Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:21 PM GMT

PDB ID	:	4OMT
Title	:	Crystal structure of human muscle phosphofructokinase (dissociated homodimer)
Authors	:	Kloos, M.; Straeter, N.
Deposited on	:	2014-01-27
Resolution	:	6.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

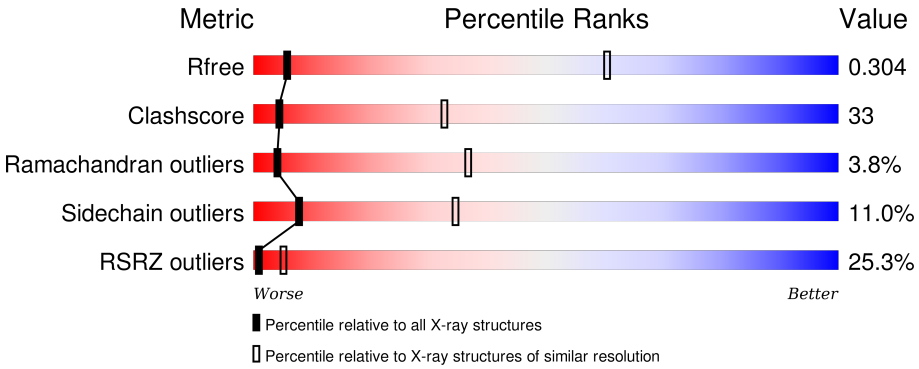
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 6.00 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	1002 (8.30-3.66)
Clashscore	102246	1050 (8.30-3.70)
Ramachandran outliers	100387	1023 (8.30-3.66)
Sidechain outliers	100360	1012 (8.30-3.64)
RSRZ outliers	91569	1001 (8.30-3.66)

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	780	24% 48% 42% 6%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 5715 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 6-phosphofructokinase, muscle type.

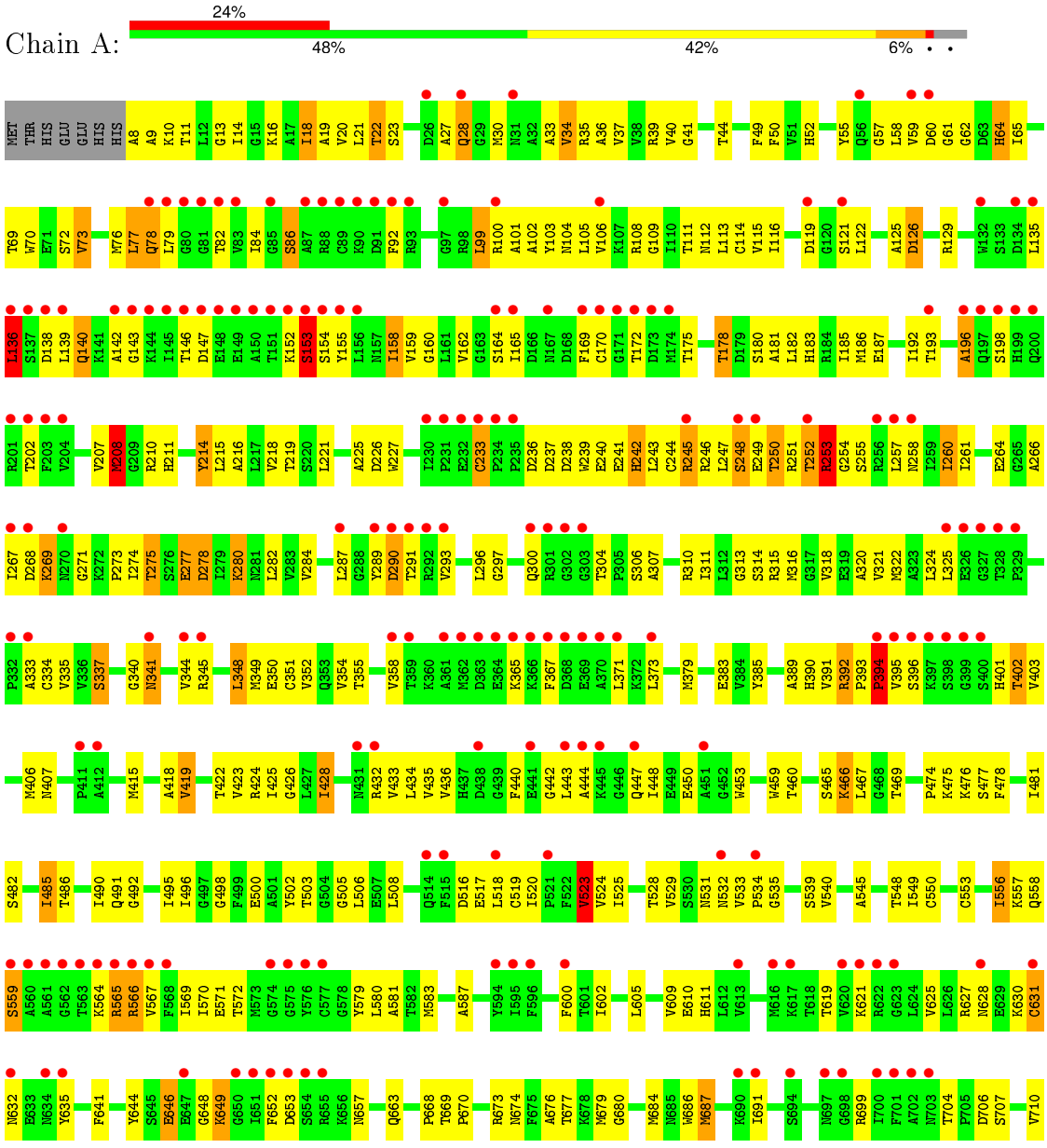
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	748	5715	3590	1018	1070	37	0	0	0

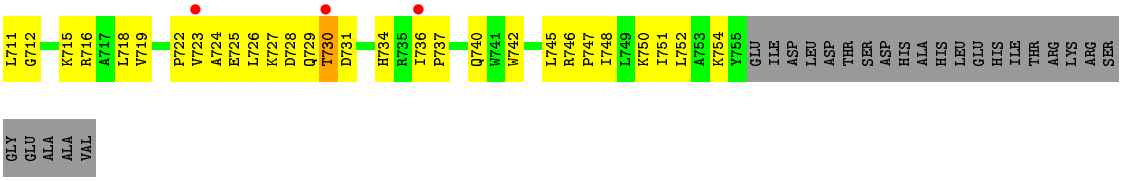
3 Residue-property plots (i)

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: 6-phosphofructokinase, muscle type

Chain A:




L711 G712 K715 R716 A717 L718 V719 P722 V723 A724 E725 L726 K727 D728 Q729 T730 D731 H734 R735 I736 P737 Q740 W741 W742 L745 R746 P747 I748 L749 K750 I751 L752 A753 K754 Y755 GLU ILE ASP LEU ASP THR SER ASP HIS ALA HIS LEU GLU HIS ILE THR ARG LYS ARG SER
GLY GLU ALA ALA VAL

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 62 2 2	Depositor
Cell constants a, b, c, α, β, γ	229.70Å 229.70Å 133.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.95 – 6.00 46.95 – 6.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (46.95-6.00) 99.9 (46.95-6.00)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	4.55 (at 6.15Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.238 , 0.274 0.272 , 0.304	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	268.6	Xtriage
Anisotropy	0.508	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 215.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 5521 reflections	Xtriage
F_o,F_c correlation	0.80	EDS
Total number of atoms	5715	wwPDB-VP
Average B, all atoms (Å^2)	194.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.61% 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

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	0.61	2/5813 (0.0%)	0.72	10/7846 (0.1%)

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	A	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	394	PRO	C-N	11.00	1.59	1.34
1	A	252	THR	CA-CB	5.18	1.66	1.53

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	394	PRO	CA-C-N	-8.24	99.07	117.20
1	A	79	LEU	CA-CB-CG	6.01	129.13	115.30
1	A	136	LEU	CA-CB-CG	5.40	127.72	115.30
1	A	99	LEU	CA-CB-CG	5.33	127.56	115.30
1	A	728	ASP	CB-CG-OD2	5.24	123.01	118.30
1	A	147	ASP	CB-CG-OD2	5.21	122.98	118.30
1	A	278	ASP	CB-CG-OD2	5.20	122.98	118.30
1	A	238	ASP	CB-CG-OD2	5.14	122.92	118.30
1	A	523	VAL	CB-CA-C	-5.13	101.66	111.40
1	A	135	LEU	CA-CB-CG	5.02	126.85	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	394	PRO	Mainchain

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	5715	0	5754	375	1
All	All	5715	0	5754	375	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 33.

All (375) 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:407:ASN:CB	1:A:469:THR:HG22	1.42	1.45
1:A:407:ASN:HB3	1:A:469:THR:CG2	1.54	1.35
1:A:275:THR:CG2	1:A:278:ASP:OD2	1.75	1.35
1:A:275:THR:HG21	1:A:278:ASP:OD2	1.24	1.31
1:A:109:GLY:HA2	1:A:152:LYS:NZ	1.42	1.29
1:A:246:ARG:O	1:A:250:THR:HG22	1.34	1.26
1:A:275:THR:HG23	1:A:278:ASP:CB	1.67	1.25
1:A:275:THR:CG2	1:A:278:ASP:CG	2.07	1.22
1:A:186:MET:CE	1:A:673:ARG:NH1	2.03	1.22
1:A:236:ASP:HA	1:A:269:LYS:CG	1.53	1.19
1:A:407:ASN:HB2	1:A:469:THR:HG22	1.33	1.09
1:A:186:MET:HE1	1:A:673:ARG:HH11	1.12	1.08
1:A:275:THR:HG23	1:A:278:ASP:HB2	1.17	1.07
1:A:99:LEU:O	1:A:103:TYR:CD2	2.08	1.05
1:A:186:MET:HE1	1:A:673:ARG:NH1	1.66	1.03
1:A:275:THR:HG21	1:A:278:ASP:CG	1.73	1.03
1:A:280:LYS:HE3	1:A:284:VAL:HG21	1.42	1.02
1:A:236:ASP:CA	1:A:269:LYS:HG2	1.90	1.01
1:A:35:ARG:HH12	1:A:752:LEU:HD13	1.22	1.01
1:A:236:ASP:HA	1:A:269:LYS:HG2	1.02	1.01
1:A:44:THR:HG21	1:A:325:LEU:HD11	1.41	1.00
1:A:175:THR:O	1:A:178:THR:HG22	1.63	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:CYS:HB2	1:A:371:LEU:HD21	1.45	0.97
1:A:247:LEU:O	1:A:250:THR:HG23	1.63	0.97
1:A:245:ARG:O	1:A:249:GLU:HG3	1.65	0.96
1:A:569:ILE:HD12	1:A:641:PHE:HA	1.48	0.96
1:A:407:ASN:CB	1:A:469:THR:CG2	2.25	0.95
1:A:407:ASN:HB3	1:A:469:THR:HG22	0.97	0.94
1:A:392:ARG:HB3	1:A:393:PRO:CA	1.97	0.94
1:A:109:GLY:HA2	1:A:152:LYS:HZ3	1.21	0.93
1:A:109:GLY:HA2	1:A:152:LYS:HZ1	1.18	0.93
1:A:335:VAL:HG23	1:A:348:LEU:HG	1.51	0.92
1:A:340:GLY:HA2	1:A:716:ARG:HA	1.49	0.92
1:A:275:THR:HG23	1:A:278:ASP:CG	1.78	0.91
1:A:99:LEU:HB2	1:A:103:TYR:HE2	1.36	0.91
1:A:233:CYS:SG	1:A:371:LEU:HD11	2.12	0.90
1:A:745:LEU:O	1:A:748:ILE:HG12	1.71	0.90
1:A:426:GLY:HA2	1:A:684:MET:HE3	1.52	0.90
1:A:407:ASN:HB3	1:A:469:THR:HG21	1.54	0.88
1:A:109:GLY:CA	1:A:152:LYS:NZ	2.35	0.88
1:A:275:THR:CG2	1:A:278:ASP:CB	2.48	0.88
1:A:506:LEU:HD22	1:A:727:LYS:HE2	1.56	0.88
1:A:275:THR:CG2	1:A:278:ASP:HB2	2.04	0.87
1:A:8:ALA:N	1:A:9:ALA:HA	1.89	0.87
1:A:99:LEU:O	1:A:103:TYR:HD2	1.55	0.86
1:A:225:ALA:HB2	1:A:261:ILE:HD13	1.57	0.86
1:A:186:MET:HE3	1:A:673:ARG:NH1	1.90	0.86
1:A:109:GLY:CA	1:A:152:LYS:HZ1	1.88	0.85
1:A:236:ASP:CA	1:A:269:LYS:CG	2.49	0.84
1:A:392:ARG:HB3	1:A:393:PRO:HA	1.57	0.84
1:A:609:VAL:C	1:A:611:HIS:H	1.82	0.81
1:A:99:LEU:C	1:A:103:TYR:CD2	2.54	0.81
1:A:241:GLU:O	1:A:245:ARG:HB3	1.81	0.80
1:A:609:VAL:O	1:A:611:HIS:N	2.14	0.80
1:A:33:ALA:O	1:A:37:VAL:HG23	1.82	0.80
1:A:392:ARG:CB	1:A:393:PRO:HA	2.10	0.80
1:A:28:GLN:H	1:A:28:GLN:HE21	1.27	0.80
1:A:524:VAL:HB	1:A:710:VAL:HG22	1.64	0.80
1:A:186:MET:CE	1:A:673:ARG:HH11	1.77	0.80
1:A:82:THR:HG21	1:A:86:SER:HB2	1.64	0.79
1:A:99:LEU:HB2	1:A:103:TYR:CE2	2.19	0.78
1:A:275:THR:HG22	1:A:278:ASP:OD2	1.81	0.78
1:A:247:LEU:HA	1:A:250:THR:CG2	2.13	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:726:LEU:O	1:A:730:THR:HG22	1.84	0.77
1:A:182:LEU:O	1:A:186:MET:HG2	1.85	0.77
1:A:236:ASP:HA	1:A:269:LYS:HG3	1.62	0.76
1:A:340:GLY:CA	1:A:716:ARG:HA	2.15	0.76
1:A:100:ARG:HA	1:A:103:TYR:HD2	1.52	0.75
1:A:106:VAL:HG13	1:A:152:LYS:HD2	1.67	0.75
1:A:100:ARG:HA	1:A:103:TYR:CD2	2.22	0.74
1:A:202:THR:HG23	1:A:258:ASN:HB2	1.66	0.74
1:A:403:VAL:HG21	1:A:684:MET:HE1	1.69	0.73
1:A:39:ARG:HD2	1:A:70:TRP:CE2	2.23	0.73
1:A:393:PRO:HG3	1:A:453:TRP:HB2	1.71	0.72
1:A:218:VAL:HG13	1:A:674:ASN:HD21	1.55	0.72
1:A:237:ASP:OD1	1:A:269:LYS:NZ	2.14	0.72
1:A:393:PRO:HB3	1:A:453:TRP:CE3	2.24	0.71
1:A:287:LEU:HB3	1:A:289:TYR:CE1	2.26	0.71
1:A:99:LEU:C	1:A:103:TYR:HD2	1.90	0.71
1:A:280:LYS:HE3	1:A:284:VAL:CG2	2.19	0.71
1:A:244:CYS:HB3	1:A:287:LEU:HD23	1.72	0.71
1:A:459:TRP:CH2	1:A:466:LYS:HB3	2.25	0.71
1:A:73:VAL:HA	1:A:76:MET:SD	2.31	0.71
1:A:280:LYS:CE	1:A:284:VAL:HG21	2.20	0.71
1:A:335:VAL:HG12	1:A:335:VAL:O	1.90	0.70
1:A:500:GLU:HA	1:A:503:THR:HB	1.73	0.70
1:A:646:GLU:HA	1:A:649:LYS:HD3	1.73	0.70
1:A:9:ALA:O	1:A:11:THR:HG22	1.92	0.70
1:A:11:THR:HA	1:A:14:ILE:HD12	1.73	0.69
1:A:175:THR:O	1:A:178:THR:CG2	2.40	0.69
1:A:243:LEU:O	1:A:247:LEU:HG	1.92	0.69
1:A:280:LYS:O	1:A:284:VAL:HG23	1.92	0.69
1:A:106:VAL:CG1	1:A:152:LYS:HD2	2.21	0.69
1:A:392:ARG:CB	1:A:393:PRO:CA	2.68	0.69
1:A:267:ILE:HA	1:A:273:PRO:HA	1.74	0.69
1:A:528:THR:HG21	1:A:532:ASN:OD1	1.93	0.69
1:A:33:ALA:HA	1:A:313:GLY:O	1.93	0.68
1:A:112:ASN:HB3	1:A:324:LEU:HD22	1.74	0.68
1:A:215:LEU:HD12	1:A:215:LEU:H	1.57	0.68
1:A:531:ASN:HA	1:A:539:SER:OG	1.94	0.68
1:A:440:PHE:C	1:A:442:GLY:H	1.96	0.68
1:A:106:VAL:HG13	1:A:152:LYS:CD	2.23	0.67
1:A:485:ILE:HG12	1:A:517:GLU:HB3	1.78	0.66
1:A:55:TYR:OH	1:A:125:ALA:HB2	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:ASP:HB3	1:A:274:ILE:HD11	1.77	0.66
1:A:82:THR:CG2	1:A:86:SER:HB2	2.26	0.65
1:A:566:ARG:HD2	1:A:653:ASP:HB3	1.78	0.65
1:A:247:LEU:C	1:A:250:THR:HG23	2.17	0.65
1:A:18:ILE:HG22	1:A:112:ASN:HB2	1.77	0.65
1:A:392:ARG:HB3	1:A:393:PRO:C	2.16	0.65
1:A:609:VAL:C	1:A:611:HIS:N	2.50	0.64
1:A:252:THR:C	1:A:254:GLY:N	2.49	0.64
1:A:20:VAL:HG23	1:A:114:CYS:HB3	1.80	0.64
1:A:252:THR:C	1:A:254:GLY:H	2.01	0.63
1:A:602:ILE:HD12	1:A:605:LEU:HB3	1.81	0.63
1:A:113:LEU:HB3	1:A:158:ILE:HG22	1.81	0.63
1:A:423:VAL:HG22	1:A:433:VAL:HG11	1.80	0.63
1:A:40:VAL:HB	1:A:321:VAL:HG21	1.80	0.63
1:A:252:THR:O	1:A:254:GLY:N	2.32	0.63
1:A:100:ARG:CA	1:A:103:TYR:HD2	2.12	0.62
1:A:415:MET:SD	1:A:469:THR:HG21	2.40	0.62
1:A:244:CYS:HB3	1:A:287:LEU:CD2	2.28	0.62
1:A:392:ARG:NH1	1:A:394:PRO:HG3	2.15	0.62
1:A:418:ALA:HA	1:A:676:ALA:O	2.00	0.62
1:A:36:ALA:O	1:A:40:VAL:HG23	2.00	0.61
1:A:506:LEU:HD22	1:A:727:LYS:CE	2.30	0.61
1:A:35:ARG:NH1	1:A:752:LEU:HD13	2.05	0.61
1:A:242:HIS:HA	1:A:245:ARG:HD2	1.82	0.61
1:A:525:ILE:HG23	1:A:679:MET:SD	2.41	0.61
1:A:280:LYS:HD3	1:A:280:LYS:C	2.21	0.61
1:A:69:THR:O	1:A:72:SER:OG	2.16	0.60
1:A:630:LYS:O	1:A:632:ASN:N	2.34	0.60
1:A:225:ALA:HB2	1:A:261:ILE:CD1	2.29	0.60
1:A:340:GLY:O	1:A:715:LYS:O	2.20	0.60
1:A:465:SER:OG	1:A:469:THR:HG23	2.01	0.60
1:A:556:ILE:HG21	1:A:570:ILE:HD11	1.84	0.59
1:A:103:TYR:CD2	1:A:139:LEU:CD1	2.86	0.59
1:A:337:SER:O	1:A:344:VAL:HG22	2.02	0.59
1:A:52:HIS:HA	1:A:84:ILE:O	2.03	0.59
1:A:186:MET:CE	1:A:673:ARG:HH12	2.08	0.58
1:A:99:LEU:CB	1:A:103:TYR:HE2	2.12	0.58
1:A:58:LEU:HG	1:A:101:ALA:HB1	1.85	0.58
1:A:39:ARG:HD2	1:A:70:TRP:CZ2	2.39	0.58
1:A:35:ARG:HH12	1:A:752:LEU:CD1	2.07	0.58
1:A:481:ILE:O	1:A:485:ILE:HG23	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:PHE:O	1:A:371:LEU:HG	2.03	0.57
1:A:186:MET:HE3	1:A:673:ARG:HH12	1.64	0.57
1:A:440:PHE:C	1:A:442:GLY:N	2.58	0.57
1:A:722:PRO:HG2	1:A:725:GLU:HB2	1.87	0.57
1:A:475:LYS:HA	1:A:478:PHE:CE2	2.40	0.57
1:A:247:LEU:CA	1:A:250:THR:CG2	2.83	0.57
1:A:296:LEU:CD1	1:A:296:LEU:H	2.17	0.57
1:A:340:GLY:O	1:A:715:LYS:C	2.43	0.57
1:A:11:THR:HA	1:A:14:ILE:CD1	2.35	0.56
1:A:502:TYR:OH	1:A:730:THR:HG21	2.06	0.56
1:A:401:HIS:ND1	1:A:491:GLN:NE2	2.53	0.56
1:A:250:THR:O	1:A:255:SER:OG	2.19	0.56
1:A:27:ALA:O	1:A:30:MET:HG3	2.05	0.56
1:A:218:VAL:HG13	1:A:674:ASN:ND2	2.21	0.56
1:A:426:GLY:CA	1:A:684:MET:HE3	2.31	0.55
1:A:605:LEU:O	1:A:609:VAL:HG23	2.06	0.55
1:A:271:GLY:O	1:A:273:PRO:HD3	2.06	0.55
1:A:481:ILE:O	1:A:485:ILE:CG2	2.54	0.55
1:A:432:ARG:HD2	1:A:450:GLU:OE2	2.06	0.55
1:A:111:THR:HG23	1:A:112:ASN:ND2	2.21	0.55
1:A:516:ASP:HA	1:A:519:CYS:SG	2.46	0.55
1:A:628:ASN:HB3	1:A:631:CYS:HB3	1.87	0.55
1:A:252:THR:HG23	1:A:253:ARG:N	2.22	0.54
1:A:182:LEU:HA	1:A:185:ILE:HD12	1.88	0.54
1:A:99:LEU:C	1:A:103:TYR:CE2	2.80	0.54
1:A:569:ILE:CD1	1:A:641:PHE:HA	2.29	0.54
1:A:296:LEU:HD12	1:A:296:LEU:H	1.71	0.54
1:A:102:ALA:HA	1:A:105:LEU:HD12	1.89	0.54
1:A:28:GLN:H	1:A:28:GLN:NE2	2.01	0.54
1:A:39:ARG:NH1	1:A:752:LEU:O	2.40	0.54
1:A:540:VAL:HG11	1:A:676:ALA:HB2	1.90	0.54
1:A:443:LEU:HA	1:A:448:ILE:HD11	1.89	0.54
1:A:99:LEU:O	1:A:139:LEU:HD11	2.07	0.53
1:A:245:ARG:O	1:A:249:GLU:CG	2.50	0.53
1:A:251:ARG:HG3	1:A:289:TYR:HE2	1.72	0.53
1:A:158:ILE:H	1:A:158:ILE:HD13	1.74	0.53
1:A:402:THR:HB	1:A:432:ARG:HE	1.73	0.53
1:A:13:GLY:CA	1:A:325:LEU:HD22	2.39	0.53
1:A:16:LYS:HD2	1:A:112:ASN:HD21	1.73	0.53
1:A:532:ASN:O	1:A:737:PRO:HD3	2.08	0.53
1:A:316:MET:SD	1:A:337:SER:HA	2.49	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:SER:HB3	1:A:121:SER:HB3	1.90	0.53
1:A:268:ASP:HB3	1:A:274:ILE:CD1	2.38	0.53
1:A:277:GLU:O	1:A:280:LYS:HB3	2.08	0.53
1:A:523:VAL:HG22	1:A:686:TRP:CZ3	2.44	0.53
1:A:44:THR:CG2	1:A:325:LEU:HD11	2.27	0.53
1:A:33:ALA:HB3	1:A:116:ILE:HD13	1.90	0.52
1:A:475:LYS:HA	1:A:478:PHE:CZ	2.43	0.52
1:A:73:VAL:HG12	1:A:76:MET:SD	2.49	0.52
1:A:69:THR:HG22	1:A:72:SER:HB3	1.92	0.52
1:A:40:VAL:HG21	1:A:318:VAL:HG22	1.91	0.52
1:A:350:GLU:O	1:A:354:VAL:HG23	2.10	0.51
1:A:495:ILE:HB	1:A:524:VAL:HG22	1.92	0.51
1:A:348:LEU:O	1:A:352:VAL:HG23	2.11	0.51
1:A:443:LEU:HD22	1:A:490:ILE:HD13	1.92	0.51
1:A:44:THR:HG21	1:A:325:LEU:CD1	2.28	0.51
1:A:21:LEU:HD11	1:A:55:TYR:HA	1.92	0.51
1:A:475:LYS:C	1:A:477:SER:H	2.14	0.51
1:A:290:ASP:CG	1:A:290:ASP:O	2.49	0.51
1:A:335:VAL:CG1	1:A:335:VAL:O	2.58	0.51
1:A:579:TYR:HD1	1:A:742:TRP:CD1	2.29	0.51
1:A:246:ARG:NH2	1:A:389:ALA:O	2.44	0.51
1:A:545:ALA:O	1:A:548:THR:HB	2.11	0.51
1:A:418:ALA:O	1:A:419:VAL:C	2.49	0.51
1:A:630:LYS:C	1:A:632:ASN:H	2.13	0.51
1:A:136:LEU:O	1:A:140:GLN:HB2	2.11	0.51
1:A:287:LEU:HB3	1:A:289:TYR:CD1	2.45	0.51
1:A:153:SER:C	1:A:155:TYR:H	2.14	0.51
1:A:275:THR:OG1	1:A:277:GLU:HG2	2.11	0.50
1:A:422:THR:HA	1:A:680:GLY:O	2.11	0.50
1:A:723:VAL:HG23	1:A:724:ALA:H	1.76	0.50
1:A:244:CYS:O	1:A:248:SER:OG	2.29	0.50
1:A:112:ASN:HB3	1:A:324:LEU:HD13	1.93	0.50
1:A:240:GLU:HB3	1:A:282:LEU:HD11	1.93	0.50
1:A:103:TYR:CD2	1:A:139:LEU:HD11	2.43	0.50
1:A:314:SER:O	1:A:318:VAL:HG23	2.12	0.50
1:A:529:VAL:HG13	1:A:545:ALA:CB	2.42	0.50
1:A:162:VAL:CG1	1:A:175:THR:HG22	2.42	0.49
1:A:482:SER:HA	1:A:485:ILE:HG23	1.94	0.49
1:A:432:ARG:HD2	1:A:450:GLU:CD	2.32	0.49
1:A:311:ILE:O	1:A:315:ARG:HG3	2.12	0.49
1:A:104:ASN:O	1:A:108:ARG:HG2	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:TRP:CD1	1:A:239:TRP:C	2.86	0.49
1:A:668:PRO:HG2	1:A:673:ARG:HE	1.78	0.49
1:A:8:ALA:N	1:A:9:ALA:CA	2.69	0.49
1:A:436:VAL:HG13	1:A:442:GLY:HA3	1.95	0.49
1:A:13:GLY:HA3	1:A:325:LEU:HD22	1.95	0.49
1:A:69:THR:CG2	1:A:72:SER:HB3	2.43	0.49
1:A:435:VAL:HG13	1:A:467:LEU:HD13	1.95	0.48
1:A:210:ARG:HG3	1:A:211:HIS:H	1.78	0.48
1:A:558:GLN:O	1:A:559:SER:O	2.32	0.48
1:A:711:LEU:HD11	1:A:718:LEU:HG	1.95	0.48
1:A:475:LYS:HG3	1:A:478:PHE:CE1	2.49	0.48
1:A:426:GLY:HA2	1:A:684:MET:CE	2.36	0.48
1:A:602:ILE:HB	1:A:635:TYR:OH	2.14	0.48
1:A:392:ARG:HB2	1:A:393:PRO:HA	1.92	0.47
1:A:35:ARG:HG3	1:A:73:VAL:HB	1.96	0.47
1:A:648:GLY:HA3	1:A:652:PHE:CZ	2.49	0.47
1:A:18:ILE:O	1:A:18:ILE:HG13	2.14	0.47
1:A:41:GLY:O	1:A:44:THR:HG22	2.13	0.47
1:A:746:ARG:N	1:A:747:PRO:HD2	2.29	0.47
1:A:35:ARG:HD3	1:A:77:LEU:HD13	1.95	0.47
1:A:159:VAL:HG11	1:A:320:ALA:HA	1.96	0.47
1:A:61:GLY:HA2	1:A:65:ILE:HD11	1.96	0.47
1:A:723:VAL:HG23	1:A:724:ALA:N	2.30	0.47
1:A:475:LYS:O	1:A:477:SER:N	2.48	0.47
1:A:424:ARG:O	1:A:425:ILE:C	2.52	0.47
1:A:395:VAL:HG12	1:A:396:SER:N	2.30	0.47
1:A:126:ASP:HB2	1:A:348:LEU:HD22	1.96	0.47
1:A:316:MET:CE	1:A:337:SER:HA	2.45	0.47
1:A:57:GLY:CA	1:A:64:HIS:HB3	2.45	0.47
1:A:40:VAL:O	1:A:44:THR:HG22	2.15	0.46
1:A:518:LEU:C	1:A:520:ILE:H	2.18	0.46
1:A:403:VAL:HG13	1:A:687:MET:HE1	1.97	0.46
1:A:225:ALA:CB	1:A:261:ILE:HD13	2.38	0.46
1:A:459:TRP:CH2	1:A:466:LYS:CB	2.97	0.46
1:A:734:HIS:O	1:A:736:ILE:HG23	2.16	0.46
1:A:103:TYR:CD1	1:A:139:LEU:HD13	2.51	0.46
1:A:492:GLY:HA3	1:A:691:ILE:HD11	1.98	0.46
1:A:55:TYR:O	1:A:58:LEU:HB3	2.15	0.46
1:A:52:HIS:O	1:A:57:GLY:HA3	2.15	0.46
1:A:340:GLY:O	1:A:341:ASN:CB	2.63	0.46
1:A:311:ILE:HD13	1:A:583:MET:CE	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:425:ILE:O	1:A:428:ILE:HG22	2.15	0.46
1:A:126:ASP:OD1	1:A:349:MET:HG2	2.16	0.45
1:A:669:THR:HB	1:A:670:PRO:HD2	1.98	0.45
1:A:13:GLY:O	1:A:16:LYS:HB2	2.16	0.45
1:A:436:VAL:HG22	1:A:448:ILE:HG12	1.98	0.45
1:A:280:LYS:HA	1:A:291:THR:HG21	1.98	0.45
1:A:242:HIS:HA	1:A:245:ARG:CD	2.46	0.45
1:A:535:GLY:O	1:A:712:GLY:HA3	2.16	0.45
1:A:159:VAL:HG22	1:A:334:CYS:HB3	1.99	0.45
1:A:78:GLN:OE1	1:A:78:GLN:N	2.46	0.45
1:A:549:ILE:O	1:A:553:CYS:SG	2.72	0.45
1:A:280:LYS:HB2	1:A:293:VAL:HG23	1.98	0.45
1:A:724:ALA:HA	1:A:727:LYS:HE3	1.99	0.45
1:A:247:LEU:HA	1:A:250:THR:HG23	1.98	0.45
1:A:340:GLY:CA	1:A:716:ARG:CA	2.93	0.45
1:A:183:HIS:O	1:A:187:GLU:HG3	2.16	0.45
1:A:109:GLY:CA	1:A:152:LYS:HZ3	2.10	0.44
1:A:403:VAL:HG13	1:A:687:MET:CE	2.47	0.44
1:A:553:CYS:O	1:A:557:LYS:HG2	2.17	0.44
1:A:407:ASN:HB2	1:A:469:THR:CG2	2.20	0.44
1:A:322:MET:HB3	1:A:345:ARG:HH21	1.81	0.44
1:A:100:ARG:N	1:A:103:TYR:HD2	2.15	0.44
1:A:602:ILE:HA	1:A:605:LEU:HB3	1.99	0.44
1:A:498:GLY:HA2	1:A:528:THR:HB	2.00	0.44
1:A:160:GLY:HA3	1:A:335:VAL:HG22	1.98	0.44
1:A:22:THR:HG21	1:A:82:THR:HG1	1.82	0.44
1:A:529:VAL:HG13	1:A:545:ALA:HB2	1.99	0.44
1:A:557:LYS:HZ3	1:A:557:LYS:HB3	1.82	0.44
1:A:34:VAL:O	1:A:35:ARG:C	2.56	0.44
1:A:122:LEU:HD22	1:A:160:GLY:HA3	1.99	0.44
1:A:311:ILE:HG21	1:A:583:MET:HE1	2.00	0.44
1:A:264:GLU:C	1:A:266:ALA:H	2.19	0.44
1:A:216:ALA:O	1:A:219:THR:HG22	2.18	0.44
1:A:196:ALA:HB3	1:A:257:LEU:HD22	2.00	0.44
1:A:246:ARG:O	1:A:250:THR:CG2	2.30	0.44
1:A:172:THR:CB	1:A:337:SER:HB2	2.48	0.44
1:A:630:LYS:C	1:A:632:ASN:N	2.72	0.44
1:A:475:LYS:C	1:A:477:SER:N	2.71	0.44
1:A:252:THR:CG2	1:A:253:ARG:N	2.80	0.43
1:A:569:ILE:HG12	1:A:625:VAL:HB	2.01	0.43
1:A:506:LEU:CD2	1:A:727:LYS:CE	2.96	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:LEU:HD13	1:A:385:TYR:HA	2.00	0.43
1:A:481:ILE:HG13	1:A:482:SER:N	2.34	0.43
1:A:55:TYR:OH	1:A:115:VAL:HG11	2.18	0.43
1:A:40:VAL:HG12	1:A:321:VAL:HG11	2.00	0.43
1:A:422:THR:O	1:A:684:MET:HG2	2.19	0.43
1:A:22:THR:HG21	1:A:82:THR:OG1	2.18	0.43
1:A:443:LEU:CD2	1:A:490:ILE:HD13	2.48	0.43
1:A:391:VAL:O	1:A:391:VAL:HG12	2.18	0.43
1:A:169:PHE:CZ	1:A:351:CYS:HB3	2.53	0.43
1:A:580:LEU:O	1:A:581:ALA:C	2.57	0.43
1:A:227:TRP:HB3	1:A:260:ILE:HG23	2.00	0.43
1:A:284:VAL:HG22	1:A:291:THR:OG1	2.19	0.43
1:A:247:LEU:HA	1:A:247:LEU:HD23	1.78	0.43
1:A:236:ASP:CB	1:A:269:LYS:HG2	2.48	0.43
1:A:403:VAL:O	1:A:434:LEU:N	2.36	0.43
1:A:406:MET:SD	1:A:495:ILE:HG12	2.59	0.43
1:A:58:LEU:HD23	1:A:92:PHE:CE1	2.54	0.43
1:A:379:MET:O	1:A:383:GLU:HG2	2.19	0.43
1:A:247:LEU:C	1:A:250:THR:CG2	2.87	0.42
1:A:352:VAL:HA	1:A:355:THR:HG22	2.00	0.42
1:A:50:PHE:CZ	1:A:84:ILE:HD11	2.54	0.42
1:A:268:ASP:O	1:A:269:LYS:C	2.57	0.42
1:A:19:ALA:HA	1:A:49:PHE:O	2.19	0.42
1:A:485:ILE:HG13	1:A:486:THR:N	2.23	0.42
1:A:505:GLY:O	1:A:508:LEU:HB2	2.20	0.42
1:A:567:VAL:N	1:A:653:ASP:O	2.48	0.42
1:A:61:GLY:HA2	1:A:65:ILE:CD1	2.49	0.42
1:A:181:ALA:O	1:A:185:ILE:HG13	2.19	0.42
1:A:600:PHE:CD1	1:A:600:PHE:N	2.87	0.42
1:A:436:VAL:CG1	1:A:442:GLY:HA3	2.49	0.42
1:A:402:THR:HB	1:A:432:ARG:HB3	2.00	0.42
1:A:247:LEU:CA	1:A:250:THR:HG23	2.49	0.42
1:A:103:TYR:CG	1:A:139:LEU:HD13	2.55	0.42
1:A:251:ARG:HG3	1:A:289:TYR:CE2	2.54	0.42
1:A:180:SER:O	1:A:183:HIS:HB2	2.20	0.42
1:A:485:ILE:HA	1:A:490:ILE:HD12	2.01	0.42
1:A:572:THR:HG21	1:A:581:ALA:HA	2.01	0.42
1:A:310:ARG:HD2	1:A:587:ALA:O	2.19	0.42
1:A:208:MET:HB2	1:A:300:GLN:OE1	2.20	0.42
1:A:571:GLU:HA	1:A:627:ARG:O	2.19	0.42
1:A:55:TYR:O	1:A:59:VAL:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:ALA:O	1:A:37:VAL:C	2.58	0.41
1:A:724:ALA:HA	1:A:727:LYS:HG3	2.02	0.41
1:A:358:VAL:HG22	1:A:373:LEU:HB3	2.01	0.41
1:A:103:TYR:OH	1:A:139:LEU:HA	2.20	0.41
1:A:609:VAL:HG22	1:A:644:TYR:CZ	2.55	0.41
1:A:333:ALA:HB1	1:A:348:LEU:HD13	2.01	0.41
1:A:140:GLN:OE1	1:A:146:THR:HB	2.20	0.41
1:A:747:PRO:O	1:A:750:LYS:HB2	2.21	0.41
1:A:306:SER:O	1:A:307:ALA:C	2.59	0.41
1:A:385:TYR:O	1:A:389:ALA:N	2.54	0.41
1:A:20:VAL:HG22	1:A:21:LEU:N	2.36	0.41
1:A:296:LEU:N	1:A:296:LEU:HD12	2.34	0.41
1:A:159:VAL:HA	1:A:334:CYS:O	2.20	0.41
1:A:287:LEU:HB3	1:A:289:TYR:HE1	1.79	0.41
1:A:214:TYR:O	1:A:215:LEU:C	2.57	0.41
1:A:440:PHE:CD1	1:A:474:PRO:HD3	2.55	0.41
1:A:207:VAL:HG12	1:A:296:LEU:HD22	2.02	0.41
1:A:646:GLU:O	1:A:649:LYS:HB2	2.21	0.41
1:A:533:VAL:HA	1:A:534:PRO:HD3	1.96	0.41
1:A:726:LEU:HD23	1:A:729:GLN:OE1	2.22	0.40
1:A:172:THR:HB	1:A:337:SER:CB	2.51	0.40
1:A:122:LEU:HD22	1:A:160:GLY:CA	2.52	0.40
1:A:106:VAL:HG13	1:A:152:LYS:HD3	2.00	0.40
1:A:340:GLY:O	1:A:715:LYS:HA	2.20	0.40
1:A:9:ALA:O	1:A:11:THR:CG2	2.64	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:396:SER:CB	1:A:396:SER:CB[4_665]	2.11	0.09

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	746/780 (96%)	619 (83%)	99 (13%)	28 (4%)	4 37

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	10	LYS
1	A	153	SER
1	A	392	ARG
1	A	444	ALA
1	A	559	SER
1	A	610	GLU
1	A	631	CYS
1	A	34	VAL
1	A	143	GLY
1	A	198	SER
1	A	208	MET
1	A	297	GLY
1	A	390	HIS
1	A	663	GLN
1	A	142	ALA
1	A	196	ALA
1	A	565	ARG
1	A	754	LYS
1	A	60	ASP
1	A	154	SER
1	A	214	TYR
1	A	476	LYS
1	A	62	GLY
1	A	253	ARG
1	A	269	LYS
1	A	341	ASN
1	A	365	LYS
1	A	419	VAL

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	607/635 (96%)	540 (89%)	67 (11%)	8 34

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ILE
1	A	22	THR
1	A	28	GLN
1	A	64	HIS
1	A	73	VAL
1	A	77	LEU
1	A	78	GLN
1	A	86	SER
1	A	119	ASP
1	A	126	ASP
1	A	129	ARG
1	A	136	LEU
1	A	138	ASP
1	A	140	GLN
1	A	153	SER
1	A	158	ILE
1	A	164	SER
1	A	165	ILE
1	A	170	CYS
1	A	178	THR
1	A	192	ILE
1	A	193	THR
1	A	208	MET
1	A	226	ASP
1	A	233	CYS
1	A	242	HIS
1	A	245	ARG
1	A	248	SER
1	A	250	THR
1	A	253	ARG
1	A	260	ILE
1	A	275	THR
1	A	277	GLU
1	A	280	LYS
1	A	290	ASP

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Mol	Chain	Res	Type
1	A	304	THR
1	A	337	SER
1	A	348	LEU
1	A	402	THR
1	A	428	ILE
1	A	447	GLN
1	A	460	THR
1	A	466	LYS
1	A	485	ILE
1	A	496	ILE
1	A	523	VAL
1	A	550	CYS
1	A	556	ILE
1	A	564	LYS
1	A	565	ARG
1	A	566	ARG
1	A	619	THR
1	A	621	LYS
1	A	646	GLU
1	A	649	LYS
1	A	657	ASN
1	A	677	THR
1	A	687	MET
1	A	699	ARG
1	A	704	THR
1	A	706	ASP
1	A	707	SER
1	A	719	VAL
1	A	730	THR
1	A	731	ASP
1	A	740	GLN
1	A	751	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	GLN
1	A	64	HIS
1	A	112	ASN
1	A	447	GLN
1	A	484	ASN
1	A	491	GLN

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Mol	Chain	Res	Type
1	A	531	ASN
1	A	642	ASN
1	A	661	HIS
1	A	674	ASN
1	A	740	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

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	748/780 (95%)	1.29	189 (25%) 1 5	60, 177, 357, 550	0

All (189) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	81	GLY	11.1
1	A	398	SER	9.0
1	A	149	GLU	9.0
1	A	302	GLY	8.0
1	A	91	ASP	7.8
1	A	89	CYS	7.4
1	A	82	THR	7.4
1	A	201	ARG	6.9
1	A	200	GLN	6.9
1	A	150	ALA	6.6
1	A	80	GLY	6.6
1	A	362	MET	6.6
1	A	153	SER	6.4
1	A	198	SER	6.2
1	A	365	LYS	6.2
1	A	565	ARG	6.1
1	A	622	ARG	6.0
1	A	154	SER	5.9
1	A	566	ARG	5.9
1	A	147	ASP	5.8
1	A	196	ALA	5.8
1	A	28	GLN	5.8
1	A	397	LYS	5.5
1	A	199	HIS	5.3
1	A	155	TYR	5.1
1	A	152	LYS	5.1
1	A	701	PHE	5.0

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Mol	Chain	Res	Type	RSRZ
1	A	146	THR	5.0
1	A	148	GLU	4.9
1	A	245	ARG	4.9
1	A	300	GLN	4.9
1	A	367	PHE	4.9
1	A	441	GLU	4.9
1	A	653	ASP	4.7
1	A	232	GLU	4.6
1	A	173	ASP	4.6
1	A	396	SER	4.5
1	A	621	LYS	4.5
1	A	138	ASP	4.5
1	A	363	ASP	4.5
1	A	165	ILE	4.4
1	A	632	ASN	4.4
1	A	233	CYS	4.4
1	A	143	GLY	4.3
1	A	394	PRO	4.3
1	A	156	LEU	4.3
1	A	563	THR	4.3
1	A	445	LYS	4.2
1	A	135	LEU	4.2
1	A	256	ARG	4.2
1	A	703	ASN	4.1
1	A	301	ARG	4.1
1	A	654	SER	4.1
1	A	170	CYS	4.0
1	A	623	GLY	4.0
1	A	287	LEU	3.9
1	A	145	ILE	3.9
1	A	92	PHE	3.8
1	A	560	ALA	3.8
1	A	652	PHE	3.8
1	A	631	CYS	3.8
1	A	136	LEU	3.8
1	A	132	TRP	3.7
1	A	257	LEU	3.7
1	A	562	GLY	3.7
1	A	333	ALA	3.6
1	A	534	PRO	3.6
1	A	87	ALA	3.6
1	A	370	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	151	THR	3.6
1	A	600	PHE	3.6
1	A	26	ASP	3.6
1	A	616	MET	3.5
1	A	364	GLU	3.5
1	A	252	THR	3.5
1	A	613	VAL	3.5
1	A	432	ARG	3.4
1	A	444	ALA	3.4
1	A	172	THR	3.4
1	A	139	LEU	3.4
1	A	651	ILE	3.4
1	A	234	PRO	3.4
1	A	635	TYR	3.3
1	A	267	ILE	3.3
1	A	561	ALA	3.3
1	A	559	SER	3.3
1	A	197	GLN	3.3
1	A	79	LEU	3.3
1	A	90	LYS	3.3
1	A	169	PHE	3.3
1	A	655	ARG	3.3
1	A	366	LYS	3.2
1	A	144	LYS	3.2
1	A	97	GLY	3.1
1	A	231	PRO	3.1
1	A	202	THR	3.1
1	A	361	ALA	3.1
1	A	690	LYS	3.1
1	A	290	ASP	3.1
1	A	617	LYS	3.1
1	A	327	GLY	3.0
1	A	400	SER	3.0
1	A	332	PRO	3.0
1	A	369	GLU	3.0
1	A	270	ASN	3.0
1	A	137	SER	2.9
1	A	577	CYS	2.9
1	A	697	ASN	2.9
1	A	514	GLN	2.9
1	A	289	TYR	2.9
1	A	358	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	567	VAL	2.9
1	A	249	GLU	2.9
1	A	171	GLY	2.9
1	A	258	ASN	2.8
1	A	83	VAL	2.8
1	A	575	GLY	2.8
1	A	576	TYR	2.8
1	A	167	ASN	2.8
1	A	447	GLN	2.8
1	A	564	LYS	2.8
1	A	164	SER	2.8
1	A	595	ILE	2.7
1	A	248	SER	2.7
1	A	78	GLN	2.7
1	A	345	ARG	2.7
1	A	371	LEU	2.7
1	A	85	GLY	2.6
1	A	650	GLY	2.6
1	A	411	PRO	2.6
1	A	325	LEU	2.6
1	A	730	THR	2.6
1	A	88	ARG	2.6
1	A	594	TYR	2.6
1	A	329	PRO	2.5
1	A	698	GLY	2.5
1	A	647	GLU	2.5
1	A	694	SER	2.5
1	A	568	PHE	2.5
1	A	341	ASN	2.5
1	A	303	GLY	2.4
1	A	399	GLY	2.4
1	A	203	PHE	2.4
1	A	368	ASP	2.4
1	A	56	GLN	2.4
1	A	359	THR	2.4
1	A	268	ASP	2.4
1	A	292	ARG	2.4
1	A	628	ASN	2.3
1	A	100	ARG	2.3
1	A	574	GLY	2.3
1	A	515	PHE	2.3
1	A	328	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	59	VAL	2.3
1	A	395	VAL	2.3
1	A	121	SER	2.2
1	A	412	ALA	2.2
1	A	596	PHE	2.2
1	A	235	PRO	2.2
1	A	702	ALA	2.2
1	A	736	ILE	2.2
1	A	344	VAL	2.2
1	A	451	ALA	2.2
1	A	700	ILE	2.2
1	A	326	GLU	2.2
1	A	532	ASN	2.2
1	A	174	MET	2.2
1	A	293	VAL	2.2
1	A	230	ILE	2.2
1	A	119	ASP	2.2
1	A	431	ASN	2.2
1	A	518	LEU	2.1
1	A	438	ASP	2.1
1	A	106	VAL	2.1
1	A	634	ASN	2.1
1	A	291	THR	2.1
1	A	723	VAL	2.1
1	A	443	LEU	2.1
1	A	620	VAL	2.1
1	A	93	ARG	2.1
1	A	60	ASP	2.1
1	A	204	VAL	2.1
1	A	31	ASN	2.0
1	A	373	LEU	2.0
1	A	134	ASP	2.0
1	A	193	THR	2.0
1	A	521	PRO	2.0
1	A	691	ILE	2.0
1	A	142	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

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.