Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 09:59 AM GMT

PDB ID	:	3KHK
Title	:	Crystal structure of type-I restriction-modification system methylation subunit (MM_0429) from Methanosarchina mazei.
Authors	:	Ramagopal, U.A.; Toro, R.; Burley, S.K.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on	:	2009-10-30
Resolution	:	2.55 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:

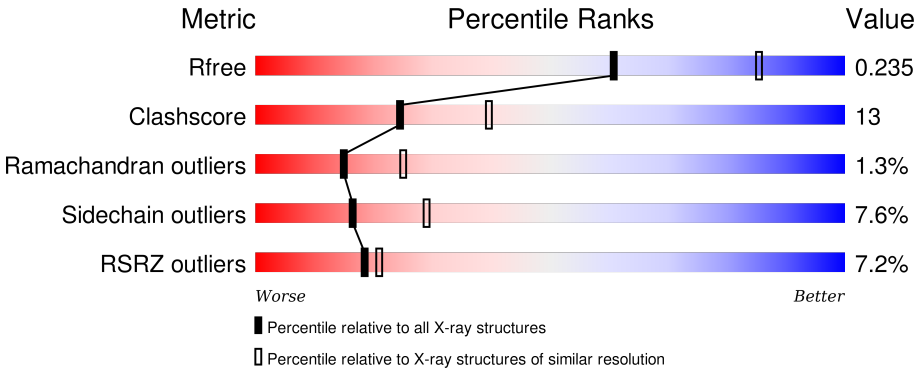
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance

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

The reported resolution of this entry is 2.55 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	4549 (2.58-2.50)
Clashscore	102246	5292 (2.58-2.50)
Ramachandran outliers	100387	5194 (2.58-2.50)
Sidechain outliers	100360	5196 (2.58-2.50)
RSRZ outliers	91569	4561 (2.58-2.50)

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	544	7%, 63%, 24%, •, 10%
1	B	544	6%, 58%, 29%, •, 10%

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	A	600	-	-	-	X
2	SO4	B	600	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7891 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.

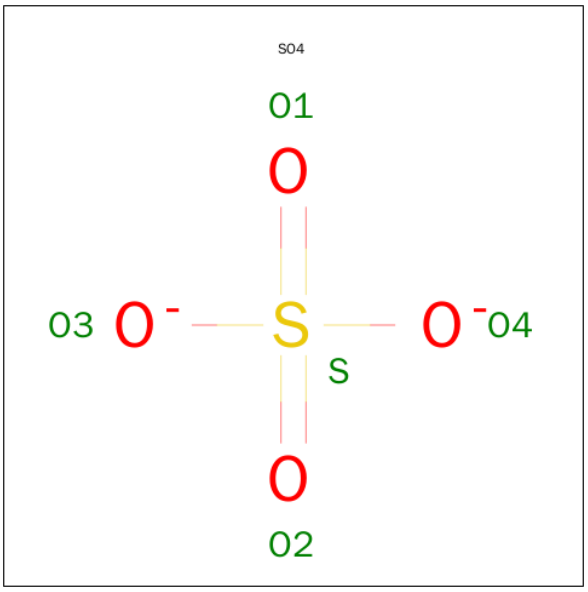
- Molecule 1 is a protein called Type I restriction-modification system methylation subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	488	Total	C	N	O	S	0	0	0
			3934	2514	669	736	15			
1	B	487	Total	C	N	O	S	0	0	0
			3929	2509	666	739	15			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	expression tag	UNP Q8PZR3
A	1	SER	-	expression tag	UNP Q8PZR3
A	2	LEU	-	expression tag	UNP Q8PZR3
A	536	GLU	-	expression tag	UNP Q8PZR3
A	537	GLY	-	expression tag	UNP Q8PZR3
A	538	HIS	-	expression tag	UNP Q8PZR3
A	539	HIS	-	expression tag	UNP Q8PZR3
A	540	HIS	-	expression tag	UNP Q8PZR3
A	541	HIS	-	expression tag	UNP Q8PZR3
A	542	HIS	-	expression tag	UNP Q8PZR3
A	543	HIS	-	expression tag	UNP Q8PZR3
B	0	MET	-	expression tag	UNP Q8PZR3
B	1	SER	-	expression tag	UNP Q8PZR3
B	2	LEU	-	expression tag	UNP Q8PZR3
B	536	GLU	-	expression tag	UNP Q8PZR3
B	537	GLY	-	expression tag	UNP Q8PZR3
B	538	HIS	-	expression tag	UNP Q8PZR3
B	539	HIS	-	expression tag	UNP Q8PZR3
B	540	HIS	-	expression tag	UNP Q8PZR3
B	541	HIS	-	expression tag	UNP Q8PZR3
B	542	HIS	-	expression tag	UNP Q8PZR3
B	543	HIS	-	expression tag	UNP Q8PZR3

- 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

- Molecule 3 is water.

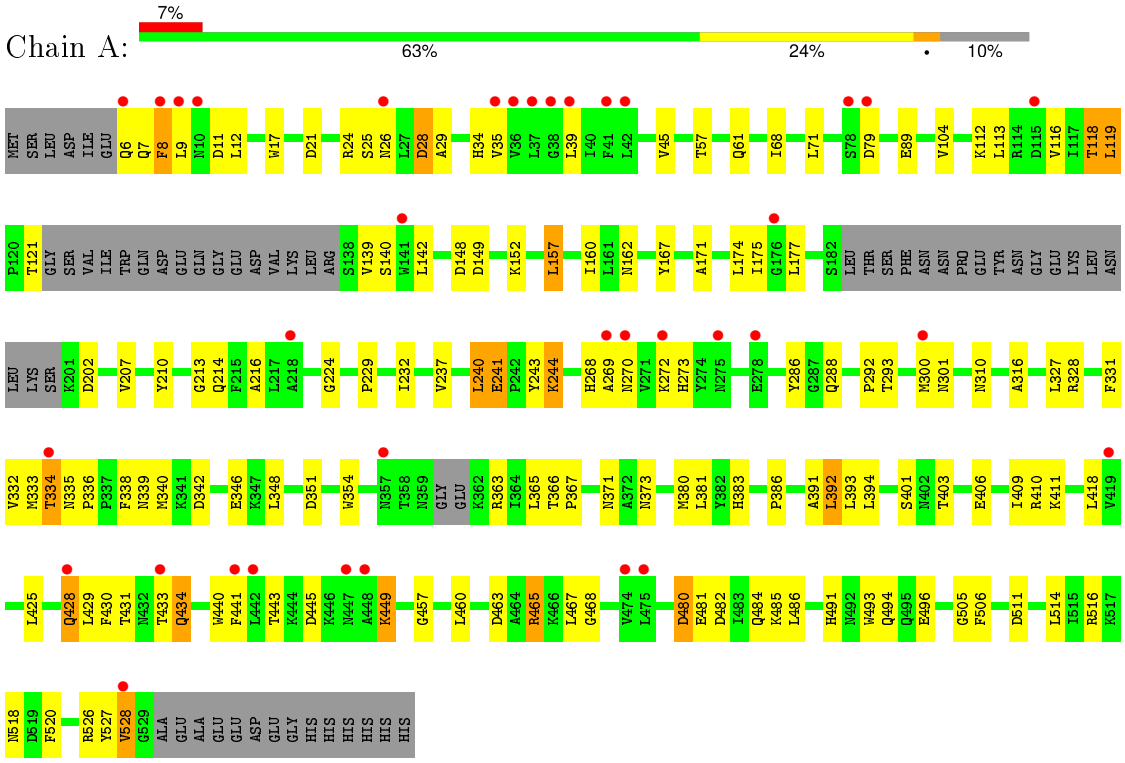
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	11	Total O 11 11	0	0
3	B	7	Total O 7 7	0	0

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.

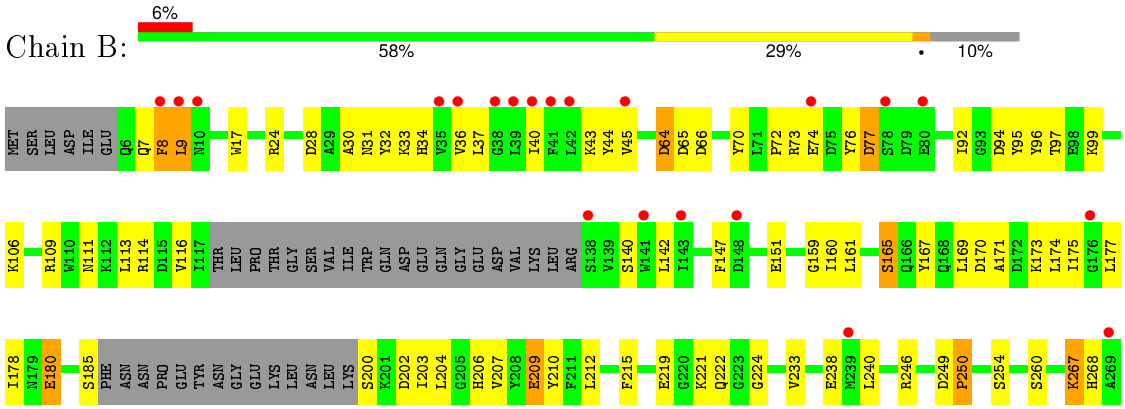
- Molecule 1: Type I restriction-modification system methylation subunit

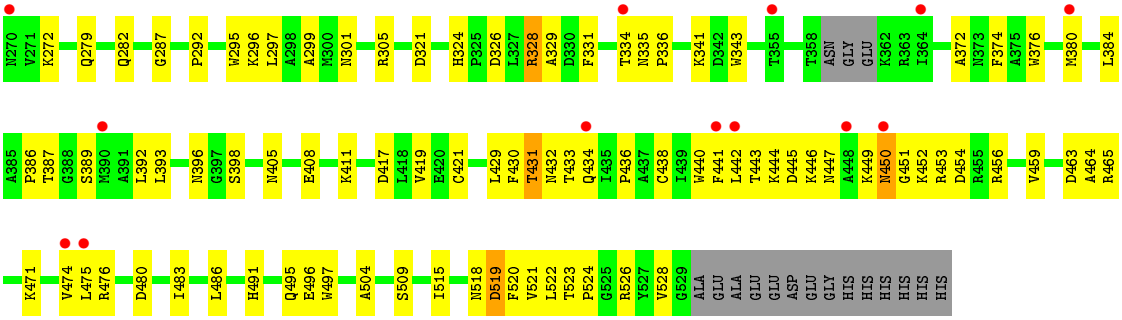
Chain A:



- Molecule 1: Type I restriction-modification system methylation subunit

Chain B:




N270 V271 K272 Q279 Q282 G287 P292 W295 K296 L297 A298 A299 N300 N301 R305 D321 H324 P325 D326 L327 R328 A329 D330 F331 T334 N335 P336 K341 D342 W343 T355 T358 ASN GLY GLU K362 R363 I364 A372 N373 F374 A375 W376 M380 L384
A385 P386 T387 G388 S389 M390 A391 L392 L393 N396 G397 S398 N405 E408 K411 D417 L418 V419 E420 C421 L429 F430 T431 N432 T433 Q434 T435 P436 A437 C438 I439 W440 F441 L442 T443 K444 D445 K446 N447 A448 K449 N450 G451 K452 R453 D454 R455 R456 V459 D463 A464 R465
K471 V474 L475 R476 D480 I483 L486 H491 Q495 E496 W497 A504 S509 I515 N518 D519 F520 V521 L522 T523 P524 G525 R526 Y527 V528 G529 ALA GLU ALA GLU GLU ASP GLU GLY HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α, β, γ	80.65Å 80.65Å 179.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.55 24.54 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.7 (25.00-2.55) 99.8 (24.54-2.55)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	3.01 (at 2.57Å)	Xtriage
Refinement program	REFMAC 5.5.0089	Depositor
R, R_{free}	0.213 , 0.242 0.211 , 0.235	Depositor DCC
R_{free} test set	1855 reflections (5.27%)	DCC
Wilson B-factor (Å^2)	53.1	Xtriage
Anisotropy	0.034	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 35.5	EDS
Estimated twinning fraction	0.509 for H, K, L 0.491 for K, H, -L 0.237 for h,-k,-l	Xtriage
Reported twinning fraction	0.509 for H, K, L 0.491 for K, H, -L	Depositor
L-test for twinning[2]	$< \|L\| > = 0.53$, $< L^2 > = 0.37$	Xtriage
Outliers	0 of 37128 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7891	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.28% 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	0.54	0/4027	0.67	0/5453
1	B	0.56	0/4021	0.67	0/5442
All	All	0.55	0/8048	0.67	0/10895

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3934	0	3783	91	0
1	B	3929	0	3764	109	0
2	A	5	0	0	1	0
2	B	5	0	0	1	0
3	A	11	0	0	0	0
3	B	7	0	0	0	0
All	All	7891	0	7547	199	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 13.

All (199) 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:334:THR:HG23	1:B:336:PRO:HD3	1.41	1.03
1:B:30:ALA:HA	1:B:219:GLU:OE2	1.61	1.00
1:A:527:TYR:O	1:A:528:VAL:HB	1.56	1.00
1:B:429:LEU:O	1:B:431:THR:HG22	1.78	0.84
1:B:279:GLN:NE2	1:B:282:GLN:HG3	1.94	0.82
1:B:279:GLN:HE21	1:B:282:GLN:HG3	1.44	0.81
1:B:431:THR:HG1	1:B:433:THR:HG1	1.19	0.80
1:B:222:GLN:HB3	1:B:432:ASN:O	1.84	0.77
1:B:160:ILE:HG22	1:B:161:LEU:HD23	1.67	0.76
1:A:139:VAL:HG11	1:A:175:ILE:HD11	1.69	0.74
1:A:431:THR:HG23	1:A:433:THR:H	1.53	0.73
1:B:328:ARG:HD3	2:B:600:SO4:O4	1.88	0.73
1:B:454:ASP:OD2	1:B:456:ARG:NH2	2.24	0.71
1:A:210:TYR:CZ	1:A:214:GLN:HG3	2.25	0.70
1:A:410:ARG:HD2	1:A:520:PHE:O	1.91	0.70
1:B:233:VAL:HG12	1:B:260:SER:HB2	1.76	0.67
1:B:36:VAL:O	1:B:40:ILE:HG13	1.94	0.67
1:A:381:LEU:HD21	1:A:418:LEU:HD13	1.77	0.67
1:B:480:ASP:HA	1:B:483:ILE:HB	1.77	0.67
1:A:365:LEU:HD13	1:A:409:ILE:HG12	1.76	0.66
1:B:109:ARG:O	1:B:113:LEU:HD13	1.96	0.65
1:A:157:LEU:HA	1:A:160:ILE:HD12	1.77	0.65
1:B:233:VAL:HG12	1:B:260:SER:CB	2.27	0.65
1:B:171:ALA:O	1:B:175:ILE:HG13	1.97	0.65
1:A:25:SER:OG	1:A:26:ASN:N	2.30	0.64
1:B:160:ILE:HD13	1:B:299:ALA:HB1	1.79	0.63
1:A:527:TYR:O	1:A:528:VAL:CB	2.36	0.63
1:B:449:LYS:O	1:B:451:GLY:N	2.31	0.62
1:B:238:GLU:O	1:B:491:HIS:HE1	1.82	0.62
1:A:232:ILE:HD11	1:A:429:LEU:CD2	2.30	0.62
1:B:453:ARG:HD3	1:B:496:GLU:HA	1.82	0.62
1:B:219:GLU:HG3	1:B:221:LYS:HG2	1.83	0.61
1:B:515:ILE:HG22	1:B:520:PHE:CD1	2.36	0.61
1:B:238:GLU:O	1:B:491:HIS:CE1	2.54	0.60
1:A:71:LEU:HD11	1:A:89:GLU:HG3	1.82	0.60
1:A:232:ILE:HD11	1:A:429:LEU:HD21	1.83	0.59
1:B:33:LYS:O	1:B:37:LEU:HG	2.02	0.59
1:B:140:SER:HB3	1:B:165:SER:OG	2.03	0.59
1:B:34:HIS:CE1	1:B:297:LEU:HD21	2.38	0.58
1:B:343:TRP:CD1	1:B:372:ALA:HB2	2.38	0.58
1:B:250:PRO:HD2	1:B:334:THR:HB	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:174:LEU:O	1:B:178:ILE:HG12	2.04	0.57
1:A:392:LEU:HD12	1:A:392:LEU:N	2.19	0.57
1:A:118:THR:HG23	1:A:119:LEU:H	1.69	0.57
1:B:8:PHE:HD2	1:B:8:PHE:C	2.08	0.57
1:A:485:LYS:HE2	1:A:506:PHE:CZ	2.40	0.57
1:B:8:PHE:CD2	1:B:8:PHE:C	2.78	0.57
1:A:354:TRP:CD1	1:A:367:PRO:HG3	2.39	0.57
1:A:232:ILE:HG21	1:A:393:LEU:HD22	1.87	0.56
1:A:113:LEU:HD22	1:A:142:LEU:HG	1.87	0.56
1:B:384:LEU:HD23	1:B:444:LYS:HG3	1.87	0.56
1:B:465:ARG:O	1:B:476:ARG:NH2	2.38	0.56
1:B:170:ASP:HB3	1:B:173:LYS:HG2	1.87	0.56
1:A:268:HIS:O	1:A:272:LYS:HG2	2.05	0.56
1:A:8:PHE:O	1:A:11:ASP:N	2.39	0.56
1:B:240:LEU:HD23	1:B:441:PHE:CZ	2.41	0.55
1:A:328:ARG:NH2	2:A:600:SO4:O1	2.31	0.55
1:B:396:ASN:ND2	1:B:436:PRO:HB2	2.21	0.55
1:A:8:PHE:HD2	1:A:9:LEU:N	2.05	0.54
1:A:240:LEU:HD13	1:A:333:MET:HE3	1.88	0.54
1:A:346:GLU:HG2	1:B:321:ASP:HA	1.89	0.54
1:A:445:ASP:OD1	1:A:449:LYS:HD2	2.06	0.54
1:B:147:PHE:O	1:B:151:GLU:HG3	2.07	0.54
1:A:505:GLY:H	1:A:528:VAL:HG22	1.74	0.53
1:A:57:THR:O	1:A:61:GLN:NE2	2.39	0.53
1:A:213:GLY:O	1:A:216:ALA:HB3	2.08	0.53
1:A:8:PHE:O	1:A:12:LEU:N	2.31	0.53
1:A:392:LEU:HD13	1:A:440:TRP:HB2	1.91	0.53
1:A:431:THR:HG23	1:A:433:THR:OG1	2.08	0.53
1:B:405:ASN:OD1	1:B:408:GLU:HB2	2.09	0.53
1:A:45:VAL:HG12	1:A:104:VAL:HG22	1.90	0.53
1:B:34:HIS:CE1	1:B:297:LEU:HD11	2.44	0.52
1:B:267:LYS:HA	1:B:267:LYS:HE2	1.90	0.52
1:A:410:ARG:HG3	1:A:440:TRP:HH2	1.74	0.52
1:A:514:LEU:O	1:A:518:ASN:ND2	2.34	0.52
1:B:9:LEU:HD12	1:B:206:HIS:CD2	2.45	0.52
1:B:233:VAL:CG1	1:B:260:SER:HB2	2.40	0.52
1:A:21:ASP:OD2	1:A:24:ARG:HD3	2.10	0.51
1:A:35:VAL:O	1:A:39:LEU:HG	2.11	0.51
1:B:421:CYS:HB3	1:B:441:PHE:HB3	1.92	0.51
1:A:237:VAL:HG22	1:A:333:MET:HE1	1.93	0.51
1:A:518:ASN:OD1	1:A:526:ARG:HD2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:467:LEU:HD12	1:A:486:LEU:HD11	1.93	0.51
1:A:334:THR:HG23	1:A:336:PRO:HD3	1.93	0.50
1:A:171:ALA:O	1:A:175:ILE:HG12	2.11	0.50
1:A:112:LYS:O	1:A:116:VAL:HG23	2.11	0.50
1:B:180:GLU:HA	1:B:180:GLU:OE2	2.10	0.50
1:B:233:VAL:CG1	1:B:260:SER:CB	2.89	0.50
1:B:443:THR:HG22	1:B:445:ASP:H	1.76	0.50
1:A:431:THR:CG2	1:A:433:THR:OG1	2.60	0.49
1:B:246:ARG:HB2	1:B:329:ALA:HA	1.93	0.49
1:A:45:VAL:HG12	1:A:104:VAL:CG2	2.42	0.49
1:B:419:VAL:O	1:B:459:VAL:HG22	2.12	0.49
1:A:338:PHE:CE1	1:A:394:LEU:HA	2.48	0.49
1:B:463:ASP:OD2	1:B:465:ARG:NH1	2.46	0.49
1:A:463:ASP:OD1	1:A:465:ARG:HB2	2.12	0.49
1:B:331:PHE:HA	1:B:389:SER:O	2.12	0.49
1:A:460:LEU:HB2	1:A:493:TRP:CD2	2.47	0.49
1:B:92:ILE:HB	1:B:95:TYR:CE2	2.49	0.48
1:A:139:VAL:HG23	1:A:174:LEU:HD22	1.93	0.48
1:A:401:SER:HG	1:A:403:THR:HG1	1.61	0.48
1:A:241:GLU:HG2	1:A:243:TYR:CE2	2.49	0.48
1:A:339:ASN:HA	1:A:371:ASN:OD1	2.12	0.48
1:B:453:ARG:HB3	1:B:495:GLN:O	2.14	0.48
1:B:287:GLY:O	1:B:324:HIS:HE1	1.97	0.48
1:A:480:ASP:O	1:A:484:GLN:HB2	2.14	0.47
1:B:34:HIS:ND1	1:B:297:LEU:HD21	2.28	0.47
1:B:209:GLU:OE2	1:B:305:ARG:NE	2.44	0.47
1:B:70:TYR:CE2	1:B:72:PRO:HA	2.48	0.47
1:A:332:VAL:HG12	1:A:380:MET:HE3	1.96	0.47
1:A:224:GLY:HA3	1:A:335:ASN:O	2.14	0.47
1:B:215:PHE:O	1:B:219:GLU:HG2	2.15	0.47
1:A:463:ASP:OD1	1:A:465:ARG:HD3	2.14	0.47
1:A:491:HIS:O	1:A:494:GLN:HB2	2.14	0.47
1:A:391:ALA:HB2	1:A:441:PHE:CD2	2.50	0.47
1:B:518:ASN:O	1:B:519:ASP:HB2	2.14	0.47
1:B:44:TYR:CD2	1:B:44:TYR:C	2.88	0.47
1:B:504:ALA:HA	1:B:528:VAL:O	2.14	0.47
1:A:425:LEU:HB3	1:A:429:LEU:HD22	1.96	0.47
1:B:44:TYR:HA	1:B:204:LEU:HD13	1.96	0.47
1:A:463:ASP:OD2	1:A:465:ARG:NH1	2.46	0.46
1:B:441:PHE:C	1:B:442:LEU:HD12	2.35	0.46
1:B:111:ASN:O	1:B:114:ARG:HB3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:TYR:CE2	1:A:214:GLN:HG3	2.50	0.46
1:B:73:ARG:HD3	1:B:73:ARG:C	2.36	0.46
1:B:92:ILE:HB	1:B:95:TYR:CD2	2.50	0.45
1:A:244:LYS:O	1:A:331:PHE:HE2	1.99	0.45
1:A:468:GLY:HA2	1:A:482:ASP:OD2	2.16	0.45
1:B:222:GLN:HE21	1:B:432:ASN:ND2	2.14	0.45
1:B:30:ALA:CA	1:B:219:GLU:OE2	2.48	0.45
1:A:338:PHE:O	1:A:339:ASN:C	2.55	0.45
1:B:445:ASP:OD2	1:B:447:ASN:HB2	2.16	0.44
1:A:457:GLY:O	1:A:511:ASP:HA	2.17	0.44
1:B:471:LYS:HB3	1:B:475:LEU:HB2	1.98	0.44
1:A:269:ALA:O	1:A:273:HIS:N	2.49	0.44
1:B:40:ILE:HD13	1:B:207:VAL:HG12	2.00	0.44
1:A:386:PRO:O	1:A:445:ASP:HB2	2.18	0.44
1:B:393:LEU:HA	1:B:438:CYS:O	2.18	0.44
1:A:34:HIS:CE1	1:A:293:THR:HG21	2.53	0.44
1:B:389:SER:OG	1:B:443:THR:HG23	2.18	0.43
1:B:376:TRP:O	1:B:380:MET:HG3	2.18	0.43
1:B:73:ARG:NH1	1:B:76:TYR:O	2.51	0.43
1:A:411:LYS:HG3	1:A:520:PHE:CE2	2.54	0.43
1:B:419:VAL:HA	1:B:442:LEU:HG	2.00	0.43
1:A:112:LYS:HD2	1:A:112:LYS:O	2.18	0.43
1:B:73:ARG:HD3	1:B:73:ARG:O	2.19	0.43
1:A:434:GLN:HB2	1:A:434:GLN:HE21	1.60	0.43
1:A:327:LEU:O	1:A:383:HIS:ND1	2.51	0.43
1:A:392:LEU:HD12	1:A:392:LEU:H	1.83	0.43
1:A:484:GLN:O	1:A:485:LYS:C	2.57	0.43
1:B:31:ASN:N	1:B:31:ASN:HD22	2.16	0.43
1:B:224:GLY:HA3	1:B:335:ASN:O	2.18	0.43
1:B:374:PHE:CE2	1:B:398:SER:HB2	2.54	0.43
1:B:449:LYS:O	1:B:452:LYS:N	2.51	0.43
1:A:516:ARG:HG3	1:A:520:PHE:CE2	2.54	0.43
1:B:173:LYS:O	1:B:177:LEU:HB2	2.19	0.43
1:B:209:GLU:CD	1:B:305:ARG:HH21	2.22	0.43
1:A:339:ASN:H	1:A:373:ASN:HD21	1.67	0.43
1:B:474:VAL:HG23	1:B:475:LEU:H	1.85	0.42
1:B:521:VAL:HG21	1:B:526:ARG:HH21	1.85	0.42
1:B:464:ALA:HB2	1:B:486:LEU:HD21	2.00	0.42
1:B:249:ASP:HA	1:B:250:PRO:HD3	1.88	0.42
1:B:106:LYS:HA	1:B:109:ARG:HD2	2.00	0.42
1:B:386:PRO:HA	1:B:444:LYS:HD3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:TYR:OH	1:A:272:LYS:HE3	2.19	0.42
1:A:332:VAL:HG11	1:A:380:MET:HB3	2.01	0.42
1:B:17:TRP:HB2	1:B:210:TYR:OH	2.19	0.42
1:A:286:TYR:HA	1:A:310:ASN:O	2.19	0.42
1:A:162:ASN:ND2	1:A:300:MET:SD	2.92	0.42
1:A:401:SER:O	1:A:410:ARG:NH2	2.43	0.42
1:B:392:LEU:HD23	1:B:440:TRP:HB2	2.01	0.42
1:B:522:LEU:O	1:B:524:PRO:HD3	2.20	0.41
1:B:268:HIS:O	1:B:272:LYS:HB2	2.20	0.41
1:B:292:PRO:O	1:B:296:LYS:HG3	2.19	0.41
1:A:207:VAL:O	1:A:207:VAL:CG1	2.67	0.41
1:B:34:HIS:HE1	1:B:297:LEU:HD11	1.85	0.41
1:B:169:LEU:HG	1:B:173:LYS:HB2	2.02	0.41
1:B:417:ASP:O	1:B:446:LYS:HE3	2.19	0.41
1:A:428:GLN:H	1:A:428:GLN:HG2	1.68	0.41
1:B:449:LYS:HB2	1:B:449:LYS:HE2	1.75	0.41
1:B:521:VAL:HG21	1:B:526:ARG:NH2	2.35	0.41
1:B:159:GLY:O	1:B:296:LYS:HE2	2.21	0.41
1:B:212:LEU:HD21	1:B:254:SER:HB2	2.03	0.41
1:B:200:SER:O	1:B:203:ILE:HB	2.21	0.41
1:B:64:ASP:C	1:B:66:ASP:H	2.22	0.41
1:A:406:GLU:O	1:A:410:ARG:HB2	2.20	0.41
1:A:288:GLN:NE2	1:A:316:ALA:O	2.39	0.41
1:A:28:ASP:O	1:A:29:ALA:C	2.58	0.41
1:A:348:LEU:O	1:A:351:ASP:HB2	2.21	0.40
1:A:339:ASN:HA	1:A:371:ASN:CG	2.42	0.40
1:B:200:SER:HA	1:B:203:ILE:HD12	2.03	0.40
1:B:96:TYR:O	1:B:97:THR:C	2.59	0.40
1:B:160:ILE:HG12	1:B:295:TRP:HZ3	1.86	0.40
1:A:139:VAL:HG23	1:A:174:LEU:CD2	2.51	0.40
1:B:450:ASN:HB2	1:B:452:LYS:HZ3	1.86	0.40
1:A:229:PRO:HB3	1:A:430:PHE:CE2	2.57	0.40
1:B:497:TRP:CD1	1:B:509:SER:HB3	2.57	0.40
1:A:17:TRP:CH2	1:A:214:GLN:HB3	2.56	0.40
1:B:64:ASP:O	1:B:66:ASP:N	2.55	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	480/544 (88%)	429 (89%)	46 (10%)	5 (1%)	19	33
1	B	479/544 (88%)	414 (86%)	58 (12%)	7 (2%)	13	22
All	All	959/1088 (88%)	843 (88%)	104 (11%)	12 (1%)	15	25

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	528	VAL
1	B	450	ASN
1	A	118	THR
1	B	65	ASP
1	B	74	GLU
1	B	116	VAL
1	B	77	ASP
1	B	430	PHE
1	A	119	LEU
1	A	496	GLU
1	B	32	TYR
1	A	270	ASN

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	413/475 (87%)	380 (92%)	33 (8%)	15	26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	411/475 (86%)	381 (93%)	30 (7%)	17 31
All	All	824/950 (87%)	761 (92%)	63 (8%)	16 29

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	7	GLN
1	A	8	PHE
1	A	28	ASP
1	A	68	ILE
1	A	79	ASP
1	A	121	THR
1	A	140	SER
1	A	148	ASP
1	A	149	ASP
1	A	152	LYS
1	A	157	LEU
1	A	167	TYR
1	A	177	LEU
1	A	202	ASP
1	A	240	LEU
1	A	241	GLU
1	A	244	LYS
1	A	292	PRO
1	A	301	ASN
1	A	334	THR
1	A	340	MET
1	A	342	ASP
1	A	363	ARG
1	A	366	THR
1	A	392	LEU
1	A	428	GLN
1	A	434	GLN
1	A	443	THR
1	A	449	LYS
1	A	465	ARG
1	A	480	ASP
1	A	481	GLU
1	B	7	GLN
1	B	8	PHE
1	B	9	LEU

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Mol	Chain	Res	Type
1	B	24	ARG
1	B	28	ASP
1	B	43	LYS
1	B	45	VAL
1	B	64	ASP
1	B	77	ASP
1	B	94	ASP
1	B	99	LYS
1	B	142	LEU
1	B	165	SER
1	B	167	TYR
1	B	180	GLU
1	B	185	SER
1	B	202	ASP
1	B	209	GLU
1	B	250	PRO
1	B	267	LYS
1	B	301	ASN
1	B	326	ASP
1	B	328	ARG
1	B	341	LYS
1	B	387	THR
1	B	411	LYS
1	B	431	THR
1	B	434	GLN
1	B	519	ASP
1	B	523	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	31	ASN
1	A	34	HIS
1	A	145	ASN
1	A	166	GLN
1	A	214	GLN
1	A	434	GLN
1	A	450	ASN
1	A	458	GLN
1	A	503	GLN
1	B	31	ASN

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Mol	Chain	Res	Type
1	B	34	HIS
1	B	83	GLN
1	B	206	HIS
1	B	279	GLN
1	B	301	ASN
1	B	324	HIS
1	B	396	ASN
1	B	432	ASN
1	B	450	ASN

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 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	600	-	4,4,4	0.61	0	6,6,6	0.51	0
2	SO4	B	600	-	4,4,4	0.81	0	6,6,6	0.47	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	600	-	-	0/0/0/0	0/0/0/0
2	SO4	B	600	-	-	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.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	600	SO4	1	0
2	B	600	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	488/544 (89%)	0.36	36 (7%)	17	20	30, 52, 68, 80	0
1	B	487/544 (89%)	0.40	34 (6%)	19	22	27, 51, 70, 82	0
All	All	975/1088 (89%)	0.38	70 (7%)	18	21	27, 52, 68, 82	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	270	ASN	5.0
1	B	9	LEU	4.3
1	A	9	LEU	4.0
1	A	141	TRP	4.0
1	B	39	LEU	4.0
1	B	36	VAL	4.0
1	A	36	VAL	3.8
1	B	442	LEU	3.8
1	A	26	ASN	3.5
1	B	42	LEU	3.3
1	A	35	VAL	3.3
1	B	441	PHE	3.3
1	A	39	LEU	3.3
1	A	176	GLY	3.2
1	A	42	LEU	3.2
1	B	38	GLY	3.0
1	A	475	LEU	3.0
1	A	115	ASP	3.0
1	B	334	THR	3.0
1	B	355	THR	2.9
1	A	442	LEU	2.9
1	B	434	GLN	2.9
1	B	45	VAL	2.9
1	A	441	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	8	PHE	2.9
1	A	278	GLU	2.9
1	B	141	TRP	2.8
1	A	218	ALA	2.8
1	A	10	ASN	2.8
1	B	10	ASN	2.8
1	A	433	THR	2.8
1	A	448	ALA	2.7
1	A	270	ASN	2.7
1	A	269	ALA	2.6
1	A	8	PHE	2.6
1	B	148	ASP	2.6
1	A	78	SER	2.6
1	B	390	MET	2.5
1	B	448	ALA	2.5
1	B	40	ILE	2.5
1	A	37	LEU	2.4
1	B	138	SER	2.4
1	A	357	ASN	2.4
1	A	38	GLY	2.4
1	A	41	PHE	2.3
1	B	78	SER	2.3
1	A	6	GLN	2.3
1	A	79	ASP	2.3
1	B	74	GLU	2.3
1	A	275	ASN	2.3
1	B	176	GLY	2.3
1	B	269	ALA	2.3
1	A	334	THR	2.3
1	B	450	ASN	2.2
1	A	474	VAL	2.2
1	B	143	ILE	2.2
1	B	474	VAL	2.2
1	B	239	MET	2.2
1	B	41	PHE	2.2
1	A	300	MET	2.1
1	A	447	ASN	2.1
1	B	364	ILE	2.1
1	A	528	VAL	2.1
1	B	35	VAL	2.1
1	B	475	LEU	2.1
1	B	380	MET	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	419	VAL	2.0
1	B	80	GLU	2.0
1	A	272	LYS	2.0
1	A	428	GLN	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 (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	SO4	B	600	5/5	0.94	0.40	10.91	39,40,44,47	0
2	SO4	A	600	5/5	0.95	0.44	8.34	44,44,48,48	0

6.5 Other polymers (i)

There are no such residues in this entry.