP	2.2
1	A	368	TYR	2.2
1	B	369	LEU	2.2
1	A	405	ILE	2.2
1	B	535	ALA	2.2
1	A	490	THR	2.2
1	B	625	PHE	2.2
1	B	558	LYS	2.2
1	B	468	LEU	2.2
1	A	493	LEU	2.2
1	A	448	LEU	2.2
1	B	569	THR	2.2
1	A	455	THR	2.2
1	A	588	LEU	2.2
1	B	515	LEU	2.2
1	B	471	ILE	2.2
1	B	612	THR	2.2
1	B	519	LEU	2.2
1	B	537	LYS	2.2
1	B	433	VAL	2.2
1	A	559	TYR	2.2
1	B	429	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	326	LEU	2.2
1	B	477	ASP	2.2
1	A	577	ASP	2.1
1	A	473	GLN	2.1
1	B	467	ILE	2.1
1	A	530	LEU	2.1
1	B	528	GLU	2.1
1	A	438	LYS	2.1
1	A	433	VAL	2.1
1	A	471	ILE	2.1
1	B	598	LYS	2.1
1	B	627	LYS	2.1
1	B	522	LYS	2.1
1	B	332	ILE	2.1
1	B	417	SER	2.1
1	B	465	SER	2.1
1	A	501	ILE	2.0
1	A	602	ARG	2.0
1	A	483	SER	2.0
1	B	314	LEU	2.0
1	B	534	TYR	2.0
1	A	347	GLU	2.0
1	A	469	VAL	2.0
1	A	356	ALA	2.0
1	A	398	ILE	2.0
1	B	385	LYS	2.0
1	B	450	PRO	2.0
1	B	565	ASP	2.0
1	A	343	ILE	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

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	SO4	A	1	5/5	0.92	0.26	-0.82	146,146,147,150	0
2	SO4	B	2	5/5	0.87	0.28	-0.89	193,195,197,202	0

6.5 Other polymers

There are no such residues in this entry.