



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 17, 2024 – 02:10 PM EDT

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](mailto: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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
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)	:	2.37.1

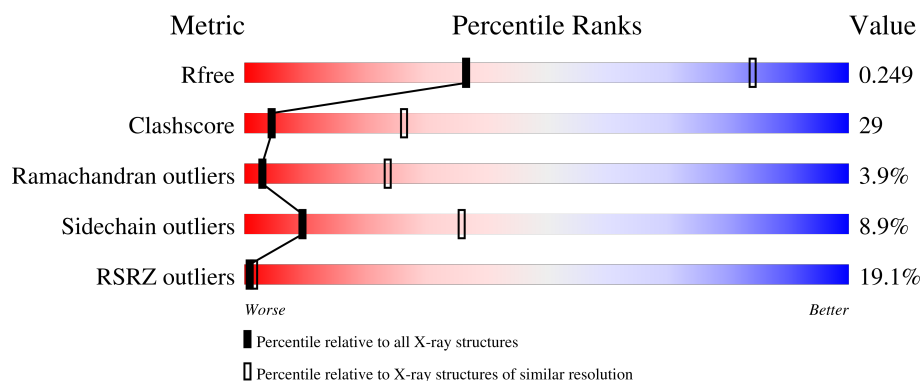
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.45 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))
$R_{free}$	130704	1291 (3.52-3.40)
Clashscore	141614	1372 (3.52-3.40)
Ramachandran outliers	138981	1337 (3.52-3.40)
Sidechain outliers	138945	1338 (3.52-3.40)
RSRZ outliers	127900	1205 (3.52-3.40)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . 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	<div> <div>16%</div> <div>49%</div> <div>42%</div> <div>6%</div> <div>.</div> </div>
1	B	336	<div> <div>20%</div> <div>49%</div> <div>40%</div> <div>7%</div> <div>.</div> </div>

## 2 Entry composition

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<sub>4</sub>S).

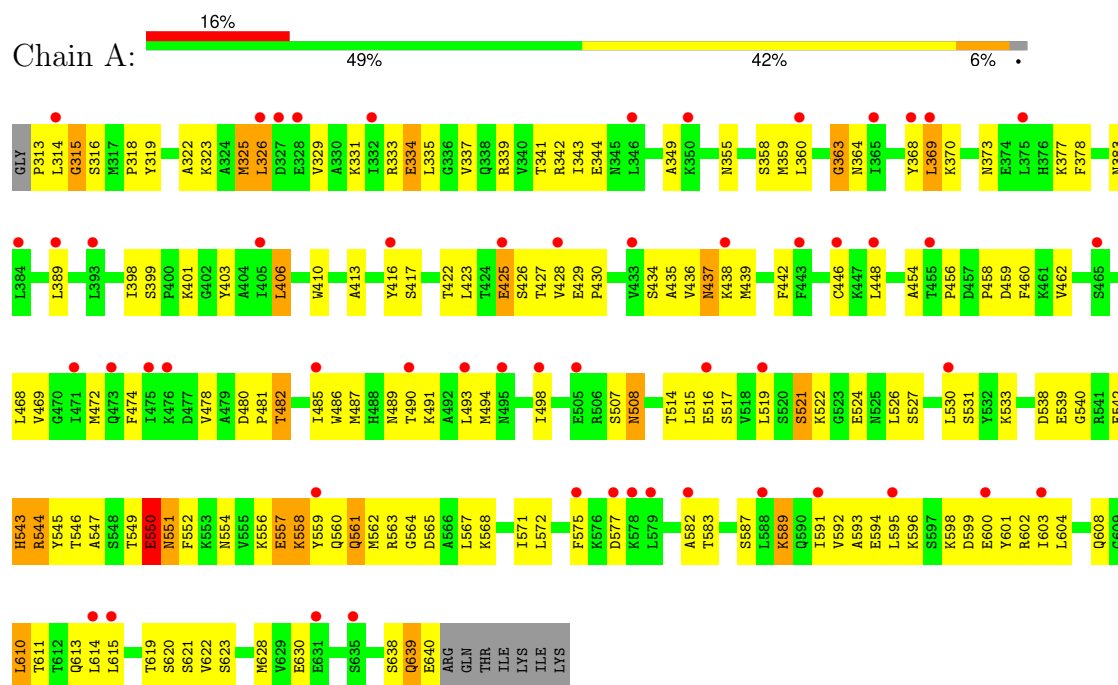


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

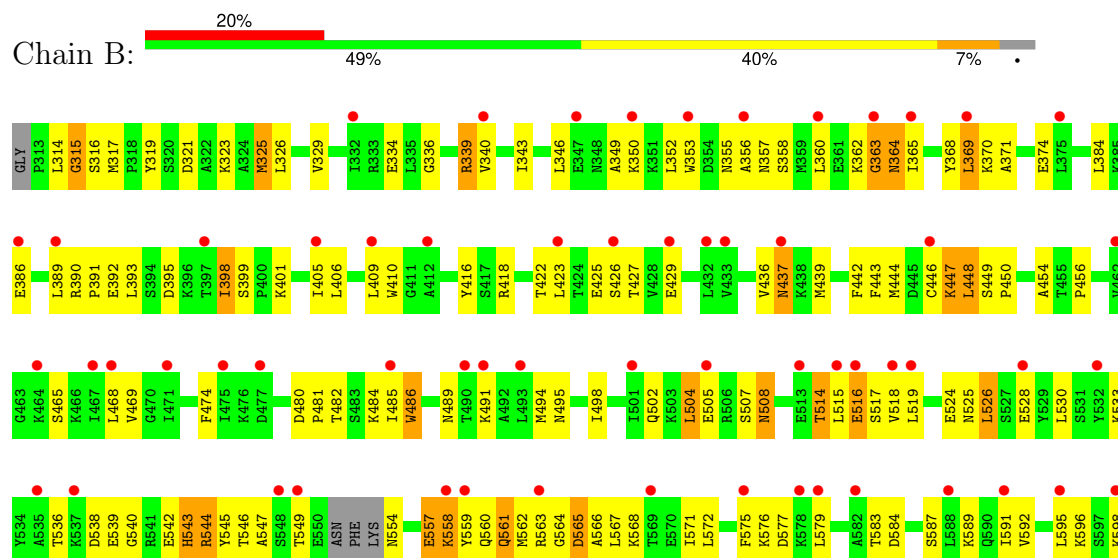
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: DrrA



#### • Molecule 1: DrrA



D599	E600	Y601	F602	T603	L604	A605	F606	Q608	G609	L610	T611	T612	Q613	L614	L615	T619	S620	S621	V622	F625	E626	F637	S638	GLN	GLU	ARG	GLN	THR	ILE	LYS	ILE	LYS

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.02 (at 3.44Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.214 , 0.241 0.229 , 0.249	Depositor DCC
$R_{free}$ test set	2728 reflections (9.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	127.1	Xtriage
Anisotropy	0.567	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 105.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.117 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5119	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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(°)	Ideal(°)
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 [i](#)

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:568:LYS:HD2	1:A:608:GLN:HE21	1.41	0.84
1:A:572:LEU:HG	1:A:628:MSE:HE1	1.60	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:H	1:A:561:GLN:HE21	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:O	1:B:339:ARG:HD3	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:429:GLU:HB2	1:A:485:ILE:HD13	1.70	0.73
1:A:604:LEU:O	1:A:619:THR:HG21	1.87	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:C	1:B:567:LEU:HD23	2.14	0.69
1:A:589:LYS:O	1:A:592:VAL:HG12	1.93	0.68
1:B:409:LEU:O	1:B:409:LEU:HD23	1.94	0.68
1:B:315:GLY:O	1:B:316:SER:HB3	1.93	0.68
1:B:494:MSE:O	1:B:498:ILE:HG13	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:A:426:SER:O	1:B:418:ARG:NH1	2.28	0.66
1:B:604:LEU:O	1:B:619:THR:HG21	1.95	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:325:MSE:O	1:B:329:VAL:HG23	1.97	0.64
1:B:571:ILE:HD12	1:B:603:ILE:HG21	1.80	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:544:ARG:CD	1:A:610:LEU:HG	2.28	0.62
1:A:549:THR:HG21	1:A:560:GLN:HA	1.81	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:HD12	1:B:530:LEU:N	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: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:B:543:HIS:CG	1:B:544:ARG:N	2.71	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: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:521:SER:O	1:A:522:LYS:HD3	2.07	0.55
1:A:544:ARG:HG2	1:A:545:TYR:CD2	2.42	0.55
1:B:346:LEU:HD23	1:B:384:LEU:HD13	1.88	0.55
1:B:584:ASP:OD1	1:B:587:SER:HB2	2.06	0.55
1:A:561:GLN:H	1:A:561:GLN:NE2	2.02	0.55
1:B:489:ASN:HB2	1:B:577:ASP:OD2	2.06	0.55
1:B:562:MSE:HE2	1:B:562:MSE:HA	1.89	0.55
1:A:325:MSE:O	1:A:325:MSE:HG2	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:A:557:GLU:HG3	1:A:558:LYS:H	1.72	0.54
1:B:568:LYS:O	1:B:572:LEU:HB2	2.08	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:A:315:GLY:O	1:A:316:SER:HB3	2.08	0.53
1:B:557:GLU:HG3	1:B:558:LYS:H	1.73	0.53
1:B:454:ALA:O	1:B:456:PRO:HD3	2.09	0.53
1:B:365:ILE:HD11	1:B:405:ILE:CG2	2.39	0.53
1:B:560:GLN:C	1:B:562:MSE:H	2.11	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:429:GLU:HB3	1:A:430:PRO:HD3	1.91	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: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:369:LEU:CD1	1:B:439:MSE:HE3	2.38	0.51
1:A:610:LEU:HD22	1:A:614:LEU:HD11	1.92	0.51
1:B:547:ALA:HB3	1:B:564:GLY:HA2	1.91	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:A:638:SER:C	1:A:640:GLU:H	2.14	0.51
1:B:465:SER:HB2	1:B:505:GLU:OE1	2.11	0.51
1:B:356:ALA:HB3	1:B:443:PHE:CE2	2.46	0.50
1:A:557:GLU:O	1:A:559:TYR:N	2.44	0.50
1:A:572:LEU:HG	1:A:628:MSE:CE	2.36	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:H	1:B:561:GLN:NE2	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:314:LEU:O	1:B:315:GLY:O	2.31	0.49
1:B:399:SER:O	1:B:401:LYS:N	2.46	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:A:550:GLU:OE2	1:A:551:ASN:HB2	2.13	0.48
1:B:334:GLU:C	1:B:336:GLY:H	2.16	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:A:478:VAL:HG21	1:B:423:LEU:HD22	1.94	0.48
1:B:436:VAL:O	1:B:437:ASN:C	2.50	0.48
1:B:449:SER:HB2	1:B:450:PRO:HD2	1.96	0.48
1:B:605:ALA:HA	1:B:619:THR:CG2	2.43	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:O	1:B:353:TRP:CE3	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:A:552:PHE:CE2	1:A:602:ARG:NH1	2.82	0.47
1:A:567:LEU:O	1:A:567:LEU:HD23	2.13	0.47
1:B:561:GLN:H	1:B:561:GLN:HE21	1.61	0.47
1:B:564:GLY:O	1:B:567:LEU:HB3	2.14	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:349:ALA:HB2	1:A:378:PHE:HE2	1.79	0.46
1:A:575:PHE:CD1	1:A:595:LEU:HD13	2.51	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:A:442:PHE:CD1	1:A:442:PHE:C	2.89	0.46
1:B:560:GLN:HA	1:B:560:GLN:NE2	2.31	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:A:339:ARG:O	1:A:343:ILE:HG13	2.16	0.46
1:B:543:HIS:CD2	1:B:544:ARG:N	2.84	0.46
1:A:413:ALA:O	1:A:417:SER:HB2	2.16	0.45
1:A:561:GLN:N	1:A:561:GLN:NE2	2.61	0.45
1:B:447:LYS:HD3	1:B:447:LYS:O	2.16	0.45
1:A:460:PHE:CE2	1:A:462:VAL:HG22	2.51	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: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
1:B:339:ARG:HD3	1:B:339:ARG:C	2.36	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:542:GLU:OE2	1:A:542:GLU:HA	2.16	0.45
1:B:448:LEU:HD13	1:B:449:SER:O	2.14	0.45
1:B:561:GLN:NE2	1:B:561:GLN:N	2.65	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: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:B:502:GLN:O	1:B:505:GLU:N	2.50	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:601:TYR:CD1	1:A:601:TYR:C	2.90	0.44
1:A:619:THR:CG2	1:A:622:VAL:HG23	2.47	0.44
1:B:362:LYS:O	1:B:362:LYS:HG3	2.17	0.44
1:B:514:THR:O	1:B:518:VAL:HG23	2.18	0.44
1:B:544:ARG:HB2	1:B:544:ARG:HH11	1.83	0.44
1:A:493:LEU:O	1:A:493:LEU:HG	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:360:LEU:HB2	1:B:368:TYR:CD1	2.53	0.43
1:B:480:ASP:C	1:B:482:THR:H	2.21	0.43
1:A:480:ASP:C	1:A:482:THR:H	2.21	0.43
1:B:349:ALA:CB	1:B:389:LEU:HD13	2.48	0.43
1:A:370:LYS:NZ	1:A:373:ASN:HD22	2.17	0.43
1:B:393:LEU:C	1:B:395:ASP:H	2.22	0.43
1:A:422:THR:HG22	1:A:423:LEU:N	2.33	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:530:LEU:N	1:A:530:LEU:HD12	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:539:GLU:CG	1:B:540:GLY:H	2.32	0.43
1:B:543:HIS:CG	1:B:546:THR:OG1	2.72	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:352:LEU:O	1:B:355:ASN:HB2	2.19	0.42
1:B:406:LEU:HD21	1:B:444:MSE:HB2	2.01	0.42
1:B:576:LYS:HD2	1:B:576:LYS:O	2.19	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: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:341:THR:HA	1:A:344:GLU:HB2	2.02	0.42
1:A:349:ALA:HB2	1:A:378:PHE:CE2	2.54	0.42
1:A:313:PRO:HB2	1:A:314:LEU:H	1.53	0.42
1:A:437:ASN:C	1:A:437:ASN:HD22	2.22	0.42
1:A:543:HIS:CG	1:A:544:ARG:N	2.86	0.42
1:B:571:ILE:HG21	1:B:600:GLU:O	2.20	0.42
1:B:386:GLU:HG3	1:B:442:PHE:CE2	2.55	0.42
1:B:436:VAL:HA	1:B:439:MSE:HE2	2.01	0.42
1:A:530:LEU:O	1:A:531:SER:HB2	2.20	0.41
1:B:355:ASN:HD22	1:B:355:ASN:HA	1.62	0.41
1:B:546:THR:HG23	1:B:564:GLY:CA	2.50	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:A:630:GLU:OE2	1:A:630:GLU:HA	2.20	0.41
1:B:484:LYS:HB3	1:B:484:LYS:HE2	1.86	0.41
1:B:557:GLU:O	1:B:559:TYR:N	2.53	0.41
1:A:389:LEU:HD23	1:A:446:CYS:HB3	2.02	0.41
1:A:399:SER:C	1:A:401:LYS:N	2.74	0.41
1:B:370:LYS:HA	1:B:370:LYS:HD2	1.93	0.41
1:B:486:TRP:HZ3	1:B:524:GLU:HA	1.85	0.41
1:B:507:SER:O	1:B:508:ASN:C	2.58	0.41
1:A:425:GLU:HG3	1:A:425:GLU:O	2.19	0.41
1:A:427:THR:OG1	1:A:428:VAL:N	2.54	0.41
1:A:568:LYS:HE2	1:A:604:LEU:HD23	2.03	0.41
1:A:619:THR:OG1	2:A:1:SO4:S	2.79	0.41
1:A:620:SER:O	1:A:623:SER:HB3	2.20	0.41
1:B:544:ARG:O	1:B:544:ARG:HG3	2.21	0.41
1:B:560:GLN:HB2	1:B:561:GLN:NE2	2.36	0.41
1:A:359:MSE:HB2	1:A:368:TYR:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:489:ASN:O	1:A:490:THR:C	2.60	0.41
1:B:389:LEU:HD23	1:B:446:CYS:HB3	2.02	0.41
1:B:549:THR:HG21	1:B:560:GLN:CA	2.50	0.41
1:B:603:ILE:HG22	1:B:604:LEU:N	2.36	0.40
1:A:468:LEU:HD23	1:A:468:LEU:HA	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:454:ALA:O	1:A:456:PRO:HD3	2.22	0.40
1:A:546:THR:HG23	1:A:564:GLY:HA3	2.02	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: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
1:B:369:LEU:HD11	1:B:436:VAL:CG1	2.50	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	326/336 (97%)	272 (83%)	42 (13%)	12 (4%)	3	25
1	B	319/336 (95%)	263 (82%)	43 (14%)	13 (4%)	3	23
All	All	645/672 (96%)	535 (83%)	85 (13%)	25 (4%)	3	24

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 [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	284/281 (101%)	257 (90%)	27 (10%)	8	33
1	B	278/281 (99%)	255 (92%)	23 (8%)	11	38
All	All	562/562 (100%)	512 (91%)	50 (9%)	9	36

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

Sometimes 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 monosaccharides 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	B	2	-	4,4,4	0.22	0	6,6,6	0.10	0
2	SO4	A	1	-	4,4,4	0.33	0	6,6,6	0.19	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 [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

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<sup>th</sup> 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 <sup>2</sup> )	Q < 0.9
1	A	317/336 (94%)	1.19	54 (17%)	1 2	69, 134, 189, 200	0
1	B	312/336 (92%)	1.21	66 (21%)	0 1	75, 151, 197, 200	0
All	All	629/672 (93%)	1.20	120 (19%)	1 1	69, 142, 193, 200	0

All (120) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	548	SER	8.0
1	B	559	TYR	5.8
1	B	603	ILE	5.1
1	B	365	ILE	3.8
1	B	363	GLY	3.7
1	B	516	GLU	3.6
1	A	332	ILE	3.6
1	B	491	LYS	3.5
1	B	501	ILE	3.5
1	B	595	LEU	3.4
1	B	588	LEU	3.3
1	A	600	GLU	3.3
1	B	579	LEU	3.3
1	B	360	LEU	3.2
1	B	340	VAL	3.2
1	B	600	GLU	3.2
1	B	405	ILE	3.1
1	A	328	GLU	3.1
1	B	582	ALA	3.1
1	B	464	LYS	3.0
1	B	437	ASN	3.0
1	B	591	ILE	3.0
1	A	505	GLU	3.0
1	A	365	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	614	LEU	2.9
1	A	314	LEU	2.9
1	A	631	GLU	2.9
1	A	360	LEU	2.8
1	B	475	ILE	2.8
1	A	476	LYS	2.8
1	A	350	LYS	2.8
1	A	603	ILE	2.8
1	A	375	LEU	2.8
1	A	346	LEU	2.7
1	B	485	ILE	2.7
1	A	485	ILE	2.7
1	B	353	TRP	2.6
1	A	615	LEU	2.6
1	B	575	PHE	2.6
1	B	462	VAL	2.6
1	A	428	VAL	2.6
1	B	611	THR	2.6
1	A	516	GLU	2.6
1	A	595	LEU	2.6
1	A	384	LEU	2.6
1	A	465	SER	2.6
1	B	549	THR	2.6
1	A	582	ALA	2.5
1	A	446	CYS	2.5
1	A	369	LEU	2.5
1	B	386	GLU	2.5
1	B	432	LEU	2.5
1	A	498	ILE	2.5
1	B	347	GLU	2.5
1	B	493	LEU	2.5
1	B	426	SER	2.5
1	B	513	GLU	2.5
1	A	393	LEU	2.4
1	B	423	LEU	2.4
1	B	563	ARG	2.4
1	B	409	LEU	2.4
1	A	443	PHE	2.4
1	B	505	GLU	2.4
1	B	446	CYS	2.4
1	B	578	LYS	2.3
1	B	356	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	375	LEU	2.3
1	A	425	GLU	2.3
1	A	495	ASN	2.3
1	A	475	ILE	2.3
1	B	412	ALA	2.3
1	A	578	LYS	2.3
1	A	575	PHE	2.3
1	A	416	TYR	2.3
1	A	591	ILE	2.3
1	B	637	LYS	2.3
1	A	519	LEU	2.3
1	A	579	LEU	2.2
1	B	350	LYS	2.2
1	B	490	THR	2.2
1	A	389	LEU	2.2
1	B	397	THR	2.2
1	B	532	TYR	2.2
1	A	635	SER	2.2
1	A	405	ILE	2.2
1	B	518	VAL	2.2
1	B	389	LEU	2.2
1	A	327	ASP	2.2
1	B	369	LEU	2.2
1	B	535	ALA	2.2
1	A	490	THR	2.2
1	B	625	PHE	2.1
1	B	558	LYS	2.1
1	A	368	TYR	2.1
1	B	468	LEU	2.1
1	A	493	LEU	2.1
1	B	471	ILE	2.1
1	A	448	LEU	2.1
1	A	455	THR	2.1
1	B	569	THR	2.1
1	B	515	LEU	2.1
1	B	429	GLU	2.1
1	B	477	ASP	2.1
1	B	433	VAL	2.1
1	A	588	LEU	2.1
1	B	612	THR	2.1
1	B	537	LYS	2.1
1	A	326	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	473	GLN	2.1
1	B	519	LEU	2.1
1	A	577	ASP	2.1
1	B	467	ILE	2.1
1	A	559	TYR	2.1
1	A	530	LEU	2.0
1	B	528	GLU	2.0
1	A	471	ILE	2.0
1	A	433	VAL	2.0
1	A	438	LYS	2.0
1	B	332	ILE	2.0
1	B	598	LYS	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 monosaccharides 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. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	SO4	B	2	5/5	0.87	0.28	193,195,197,202	0
2	SO4	A	1	5/5	0.92	0.26	146,146,147,150	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.