Full wwPDB X-ray Structure Validation Report (i)

Feb 22, 2024 – 04:00 AM EST

PDB ID	:	4R5L
Title	:	Crystal structure of the DnaK C-terminus (Dnak-SBD-C)
Authors	:	Leu, J.I.; Zhang, P.; Murphy, M.E.; Marmorstein, R.; George, D.L.
Deposited on	:	2014-08-21
Resolution	:	2.97 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

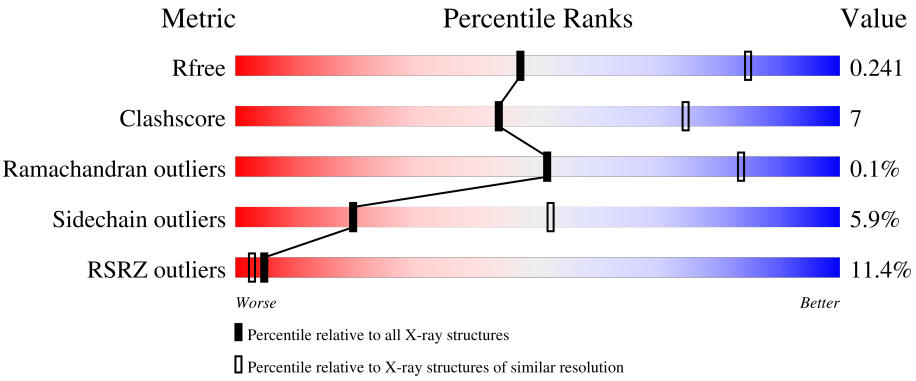
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.97 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	2754 (3.00-2.96)
Clashscore	141614	3103 (3.00-2.96)
Ramachandran outliers	138981	2993 (3.00-2.96)
Sidechain outliers	138945	2996 (3.00-2.96)
RSRZ outliers	127900	2644 (3.00-2.96)

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 >=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	230	81% 15%
1	B	230	20% 78% 16%
1	C	230	20% 79% 15%
1	D	230	3% 86% 12%

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	SO4	B	701	-	-	-	X
2	SO4	D	702	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 6651 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 Chaperone protein DnaK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	222	Total	C	N	O	S	0	0	0
			1660	1021	297	336	6			
1	B	226	Total	C	N	O	S	0	0	0
			1583	976	288	314	5			
1	C	223	Total	C	N	O	S	0	0	0
			1624	997	292	330	5			
1	D	227	Total	C	N	O	S	0	0	0
			1696	1040	300	350	6			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	378	MET	-	expression tag	UNP P0A6Y8
A	379	HIS	-	expression tag	UNP P0A6Y8
A	380	HIS	-	expression tag	UNP P0A6Y8
A	381	HIS	-	expression tag	UNP P0A6Y8
A	382	HIS	-	expression tag	UNP P0A6Y8
A	383	HIS	-	expression tag	UNP P0A6Y8
A	384	HIS	-	expression tag	UNP P0A6Y8
A	385	ILE	-	expression tag	UNP P0A6Y8
A	386	GLU	-	expression tag	UNP P0A6Y8
A	387	GLY	-	expression tag	UNP P0A6Y8
A	388	ARG	-	expression tag	UNP P0A6Y8
B	378	MET	-	expression tag	UNP P0A6Y8
B	379	HIS	-	expression tag	UNP P0A6Y8
B	380	HIS	-	expression tag	UNP P0A6Y8
B	381	HIS	-	expression tag	UNP P0A6Y8
B	382	HIS	-	expression tag	UNP P0A6Y8
B	383	HIS	-	expression tag	UNP P0A6Y8
B	384	HIS	-	expression tag	UNP P0A6Y8
B	385	ILE	-	expression tag	UNP P0A6Y8
B	386	GLU	-	expression tag	UNP P0A6Y8
B	387	GLY	-	expression tag	UNP P0A6Y8

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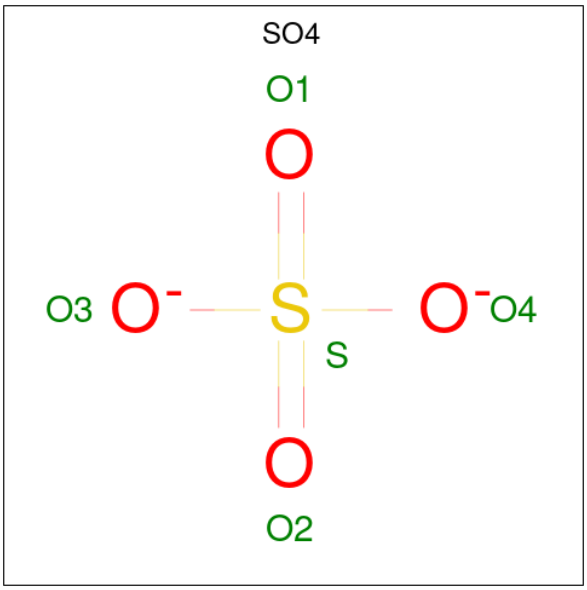
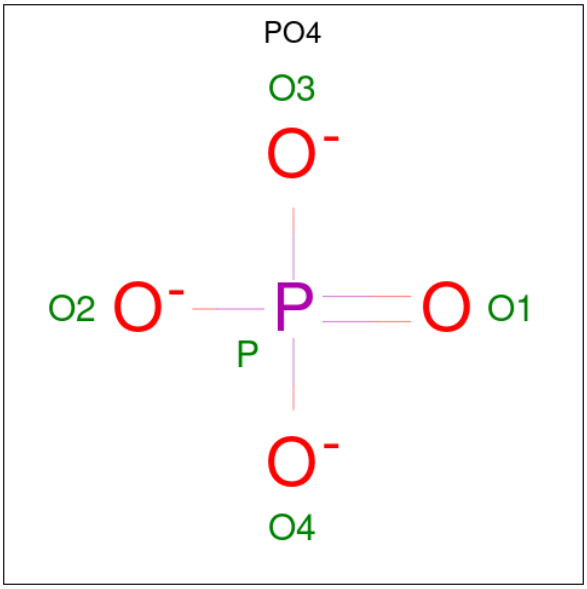
Chain	Residue	Modelled	Actual	Comment	Reference
B	388	ARG	-	expression tag	UNP P0A6Y8
C	378	MET	-	expression tag	UNP P0A6Y8
C	379	HIS	-	expression tag	UNP P0A6Y8
C	380	HIS	-	expression tag	UNP P0A6Y8
C	381	HIS	-	expression tag	UNP P0A6Y8
C	382	HIS	-	expression tag	UNP P0A6Y8
C	383	HIS	-	expression tag	UNP P0A6Y8
C	384	HIS	-	expression tag	UNP P0A6Y8
C	385	ILE	-	expression tag	UNP P0A6Y8
C	386	GLU	-	expression tag	UNP P0A6Y8
C	387	GLY	-	expression tag	UNP P0A6Y8
C	388	ARG	-	expression tag	UNP P0A6Y8
D	378	MET	-	expression tag	UNP P0A6Y8
D	379	HIS	-	expression tag	UNP P0A6Y8
D	380	HIS	-	expression tag	UNP P0A6Y8
D	381	HIS	-	expression tag	UNP P0A6Y8
D	382	HIS	-	expression tag	UNP P0A6Y8
D	383	HIS	-	expression tag	UNP P0A6Y8
D	384	HIS	-	expression tag	UNP P0A6Y8
D	385	ILE	-	expression tag	UNP P0A6Y8
D	386	GLU	-	expression tag	UNP P0A6Y8
D	387	GLY	-	expression tag	UNP P0A6Y8
D	388	ARG	-	expression tag	UNP P0A6Y8

- 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	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total O P 5 4 1	0	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total Ca 1 1	0	0

- Molecule 5 is water.

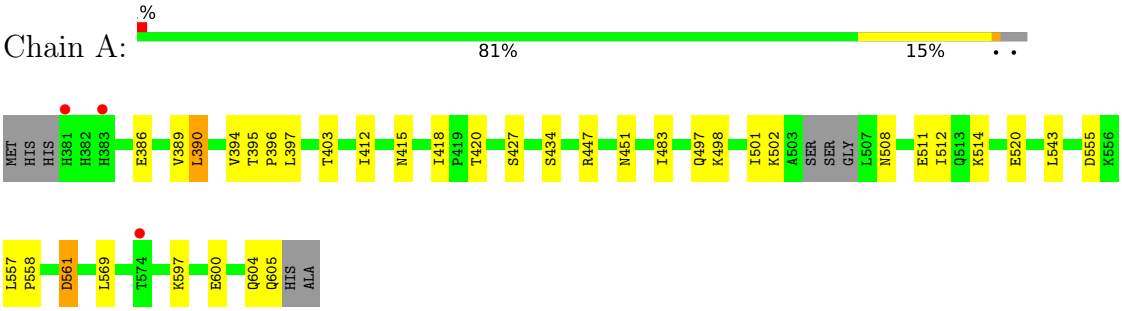
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	10	Total O 10 10	0	0
5	B	8	Total O 8 8	0	0
5	C	1	Total O 1 1	0	0
5	D	3	Total O 3 3	0	0

3 Residue-property plots (i)

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.

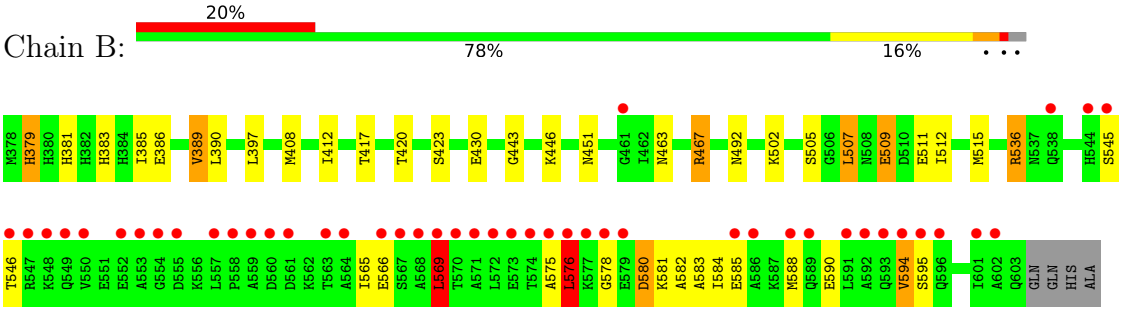
• Molecule 1: Chaperone protein DnaK

Chain A:



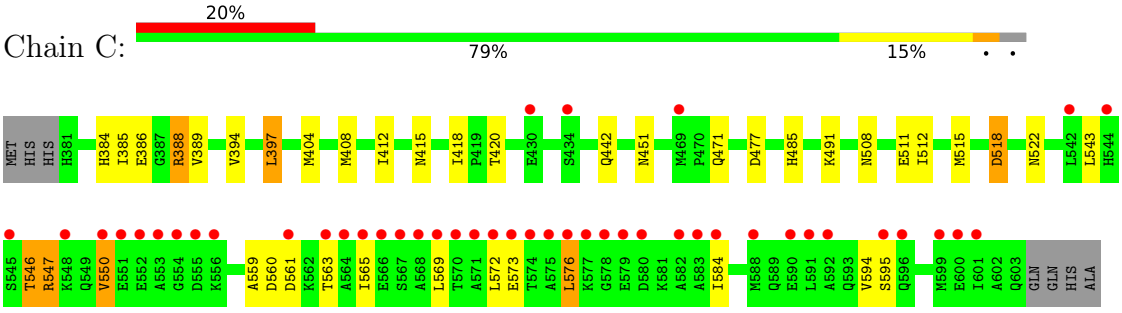
• Molecule 1: Chaperone protein DnaK

Chain B:



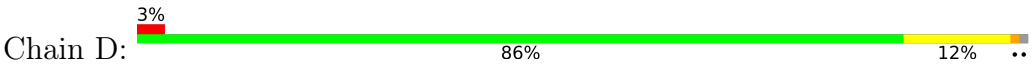
• Molecule 1: Chaperone protein DnaK

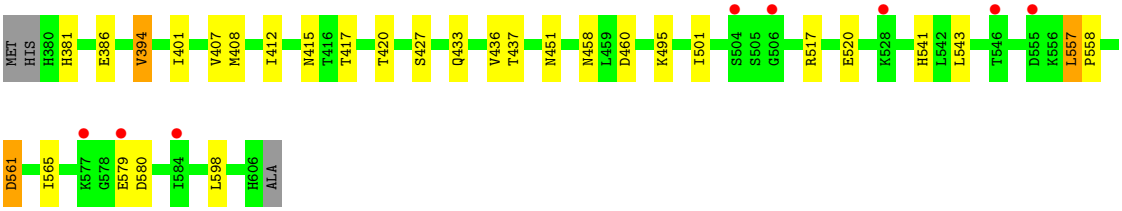
Chain C:



• Molecule 1: Chaperone protein DnaK

Chain D:




MET
HIS
H380
H381
E386
V394
I401
V407
M408
I412
N415
T416
T417
T420
S427
Q433
V436
T437
N451
N458
L459
D460
K495
I501
S504
S505
G506
R517
E520
K528
H541
L542
L543
T546
D555
K556
L557
P558

D561
I565
K577
G578
E579
D580
I584
L598
H606
ALA

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	92.31Å 99.91Å 133.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.90 – 2.97 43.93 – 2.96	Depositor EDS
% Data completeness (in resolution range)	99.9 (41.90-2.97) 99.6 (43.93-2.96)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.63 (at 2.96Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.205 , 0.243 0.206 , 0.241	Depositor DCC
R_{free} test set	1344 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å^2)	53.8	Xtriage
Anisotropy	0.613	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 69.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	6651	wwPDB-VP
Average B, all atoms (Å^2)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.82% 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: PO4, CA, 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	0.25	0/1676	0.45	0/2265
1	B	0.27	0/1602	0.59	2/2179 (0.1%)
1	C	0.26	0/1642	0.47	0/2228
1	D	0.25	0/1713	0.46	0/2314
All	All	0.26	0/6633	0.49	2/8986 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	569	LEU	CA-CB-CG	6.00	129.11	115.30
1	B	580	ASP	N-CA-CB	-5.02	101.57	110.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	576	LEU	Peptide

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	1660	0	1631	21	1
1	B	1583	0	1474	34	0
1	C	1624	0	1553	25	1
1	D	1696	0	1659	17	0
2	A	15	0	0	1	0
2	B	15	0	0	0	0
2	C	10	0	0	0	0
2	D	10	0	0	0	0
3	A	10	0	0	0	0
3	C	5	0	0	0	0
4	C	1	0	0	0	0
5	A	10	0	0	1	0
5	B	8	0	0	1	0
5	C	1	0	0	0	0
5	D	3	0	0	0	0
All	All	6651	0	6317	87	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 7.

All (87) 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:511:GLU:HA	1:A:514:LYS:HB3	1.57	0.84
1:B:581:LYS:HG3	1:B:582:ALA:H	1.43	0.83
1:C:547:ARG:HG2	1:C:569:LEU:HD13	1.67	0.75
1:D:394:VAL:HG13	1:D:415:ASN:HA	1.74	0.70
1:B:580:ASP:CG	1:B:581:LYS:HB2	2.14	0.68
1:B:509:GLU:HA	1:B:512:ILE:HD13	1.75	0.67
1:C:386:GLU:OE2	1:D:541:HIS:NE2	2.29	0.66
1:D:460:ASP:OD1	1:D:495:LYS:NZ	2.29	0.66
1:C:543:LEU:HD21	1:C:573:GLU:HG2	1.80	0.63
1:A:520:GLU:OE2	1:D:517:ARG:NH1	2.31	0.62
1:A:558:PRO:HB2	1:A:561:ASP:HB2	1.83	0.61
1:C:384:HIS:O	1:D:433:GLN:NE2	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:581:LYS:HG3	1:B:582:ALA:N	2.14	0.59
1:C:404:MET:HE1	1:D:386:GLU:HG3	1.85	0.59
1:C:518:ASP:O	1:C:522:ASN:ND2	2.30	0.59
1:B:397:LEU:HD12	1:B:443:GLY:HA2	1.85	0.58
1:C:394:VAL:HG13	1:C:415:ASN:HA	1.84	0.58
1:B:446:LYS:NZ	5:B:808:HOH:O	2.36	0.58
1:C:508:ASN:N	1:C:511:GLU:OE1	2.27	0.58
1:B:581:LYS:CG	1:B:582:ALA:H	2.14	0.58
1:A:394:VAL:HG13	1:A:415:ASN:HA	1.86	0.58
1:B:581:LYS:HB3	1:B:583:ALA:H	1.69	0.57
1:A:386:GLU:OE2	1:B:467:ARG:NH1	2.38	0.56
1:A:427:SER:N	1:B:386:GLU:O	2.26	0.56
1:A:447:ARG:O	1:A:451:ASN:ND2	2.39	0.56
1:B:512:ILE:HD12	1:B:512:ILE:H	1.70	0.55
1:A:555:ASP:OD1	1:A:555:ASP:N	2.38	0.54
1:C:408:MET:SD	1:C:451:ASN:ND2	2.81	0.54
1:B:507:LEU:HB3	1:B:512:ILE:HD11	1.89	0.53
1:A:395:THR:HG23	1:A:418:ILE:HD11	1.91	0.53
1:A:403:THR:HG22	1:B:385:ILE:HG22	1.93	0.51
1:B:408:MET:SD	1:B:451:ASN:ND2	2.83	0.51
1:C:559:ALA:O	1:C:563:THR:HG23	2.10	0.51
1:A:434:SER:OG	2:A:703:SO4:O2	2.21	0.51
1:B:580:ASP:OD2	1:B:581:LYS:HB2	2.11	0.50
1:B:582:ALA:HA	1:B:585:GLU:HB2	1.94	0.50
1:C:560:ASP:O	1:C:563:THR:OG1	2.30	0.49
1:D:437:THR:OG1	1:D:458:ASN:OD1	2.28	0.49
1:A:396:PRO:HB2	1:A:397:LEU:HD22	1.93	0.49
1:A:397:LEU:HD21	1:A:512:ILE:HG12	1.95	0.49
1:B:507:LEU:CB	1:B:512:ILE:HD11	2.42	0.49
1:C:389:VAL:HG22	1:D:427:SER:HB2	1.96	0.48
1:C:412:ILE:HD13	1:C:420:THR:HG23	1.94	0.48
1:B:581:LYS:CG	1:B:582:ALA:N	2.75	0.48
1:B:575:ALA:HB1	1:B:584:ILE:HD12	1.96	0.48
1:B:463:ASN:ND2	1:B:492:ASN:OD1	2.47	0.48
1:D:412:ILE:HD13	1:D:420:THR:HG23	1.96	0.48
1:C:397:LEU:HD13	1:C:512:ILE:HG23	1.96	0.47
1:C:397:LEU:HD23	1:C:442:GLN:HG2	1.96	0.47
1:C:550:VAL:HG11	1:C:565:ILE:HG21	1.97	0.46
1:C:385:ILE:HD11	1:D:401:ILE:HD12	1.96	0.46
1:D:408:MET:SD	1:D:451:ASN:ND2	2.89	0.46
1:B:430:GLU:HA	1:B:467:ARG:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:412:ILE:HD13	1:B:420:THR:HG23	1.98	0.46
1:A:483:ILE:HD12	1:A:502:LYS:HD3	1.97	0.45
1:B:511:GLU:O	1:B:515:MET:HG3	2.17	0.45
1:A:412:ILE:HD13	1:A:420:THR:HG23	1.98	0.45
1:C:546:THR:O	1:C:550:VAL:HG13	2.15	0.45
1:C:477:ASP:HB3	1:C:485:HIS:HB2	1.98	0.45
1:B:536:ARG:HG3	1:B:576:LEU:HD22	1.99	0.45
1:C:511:GLU:O	1:C:515:MET:HG3	2.17	0.45
1:A:508:ASN:N	1:A:508:ASN:OD1	2.50	0.44
1:A:543:LEU:HD12	1:A:569:LEU:HD22	2.00	0.44
1:B:502:LYS:HE3	1:B:505:SER:HB2	1.98	0.44
1:A:557:LEU:HD12	1:A:558:PRO:HD2	2.00	0.44
1:A:561:ASP:OD2	1:A:597:LYS:HD2	2.18	0.44
1:B:536:ARG:NH1	1:B:578:GLY:O	2.50	0.43
1:C:385:ILE:HG22	1:D:436:VAL:HB	2.01	0.43
1:D:579:GLU:HG2	1:D:580:ASP:H	1.83	0.43
1:C:418:ILE:HG22	1:C:420:THR:HG22	1.99	0.43
1:C:565:ILE:O	1:C:569:LEU:HG	2.19	0.43
1:B:594:VAL:HG23	1:B:595:SER:H	1.83	0.43
1:D:565:ILE:HD13	1:D:598:LEU:HD22	2.00	0.43
1:B:507:LEU:HD12	1:B:507:LEU:HA	1.91	0.43
1:C:576:LEU:HD12	1:C:584:ILE:HD13	2.01	0.43
1:D:558:PRO:HG2	1:D:561:ASP:HB2	2.00	0.43
1:C:471:GLN:HB2	1:C:491:LYS:HB2	2.00	0.42
1:B:584:ILE:O	1:B:588:MET:HG3	2.19	0.42
5:A:809:HOH:O	1:B:379:HIS:HE1	2.01	0.42
1:B:389:VAL:CG1	1:B:417:THR:HG21	2.49	0.42
1:B:545:SER:OG	1:B:546:THR:N	2.52	0.42
1:B:566:GLU:O	1:B:569:LEU:HD22	2.20	0.42
1:A:497:GLN:OE1	1:A:498:LYS:N	2.52	0.41
1:D:557:LEU:HA	1:D:558:PRO:HD2	1.95	0.41
1:A:390:LEU:H	1:A:390:LEU:HG	1.45	0.40
1:B:565:ILE:O	1:B:569:LEU:HD13	2.21	0.40
1:D:557:LEU:HD23	1:D:558:PRO:HD2	2.04	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:A:600:GLU:OE1	1:C:388:ARG:NH2[2_764]	2.09	0.11

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	218/230 (95%)	213 (98%)	5 (2%)	0	100 100
1	B	224/230 (97%)	206 (92%)	17 (8%)	1 (0%)	34 70
1	C	221/230 (96%)	211 (96%)	10 (4%)	0	100 100
1	D	225/230 (98%)	214 (95%)	11 (5%)	0	100 100
All	All	888/920 (96%)	844 (95%)	43 (5%)	1 (0%)	51 83

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	509	GLU

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	174/191 (91%)	168 (97%)	6 (3%)	37 70
1	B	149/191 (78%)	136 (91%)	13 (9%)	10 35
1	C	164/191 (86%)	153 (93%)	11 (7%)	16 47
1	D	179/191 (94%)	170 (95%)	9 (5%)	24 58
All	All	666/764 (87%)	627 (94%)	39 (6%)	19 52

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	389	VAL
1	A	390	LEU
1	A	501	ILE
1	A	561	ASP
1	A	604	GLN
1	A	605	GLN
1	B	379	HIS
1	B	381	HIS
1	B	383	HIS
1	B	389	VAL
1	B	390	LEU
1	B	423	SER
1	B	467	ARG
1	B	507	LEU
1	B	536	ARG
1	B	569	LEU
1	B	576	LEU
1	B	590	GLU
1	B	594	VAL
1	C	388	ARG
1	C	397	LEU
1	C	518	ASP
1	C	546	THR
1	C	547	ARG
1	C	550	VAL
1	C	561	ASP
1	C	572	LEU
1	C	576	LEU
1	C	594	VAL
1	C	595	SER
1	D	381	HIS
1	D	394	VAL
1	D	407	VAL
1	D	417	THR
1	D	501	ILE
1	D	520	GLU
1	D	543	LEU
1	D	557	LEU
1	D	561	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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)

Of 14 ligands modelled in this entry, 1 is monoatomic - leaving 13 for Mogul analysis.

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	703	-	4,4,4	0.15	0	6,6,6	0.06	0
2	SO4	A	703	-	4,4,4	0.14	0	6,6,6	0.08	0
2	SO4	A	702	-	4,4,4	0.13	0	6,6,6	0.07	0
2	SO4	C	702	-	4,4,4	0.14	0	6,6,6	0.07	0
3	PO4	A	704	-	4,4,4	0.93	0	6,6,6	0.45	0
2	SO4	B	702	-	4,4,4	0.15	0	6,6,6	0.05	0
3	PO4	A	705	-	4,4,4	0.94	0	6,6,6	0.41	0
2	SO4	D	701	-	4,4,4	0.16	0	6,6,6	0.07	0
2	SO4	D	702	-	4,4,4	0.13	0	6,6,6	0.08	0
2	SO4	C	701	-	4,4,4	0.14	0	6,6,6	0.06	0
2	SO4	B	701	-	4,4,4	0.14	0	6,6,6	0.07	0
2	SO4	A	701	-	4,4,4	0.15	0	6,6,6	0.05	0
3	PO4	C	703	-	4,4,4	0.95	0	6,6,6	0.39	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	703	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^{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	222/230 (96%)	0.28	3 (1%) 75 57	49, 73, 99, 115	0
1	B	226/230 (98%)	1.06	46 (20%) 1 0	51, 90, 144, 172	0
1	C	223/230 (96%)	0.86	45 (20%) 1 0	54, 86, 134, 151	0
1	D	227/230 (98%)	0.37	8 (3%) 44 26	48, 74, 103, 135	0
All	All	898/920 (97%)	0.64	102 (11%) 5 3	48, 77, 135, 172	0

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	553	ALA	8.8
1	B	592	ALA	7.7
1	B	589	GLN	7.4
1	B	570	THR	6.7
1	B	588	MET	6.2
1	B	567	SER	5.5
1	B	574	THR	5.3
1	B	593	GLN	4.9
1	B	555	ASP	4.7
1	B	586	ALA	4.7
1	B	560	ASP	4.5
1	B	595	SER	4.5
1	C	601	ILE	4.4
1	C	564	ALA	4.4
1	B	578	GLY	4.3
1	B	564	ALA	4.2
1	B	545	SER	4.2
1	C	568	ALA	4.2
1	A	381	HIS	4.1
1	B	591	LEU	4.1
1	B	573	GLU	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	554	GLY	4.0
1	C	576	LEU	3.9
1	B	585	GLU	3.9
1	B	571	ALA	3.8
1	C	561	ASP	3.8
1	B	569	LEU	3.7
1	B	550	VAL	3.7
1	B	552	GLU	3.7
1	C	554	GLY	3.7
1	B	544	HIS	3.6
1	C	565	ILE	3.5
1	C	570	THR	3.5
1	B	538	GLN	3.4
1	B	558	PRO	3.4
1	B	575	ALA	3.4
1	B	563	THR	3.4
1	B	601	ILE	3.3
1	C	575	ALA	3.3
1	D	504	SER	3.3
1	C	553	ALA	3.3
1	C	544	HIS	3.3
1	C	600	GLU	3.2
1	C	580	ASP	3.2
1	B	546	THR	3.2
1	C	578	GLY	3.1
1	C	595	SER	3.0
1	C	551	GLU	3.0
1	B	576	LEU	3.0
1	C	584	ILE	3.0
1	B	566	GLU	2.9
1	D	577	LYS	2.9
1	B	561	ASP	2.9
1	B	549	GLN	2.9
1	C	591	LEU	2.8
1	C	567	SER	2.8
1	B	568	ALA	2.8
1	C	542	LEU	2.8
1	C	572	LEU	2.8
1	C	545	SER	2.7
1	B	461	GLY	2.7
1	C	596	GLN	2.7
1	D	579	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	430	GLU	2.6
1	B	572	LEU	2.6
1	B	577	LYS	2.6
1	C	573	GLU	2.6
1	D	546	THR	2.6
1	C	563	THR	2.6
1	C	583	ALA	2.6
1	B	602	ALA	2.5
1	C	550	VAL	2.5
1	C	574	THR	2.5
1	C	577	LYS	2.5
1	D	555	ASP	2.5
1	B	548	LYS	2.5
1	C	579	GLU	2.4
1	D	506	GLY	2.4
1	C	599	MET	2.4
1	C	552	GLU	2.4
1	C	555	ASP	2.4
1	C	592	ALA	2.4
1	C	469	MET	2.3
1	C	556	LYS	2.3
1	A	574	THR	2.3
1	B	596	GLN	2.3
1	B	579	GLU	2.3
1	B	547	ARG	2.2
1	C	434	SER	2.2
1	C	582	ALA	2.2
1	C	569	LEU	2.2
1	D	584	ILE	2.2
1	B	594	VAL	2.2
1	C	548	LYS	2.1
1	C	571	ALA	2.1
1	B	559	ALA	2.1
1	C	566	GLU	2.1
1	C	590	GLU	2.0
1	A	383	HIS	2.0
1	C	588	MET	2.0
1	B	557	LEU	2.0
1	D	528	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^{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
2	SO4	B	703	5/5	0.71	0.31	127,157,171,177	0
2	SO4	B	701	5/5	0.73	0.42	107,109,129,153	0
2	SO4	D	702	5/5	0.78	0.44	130,135,146,148	0
2	SO4	A	702	5/5	0.84	0.39	115,120,131,149	0
3	PO4	A	704	5/5	0.84	0.27	80,86,104,134	0
3	PO4	A	705	5/5	0.84	0.28	113,114,147,149	0
2	SO4	C	702	5/5	0.89	0.18	107,115,129,138	0
3	PO4	C	703	5/5	0.89	0.26	85,89,109,129	0
2	SO4	A	703	5/5	0.90	0.18	108,120,141,153	0
2	SO4	C	701	5/5	0.91	0.30	120,125,141,141	0
4	CA	C	704	1/1	0.91	0.13	114,114,114,114	0
2	SO4	D	701	5/5	0.92	0.32	93,105,115,117	0
2	SO4	B	702	5/5	0.94	0.20	116,126,143,149	0
2	SO4	A	701	5/5	0.95	0.28	84,98,118,120	0

6.5 Other polymers (i)

There are no such residues in this entry.