Full wwPDB X-ray Structure Validation Report (i)

Jun 15, 2024 – 06:56 AM EDT

PDB ID	:	1SZQ
Title	:	Crystal Structure of 2-methylcitrate dehydratase
Authors	:	Rajashankar, K.R.; Kniewel, R.; Solorzano, V.; Lima, C.D.; Burley, S.K.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on	:	2004-04-06
Resolution	:	2.70 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 (i)) were used in the production of this report:

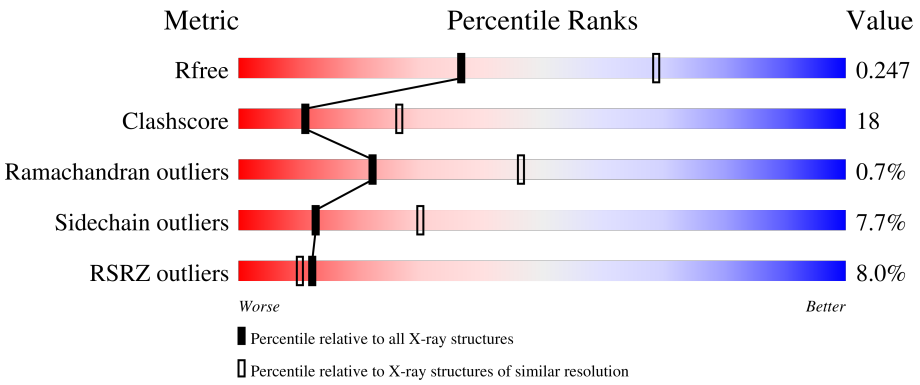
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	483	3% 66% 28%
1	B	483	13% 60% 32% 6%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 7600 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 2-methylcitrate dehydratase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	473	3719	2364	644	692	7	12	0	0	0
1	B	473	3719	2364	644	692	7	12	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	24	MSE	MET	modified residue	UNP P77243
A	95	MSE	MET	modified residue	UNP P77243
A	141	MSE	MET	modified residue	UNP P77243
A	148	MSE	MET	modified residue	UNP P77243
A	186	MSE	MET	modified residue	UNP P77243
A	238	MSE	MET	modified residue	UNP P77243
A	244	MSE	MET	modified residue	UNP P77243
A	278	MSE	MET	modified residue	UNP P77243
A	301	MSE	MET	modified residue	UNP P77243
A	307	MSE	MET	modified residue	UNP P77243
A	351	MSE	MET	modified residue	UNP P77243
A	472	MSE	MET	modified residue	UNP P77243
B	24	MSE	MET	modified residue	UNP P77243
B	95	MSE	MET	modified residue	UNP P77243
B	141	MSE	MET	modified residue	UNP P77243
B	148	MSE	MET	modified residue	UNP P77243
B	186	MSE	MET	modified residue	UNP P77243
B	238	MSE	MET	modified residue	UNP P77243
B	244	MSE	MET	modified residue	UNP P77243
B	278	MSE	MET	modified residue	UNP P77243
B	301	MSE	MET	modified residue	UNP P77243
B	307	MSE	MET	modified residue	UNP P77243
B	351	MSE	MET	modified residue	UNP P77243
B	472	MSE	MET	modified residue	UNP P77243

- Molecule 2 is water.

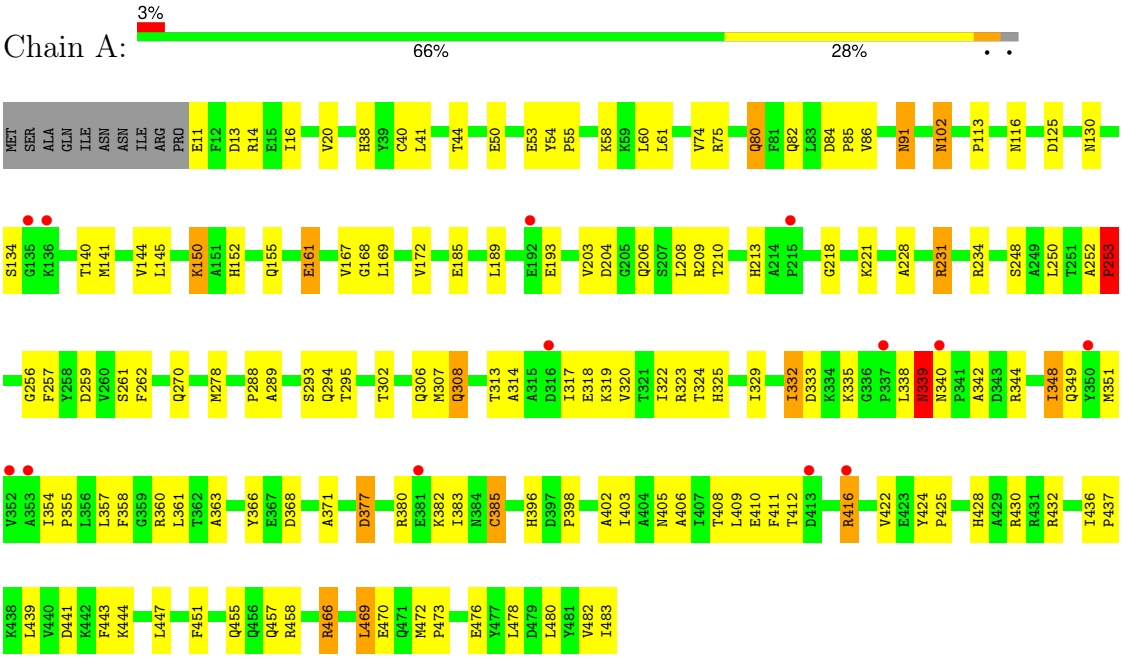
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	93	93	93	0	0
			Total	O		
2	B	69	69	69	0	0

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.

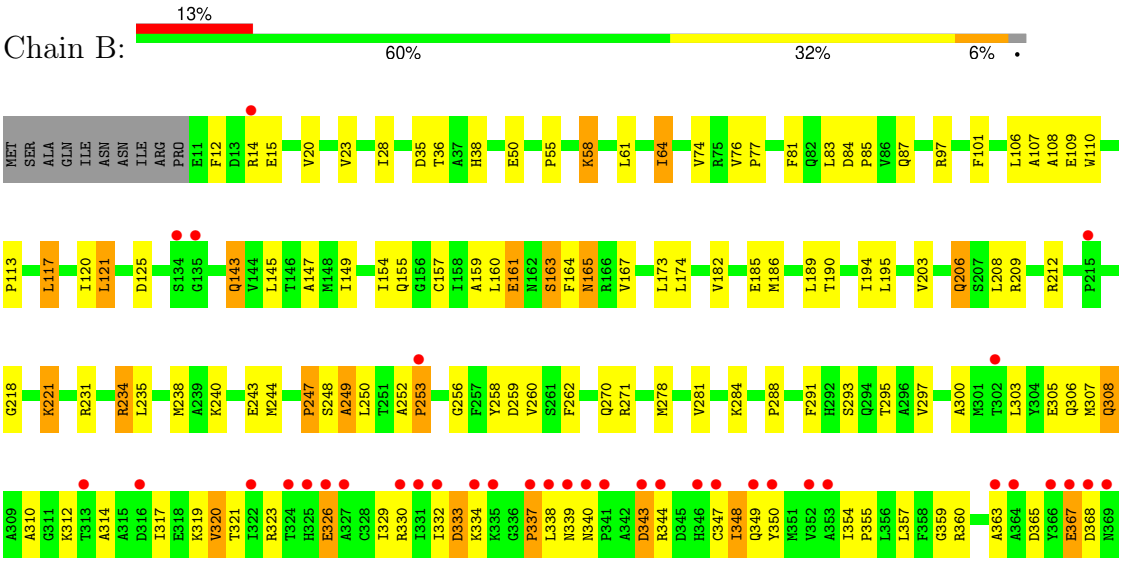
- Molecule 1: 2-methylcitrate dehydratase

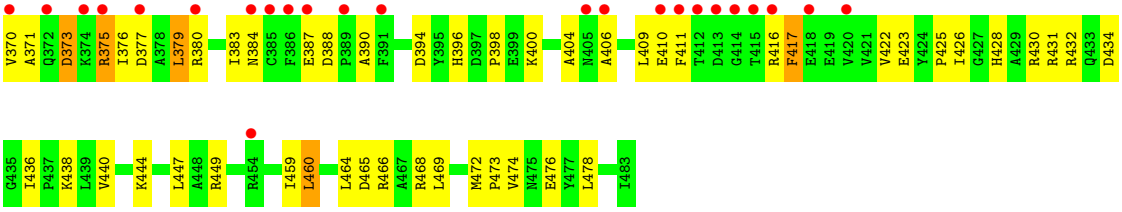
Chain A:



- Molecule 1: 2-methylcitrate dehydratase

Chain B:




V370
A371
Q372
D373
K374
R375
I376
D377
A378
L379
R380
I383
N384
G385
F386
E387
D388
P389
A390
F391
D394
Y395
H396
D397
P398
E399
K400
A404
N405
A406
L409
E410
F411
T412
D413
G414
T415
R416
F417
E418
E419
V420
V421
V422
E423
Y424
P425
I426
G427
H428
A429
R430
R431
R432
Q433
D434
G435
I436
P437
K438
L439
V440
K444
L447
A448
R449
R454
I459
L460
L464
D465
R466
A467
R468
L469
M472
P473
V474
N475
E476
Y477
L478
I483

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α, β, γ	97.58Å 97.58Å 219.75Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.70 20.04 – 2.71	Depositor EDS
% Data completeness (in resolution range)	95.4 (20.00-2.70) 98.8 (20.04-2.71)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	2.75 (at 2.71Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.204 , 0.247 0.207 , 0.247	Depositor DCC
R_{free} test set	3106 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å^2)	42.5	Xtriage
Anisotropy	0.459	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 55.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.043 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7600	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.71% 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 (i)

5.1 Standard geometry (i)

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	0.40	0/3788	0.58	0/5125
1	B	0.38	0/3788	0.56	0/5125
All	All	0.39	0/7576	0.57	0/10250

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 (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	3719	0	3689	113	0
1	B	3719	0	3689	164	0
2	A	93	0	0	5	0
2	B	69	0	0	7	0
All	All	7600	0	7378	268	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 18.

All (268) 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:322:ILE:HB	1:A:385:CYS:HB3	1.57	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:THR:HG23	1:A:422:VAL:HB	1.56	0.87
1:A:85:PRO:HG2	1:B:64:ILE:HD11	1.60	0.84
1:B:472:MSE:HE2	1:B:476:GLU:HB3	1.59	0.84
1:B:36:THR:HG22	1:B:278:MSE:HE2	1.62	0.81
1:A:307:MSE:HE3	1:A:411:PHE:CE1	2.16	0.79
1:A:44:THR:HG23	1:A:102:ASN:HD21	1.53	0.72
1:A:354:ILE:HB	1:A:355:PRO:HD3	1.71	0.72
1:B:354:ILE:HB	1:B:355:PRO:HD3	1.72	0.71
1:A:295:THR:HG22	1:A:405:ASN:HB2	1.72	0.71
1:A:172:VAL:HG13	1:A:228:ALA:HB2	1.73	0.71
1:A:332:ILE:HG23	1:A:348:ILE:HB	1.72	0.70
1:B:218:GLY:O	1:B:221:LYS:HD2	1.92	0.70
1:B:365:ASP:HA	1:B:370:VAL:HG11	1.73	0.69
1:B:373:ASP:HB2	1:B:376:ILE:HG12	1.74	0.69
1:B:320:VAL:HG13	1:B:409:LEU:HD23	1.74	0.69
1:B:338:LEU:HB2	1:B:343:ASP:HB3	1.75	0.69
1:A:332:ILE:CG2	1:A:348:ILE:HB	2.22	0.69
1:B:357:LEU:HD21	1:B:379:LEU:HD12	1.75	0.69
1:B:375:ARG:HD2	1:B:375:ARG:H	1.59	0.68
1:B:348:ILE:HD13	1:B:348:ILE:O	1.94	0.67
1:B:161:GLU:OE2	1:B:270:GLN:HB3	1.94	0.67
1:B:339:ASN:HA	1:B:344:ARG:HH12	1.58	0.67
1:B:338:LEU:HD12	1:B:338:LEU:O	1.95	0.66
1:B:323:ARG:HB3	1:B:406:ALA:HB3	1.78	0.66
1:B:165:ASN:N	1:B:165:ASN:HD22	1.92	0.66
1:B:155:GLN:HG3	1:B:174:LEU:HB3	1.77	0.66
1:B:350:TYR:HE1	1:B:376:ILE:HG23	1.60	0.66
1:A:116:ASN:HD21	1:A:155:GLN:NE2	1.93	0.65
1:B:234:ARG:HD3	1:B:238:MSE:HE2	1.78	0.65
1:A:116:ASN:HD21	1:A:155:GLN:HE21	1.45	0.65
1:A:253:PRO:O	1:A:259:ASP:OD2	2.15	0.64
1:A:295:THR:HG21	1:A:422:VAL:O	1.97	0.64
1:A:308:GLN:HE21	1:A:308:GLN:HA	1.61	0.64
1:B:189:LEU:HD21	1:B:240:LYS:HG2	1.79	0.64
1:A:13:ASP:OD1	1:A:248:SER:HA	1.98	0.63
1:B:55:PRO:HA	1:B:58:LYS:HG2	1.80	0.63
1:B:321:THR:HG22	1:B:384:ASN:HB3	1.81	0.62
1:B:329:ILE:HG13	1:B:387:GLU:HG2	1.80	0.62
1:A:86:VAL:HG23	1:B:64:ILE:HD12	1.81	0.62
1:A:55:PRO:HA	1:A:58:LYS:HG2	1.82	0.62
1:A:218:GLY:O	1:A:221:LYS:HG2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:307:MSE:HE2	1:B:312:LYS:O	2.01	0.61
1:A:368:ASP:HA	1:A:371:ALA:HB3	1.83	0.61
1:A:320:VAL:HB	1:A:383:ILE:HD13	1.83	0.60
1:B:84:ASP:HB2	1:B:85:PRO:HD2	1.82	0.60
1:A:141:MSE:HA	1:A:144:VAL:HG13	1.84	0.60
1:B:295:THR:HB	1:B:422:VAL:HB	1.82	0.60
1:B:340:ASN:HB2	1:B:343:ASP:OD1	2.02	0.60
1:A:432:ARG:O	1:A:436:ILE:HG12	2.02	0.59
1:B:36:THR:CG2	1:B:278:MSE:HE2	2.33	0.59
1:B:209:ARG:HD2	2:B:503:HOH:O	2.03	0.59
1:A:150:LYS:HD3	2:A:522:HOH:O	2.03	0.58
1:B:190:THR:O	1:B:194:ILE:HG13	2.02	0.58
1:B:404:ALA:HB2	1:B:423:GLU:HA	1.86	0.58
1:A:323:ARG:HB3	1:A:406:ALA:HB3	1.85	0.58
1:B:108:ALA:HB3	1:B:159:ALA:O	2.03	0.58
1:B:117:LEU:O	1:B:121:LEU:HB2	2.02	0.58
1:A:348:ILE:HD13	1:A:348:ILE:O	2.04	0.58
1:B:306:GLN:HB3	1:B:417:PHE:HE2	1.69	0.58
1:A:307:MSE:HE3	1:A:411:PHE:HE1	1.67	0.57
1:A:209:ARG:HH21	1:A:213:HIS:CE1	2.23	0.56
1:B:15:GLU:HG3	1:B:250:LEU:HD13	1.86	0.56
1:A:348:ILE:HG22	1:A:349:GLN:HE21	1.68	0.56
1:B:375:ARG:HB3	1:B:379:LEU:HB2	1.86	0.56
1:B:432:ARG:O	1:B:436:ILE:HG12	2.05	0.56
1:B:307:MSE:HE1	1:B:314:ALA:HA	1.88	0.56
1:B:400:LYS:HG2	1:B:430:ARG:NH1	2.21	0.56
1:A:168:GLY:HA3	1:B:260:VAL:HG13	1.88	0.56
1:B:23:VAL:HG12	1:B:185:GLU:HG3	1.88	0.56
1:A:74:VAL:O	1:A:82:GLN:HA	2.05	0.55
1:B:344:ARG:HG3	1:B:344:ARG:HH11	1.70	0.55
1:B:189:LEU:CD2	1:B:240:LYS:HG2	2.37	0.55
1:B:432:ARG:HD2	1:B:436:ILE:HD11	1.88	0.55
1:B:375:ARG:HH11	1:B:375:ARG:HG2	1.72	0.55
1:A:289:ALA:HA	1:A:351:MSE:HE2	1.89	0.55
1:A:16:ILE:O	1:A:20:VAL:HG23	2.08	0.54
1:B:293:SER:O	1:B:297:VAL:HG23	2.07	0.54
1:A:436:ILE:HB	1:A:437:PRO:HD3	1.89	0.54
1:B:339:ASN:CA	1:B:344:ARG:HH12	2.20	0.54
1:B:357:LEU:HD11	1:B:375:ARG:HB2	1.89	0.54
1:A:141:MSE:HG3	1:A:469:LEU:CD2	2.38	0.54
1:A:408:THR:HA	2:A:499:HOH:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:404:ALA:HA	1:B:422:VAL:O	2.07	0.54
1:B:447:LEU:HD21	1:B:459:ILE:HG21	1.90	0.54
1:A:458:ARG:HD2	1:A:480:LEU:HD22	1.88	0.54
1:B:23:VAL:CG2	1:B:154:ILE:HD11	2.38	0.54
1:B:460:LEU:HD22	1:B:464:LEU:HG	1.91	0.53
1:B:87:GLN:NE2	1:B:87:GLN:HA	2.23	0.53
1:B:147:ALA:HB1	1:B:182:VAL:HG11	1.89	0.53
1:B:350:TYR:CZ	1:B:354:ILE:HD11	2.44	0.53
1:A:40:CYS:HB2	1:A:278:MSE:HE1	1.91	0.53
1:A:206:GLN:HA	1:A:206:GLN:OE1	2.09	0.53
1:B:278:MSE:HE3	1:B:281:VAL:HG21	1.90	0.53
1:A:140:THR:HB	1:A:470:GLU:O	2.09	0.53
1:B:81:PHE:HB3	1:B:83:LEU:HD21	1.90	0.53
1:A:189:LEU:HB3	1:A:193:GLU:HB2	1.91	0.53
1:B:212:ARG:HG2	1:B:221:LYS:HB2	1.91	0.53
1:B:340:ASN:O	1:B:343:ASP:HB2	2.09	0.53
1:A:351:MSE:HE2	1:A:366:TYR:OH	2.09	0.52
1:A:252:ALA:HB3	1:A:256:GLY:CA	2.39	0.52
1:A:314:ALA:HB3	1:A:357:LEU:HD23	1.91	0.52
1:A:424:TYR:CZ	1:A:430:ARG:HD2	2.45	0.52
1:B:50:GLU:HG3	1:B:449:ARG:NE	2.25	0.52
1:A:329:ILE:O	1:A:333:ASP:HB3	2.10	0.52
1:B:163:SER:OG	1:B:165:ASN:ND2	2.42	0.52
1:A:324:THR:OG1	1:A:325:HIS:N	2.42	0.52
1:B:388:ASP:OD2	1:B:390:ALA:HB3	2.09	0.52
1:A:295:THR:CG2	1:A:405:ASN:HB2	2.39	0.52
1:A:134:SER:HB2	2:A:558:HOH:O	2.10	0.51
1:B:344:ARG:HH21	1:B:371:ALA:HB1	1.75	0.51
1:A:354:ILE:HG23	1:A:358:PHE:HD2	1.75	0.51
1:B:20:VAL:HG21	1:B:195:LEU:HD23	1.92	0.51
1:B:165:ASN:HD22	1:B:165:ASN:H	1.59	0.51
1:B:161:GLU:HB2	2:B:484:HOH:O	2.10	0.51
1:A:91:ASN:N	1:A:91:ASN:HD22	2.09	0.51
1:A:172:VAL:CG1	1:A:228:ALA:HB2	2.41	0.51
1:A:338:LEU:HB3	1:A:344:ARG:HG3	1.93	0.51
1:B:307:MSE:HE3	1:B:411:PHE:CE1	2.45	0.50
1:B:307:MSE:HE3	1:B:411:PHE:CZ	2.46	0.50
1:B:300:ALA:HB1	1:B:355:PRO:HB2	1.93	0.50
1:B:436:ILE:O	1:B:440:VAL:HG23	2.11	0.50
1:B:15:GLU:CD	1:B:15:GLU:H	2.13	0.50
1:A:84:ASP:HB2	1:B:64:ILE:HD13	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:402:ALA:HB2	1:A:424:TYR:CE1	2.47	0.50
1:B:337:PRO:HG3	1:B:377:ASP:OD2	2.12	0.50
1:A:172:VAL:HG13	1:A:228:ALA:CB	2.42	0.49
1:B:293:SER:HB3	1:B:332:ILE:HD12	1.94	0.49
1:B:235:LEU:HD23	1:B:238:MSE:HE3	1.95	0.49
1:B:55:PRO:HA	1:B:58:LYS:CG	2.42	0.49
1:B:165:ASN:HB3	2:B:503:HOH:O	2.13	0.49
1:B:338:LEU:HG	1:B:380:ARG:HH12	1.77	0.49
1:B:143:GLN:HG3	2:B:536:HOH:O	2.13	0.48
1:B:165:ASN:N	1:B:165:ASN:ND2	2.61	0.48
1:B:258:TYR:HA	1:B:262:PHE:HB3	1.95	0.48
1:A:416:ARG:H	1:A:416:ARG:HD3	1.78	0.48
1:A:86:VAL:CG2	1:B:64:ILE:HD12	2.43	0.48
1:B:339:ASN:HA	1:B:344:ARG:NH1	2.28	0.48
1:B:288:PRO:HG3	1:B:363:ALA:N	2.28	0.48
1:B:278:MSE:HE3	1:B:281:VAL:CG2	2.43	0.48
1:B:317:ILE:CG2	1:B:320:VAL:HG22	2.44	0.48
1:B:319:LYS:CD	1:B:321:THR:HG23	2.44	0.48
1:B:332:ILE:O	1:B:333:ASP:HB2	2.12	0.48
1:B:375:ARG:H	1:B:375:ARG:CD	2.20	0.48
2:A:492:HOH:O	1:B:244:MSE:HE3	2.14	0.48
1:B:317:ILE:HD12	1:B:409:LEU:HB3	1.95	0.48
1:B:106:LEU:HD22	1:B:110:TRP:CE2	2.49	0.47
1:A:441:ASP:HA	1:A:444:LYS:HD3	1.95	0.47
1:A:451:PHE:HB3	1:A:455:GLN:HB3	1.97	0.47
1:B:35:ASP:O	1:B:38:HIS:HB3	2.15	0.47
1:B:203:VAL:HG23	1:B:249:ALA:HB1	1.96	0.47
1:A:250:LEU:HD23	1:A:257:PHE:HB3	1.97	0.47
1:B:317:ILE:HG21	1:B:320:VAL:HG22	1.96	0.47
1:B:425:PRO:HG2	1:B:428:HIS:HB2	1.95	0.47
1:A:358:PHE:HB3	1:A:360:ARG:NH1	2.29	0.47
1:A:295:THR:CG2	1:A:422:VAL:O	2.63	0.47
1:B:145:LEU:O	1:B:149:ILE:HG13	2.15	0.47
1:B:306:GLN:HB3	1:B:417:PHE:CE2	2.50	0.47
1:A:339:ASN:HB2	1:A:340:ASN:H	1.52	0.47
1:B:319:LYS:HE2	1:B:410:GLU:HG3	1.97	0.47
1:A:102:ASN:HD22	1:A:102:ASN:HA	1.51	0.47
1:A:113:PRO:HA	1:A:155:GLN:NE2	2.30	0.46
1:A:257:PHE:CE1	1:A:261:SER:HB2	2.51	0.46
1:A:289:ALA:HA	1:A:351:MSE:CE	2.45	0.46
1:A:340:ASN:OD1	1:A:342:ALA:HB3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:338:LEU:HB2	1:B:343:ASP:CB	2.42	0.46
1:A:203:VAL:HA	1:B:208:LEU:HD12	1.97	0.46
1:B:12:PHE:CD1	1:B:247:PRO:HA	2.50	0.46
1:B:28:ILE:HD13	1:B:149:ILE:HG21	1.97	0.46
1:B:161:GLU:N	2:B:484:HOH:O	2.39	0.46
1:B:326:GLU:HG2	1:B:330:ARG:HH12	1.80	0.46
1:B:117:LEU:HD22	1:B:121:LEU:HG	1.97	0.46
1:B:120:ILE:HA	1:B:186:MSE:HE1	1.98	0.46
1:A:443:PHE:CE2	1:A:447:LEU:HD11	2.50	0.46
1:B:357:LEU:CD1	1:B:375:ARG:HB2	2.46	0.46
1:B:426:ILE:CD1	1:B:438:LYS:HG3	2.46	0.46
1:A:38:HIS:ND1	1:A:466:ARG:HG3	2.31	0.46
1:A:55:PRO:HA	1:A:58:LYS:CG	2.44	0.46
1:B:344:ARG:HG3	1:B:344:ARG:NH1	2.31	0.46
1:B:375:ARG:HD2	1:B:375:ARG:N	2.30	0.46
1:A:50:GLU:O	1:A:53:GLU:HG2	2.16	0.46
1:A:428:HIS:CE1	1:A:430:ARG:HG3	2.51	0.46
1:B:270:GLN:HE21	1:B:271:ARG:HD2	1.81	0.46
1:A:75:ARG:CD	1:A:82:GLN:HG2	2.46	0.45
1:A:302:THR:O	1:A:306:GLN:HB2	2.15	0.45
1:A:313:THR:HG22	1:A:314:ALA:N	2.31	0.45
1:A:319:LYS:HB3	1:A:410:GLU:HB2	1.97	0.45
1:A:396:HIS:O	1:A:398:PRO:HD3	2.16	0.45
1:B:253:PRO:O	1:B:259:ASP:OD2	2.34	0.45
1:B:375:ARG:HA	1:B:379:LEU:H	1.81	0.45
1:A:53:GLU:HG3	1:A:54:TYR:CE1	2.51	0.45
1:B:155:GLN:HG3	1:B:174:LEU:CB	2.43	0.45
1:B:14:ARG:HD3	2:B:497:HOH:O	2.16	0.45
1:B:74:VAL:HA	1:B:125:ASP:OD1	2.15	0.45
1:B:109:GLU:HB3	1:B:159:ALA:HB1	1.97	0.45
1:B:125:ASP:OD2	1:B:478:LEU:HD12	2.16	0.45
1:B:367:GLU:HB2	1:B:368:ASP:H	1.60	0.45
1:A:482:VAL:HG12	1:A:483:ILE:N	2.31	0.45
1:A:403:ILE:HD12	1:A:425:PRO:HG2	1.98	0.45
1:A:85:PRO:CG	1:B:64:ILE:HD11	2.38	0.44
1:A:318:GLU:HA	1:A:382:LYS:HD3	1.99	0.44
1:B:404:ALA:CB	1:B:423:GLU:HA	2.47	0.44
1:B:472:MSE:HA	1:B:473:PRO:HD3	1.88	0.44
1:B:173:LEU:HB3	1:B:206:GLN:HG3	1.98	0.44
1:A:169:LEU:HD11	1:A:261:SER:HB3	1.99	0.44
1:A:348:ILE:CG2	1:A:349:GLN:N	2.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:338:LEU:HD22	1:B:343:ASP:HB3	1.99	0.44
1:A:14:ARG:HG2	1:A:14:ARG:HH11	1.83	0.44
1:B:161:GLU:CD	1:B:270:GLN:HB3	2.38	0.44
1:B:252:ALA:HB3	1:B:256:GLY:CA	2.48	0.44
1:B:303:LEU:HB3	1:B:409:LEU:HD11	2.00	0.44
1:B:64:ILE:HG22	2:B:530:HOH:O	2.18	0.44
1:B:320:VAL:HB	1:B:383:ILE:HD13	2.00	0.43
1:B:147:ALA:HB1	1:B:182:VAL:CG1	2.47	0.43
1:A:482:VAL:CG1	1:A:483:ILE:N	2.81	0.43
1:A:208:LEU:HD22	1:B:260:VAL:HG11	2.01	0.43
1:A:354:ILE:HG22	1:A:360:ARG:O	2.18	0.43
1:B:334:LYS:H	1:B:349:GLN:NE2	2.15	0.43
1:B:426:ILE:HD11	1:B:438:LYS:HG3	1.99	0.43
1:A:60:LEU:HD21	1:B:243:GLU:HG2	2.01	0.43
1:B:164:PHE:O	1:B:167:VAL:HG22	2.19	0.43
1:B:344:ARG:HB3	1:B:350:TYR:CD2	2.54	0.42
1:B:473:PRO:O	1:B:474:VAL:C	2.57	0.42
1:B:157:CYS:O	1:B:160:LEU:HB2	2.19	0.42
1:A:288:PRO:HD2	1:A:361:LEU:O	2.18	0.42
1:A:348:ILE:HG23	1:A:349:GLN:N	2.34	0.42
1:A:58:LYS:HA	1:A:61:LEU:HG	2.01	0.42
1:B:339:ASN:HA	1:B:344:ARG:HH22	1.84	0.42
1:B:248:SER:O	1:B:250:LEU:N	2.53	0.42
1:B:400:LYS:HG2	1:B:430:ARG:HH12	1.83	0.42
1:A:363:ALA:HA	1:A:366:TYR:HD2	1.85	0.42
1:B:314:ALA:CB	1:B:357:LEU:HD23	2.50	0.42
1:A:125:ASP:CG	1:A:478:LEU:HD12	2.40	0.42
1:A:318:GLU:OE1	1:A:412:THR:HA	2.20	0.42
1:B:317:ILE:CD1	1:B:409:LEU:HD22	2.50	0.42
1:B:76:VAL:HA	1:B:77:PRO:HD3	1.93	0.41
1:B:375:ARG:HG2	1:B:375:ARG:NH1	2.34	0.41
1:A:161:GLU:OE1	1:A:270:GLN:HB3	2.19	0.41
1:A:293:SER:O	1:A:294:GLN:C	2.58	0.41
1:A:377:ASP:CG	1:A:380:ARG:HH21	2.24	0.41
1:B:165:ASN:ND2	1:B:165:ASN:H	2.18	0.41
1:A:320:VAL:HG22	1:A:409:LEU:CD2	2.50	0.41
1:B:125:ASP:HB2	1:B:478:LEU:HD12	2.03	0.41
1:B:396:HIS:O	1:B:398:PRO:HD3	2.20	0.41
1:A:141:MSE:O	1:A:144:VAL:HG13	2.21	0.41
1:B:58:LYS:HA	1:B:61:LEU:HG	2.02	0.41
1:B:107:ALA:O	1:B:108:ALA:C	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:ARG:HD2	2:A:536:HOH:O	2.20	0.41
1:A:80:GLN:N	1:A:80:GLN:CD	2.75	0.41
1:A:439:LEU:HD23	1:A:439:LEU:C	2.41	0.41
1:A:472:MSE:HE3	1:A:472:MSE:HB2	2.02	0.41
1:B:113:PRO:HA	1:B:155:GLN:HE22	1.86	0.41
1:B:355:PRO:O	1:B:359:GLY:HA2	2.21	0.41
1:B:320:VAL:CG1	1:B:409:LEU:HD23	2.49	0.41
1:B:329:ILE:HG13	1:B:387:GLU:CG	2.50	0.41
1:B:329:ILE:CG1	1:B:387:GLU:HG2	2.50	0.41
1:B:431:ARG:NH1	1:B:434:ASP:OD2	2.54	0.41
1:A:141:MSE:HA	1:A:144:VAL:CG1	2.50	0.40
1:A:472:MSE:HA	1:A:473:PRO:HD3	1.93	0.40
1:A:473:PRO:HG2	1:A:476:GLU:OE2	2.22	0.40
1:B:308:GLN:C	1:B:310:ALA:H	2.24	0.40
1:B:465:ASP:HB3	1:B:468:ARG:HB3	2.03	0.40
1:B:101:PHE:HA	1:B:284:LYS:HD2	2.03	0.40
1:A:54:TYR:HA	1:A:55:PRO:HD2	1.97	0.40
1:A:307:MSE:SE	1:A:317:ILE:HD11	2.72	0.40
1:A:204:ASP:OD1	1:A:231:ARG:NH1	2.55	0.40
1:B:278:MSE:HA	1:B:281:VAL:CG2	2.51	0.40
1:B:440:VAL:O	1:B:444:LYS:HG3	2.21	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	471/483 (98%)	440 (93%)	29 (6%)	2 (0%)	34 60
1	B	471/483 (98%)	423 (90%)	43 (9%)	5 (1%)	14 34
All	All	942/966 (98%)	863 (92%)	72 (8%)	7 (1%)	22 46

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	326	GLU
1	B	249	ALA
1	B	333	ASP
1	A	253	PRO
1	A	339	ASN
1	B	373	ASP
1	B	337	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	391/388 (101%)	363 (93%)	28 (7%)	14	34
1	B	391/388 (101%)	359 (92%)	32 (8%)	11	26
All	All	782/776 (101%)	722 (92%)	60 (8%)	13	30

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	GLU
1	A	41	LEU
1	A	80	GLN
1	A	91	ASN
1	A	102	ASN
1	A	130	ASN
1	A	145	LEU
1	A	150	LYS
1	A	152	HIS
1	A	161	GLU
1	A	167	VAL
1	A	185	GLU
1	A	210	THR
1	A	231	ARG
1	A	234	ARG
1	A	253	PRO

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Mol	Chain	Res	Type
1	A	262	PHE
1	A	308	GLN
1	A	332	ILE
1	A	335	LYS
1	A	339	ASN
1	A	348	ILE
1	A	377	ASP
1	A	385	CYS
1	A	416	ARG
1	A	457	GLN
1	A	466	ARG
1	A	469	LEU
1	B	58	LYS
1	B	64	ILE
1	B	97	ARG
1	B	117	LEU
1	B	121	LEU
1	B	143	GLN
1	B	161	GLU
1	B	163	SER
1	B	165	ASN
1	B	206	GLN
1	B	221	LYS
1	B	231	ARG
1	B	234	ARG
1	B	247	PRO
1	B	253	PRO
1	B	291	PHE
1	B	305	GLU
1	B	308	GLN
1	B	320	VAL
1	B	343	ASP
1	B	347	CYS
1	B	348	ILE
1	B	360	ARG
1	B	367	GLU
1	B	375	ARG
1	B	379	LEU
1	B	394	ASP
1	B	416	ARG
1	B	417	PHE
1	B	460	LEU

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Mol	Chain	Res	Type
1	B	466	ARG
1	B	469	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	87	GLN
1	A	102	ASN
1	A	155	GLN
1	A	294	GLN
1	A	308	GLN
1	A	349	GLN
1	A	372	GLN
1	B	87	GLN
1	B	155	GLN
1	B	165	ASN
1	B	196	ASN
1	B	206	GLN
1	B	270	GLN
1	B	306	GLN
1	B	349	GLN

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)

There are no ligands in this entry.

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 (i)

6.1 Protein, DNA and RNA chains (i)

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, 95th 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	461/483 (95%)	-0.10	13 (2%) 53 54	22, 39, 78, 87	0
1	B	461/483 (95%)	0.38	61 (13%) 3 2	22, 44, 118, 125	0
All	All	922/966 (95%)	0.14	74 (8%) 12 10	22, 41, 112, 125	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	337	PRO	6.3
1	B	414	GLY	5.7
1	B	389	PRO	5.2
1	B	334	LYS	4.9
1	B	352	VAL	4.5
1	B	374	LYS	4.5
1	B	339	ASN	4.4
1	B	368	ASP	4.1
1	B	372	GLN	4.0
1	B	330	ARG	4.0
1	B	411	PHE	3.8
1	B	135	GLY	3.8
1	B	322	ILE	3.7
1	B	387	GLU	3.7
1	B	418	GLU	3.5
1	B	413	ASP	3.4
1	A	337	PRO	3.4
1	B	370	VAL	3.2
1	B	415	THR	3.1
1	B	335	LYS	3.1
1	B	350	TYR	3.0
1	B	327	ALA	3.0
1	B	341	PRO	3.0
1	B	420	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	367	GLU	3.0
1	B	353	ALA	2.9
1	B	363	ALA	2.9
1	B	412	THR	2.9
1	B	340	ASN	2.9
1	B	343	ASP	2.8
1	B	313	THR	2.8
1	B	326	GLU	2.7
1	A	352	VAL	2.7
1	B	344	ARG	2.7
1	B	325	HIS	2.7
1	B	14	ARG	2.6
1	B	331	ILE	2.6
1	B	316	ASP	2.6
1	B	391	PHE	2.6
1	B	380	ARG	2.6
1	B	366	TYR	2.5
1	A	353	ALA	2.5
1	B	385	CYS	2.5
1	B	369	ASN	2.4
1	B	215	PRO	2.4
1	B	377	ASP	2.4
1	B	375	ARG	2.4
1	B	302	THR	2.3
1	A	416	ARG	2.3
1	B	405	ASN	2.3
1	B	410	GLU	2.3
1	A	413	ASP	2.3
1	B	338	LEU	2.3
1	A	136	LYS	2.3
1	B	134	SER	2.3
1	B	386	PHE	2.3
1	B	454	ARG	2.3
1	B	349	GLN	2.2
1	B	346	HIS	2.2
1	A	381	GLU	2.2
1	B	416	ARG	2.2
1	A	316	ASP	2.2
1	B	347	CYS	2.2
1	B	364	ALA	2.2
1	B	332	ILE	2.2
1	B	324	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	135	GLY	2.1
1	B	253	PRO	2.1
1	A	340	ASN	2.1
1	A	215	PRO	2.1
1	A	350	TYR	2.1
1	B	384	ASN	2.1
1	A	192	GLU	2.0
1	B	406	ALA	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.