Full wwPDB X-ray Structure Validation Report ⓘ

Oct 25, 2023 – 04:33 AM EDT

PDB ID	:	2ZAM
Title	:	Crystal structure of mouse SKD1/VPS4B apo-form
Authors	:	Inoue, M.; Kawasaki, M.; Kamikubo, H.; Kataoka, M.; Kato, R.; Yoshimori, T.; Wakatsuki, S.
Deposited on	:	2007-10-08
Resolution	:	3.50 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 ⓘ 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 ⓘ) were used in the production of this report:

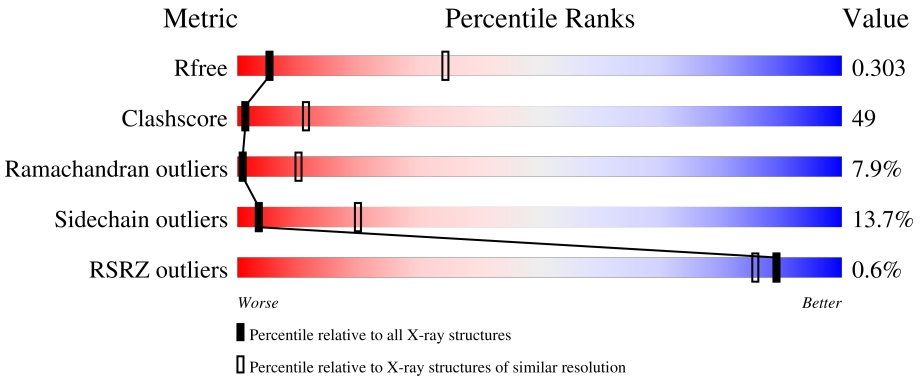
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 3.50 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	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=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	444	23% 38% 8% · 31%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2396 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 Vacuolar protein sorting-associating protein 4B.

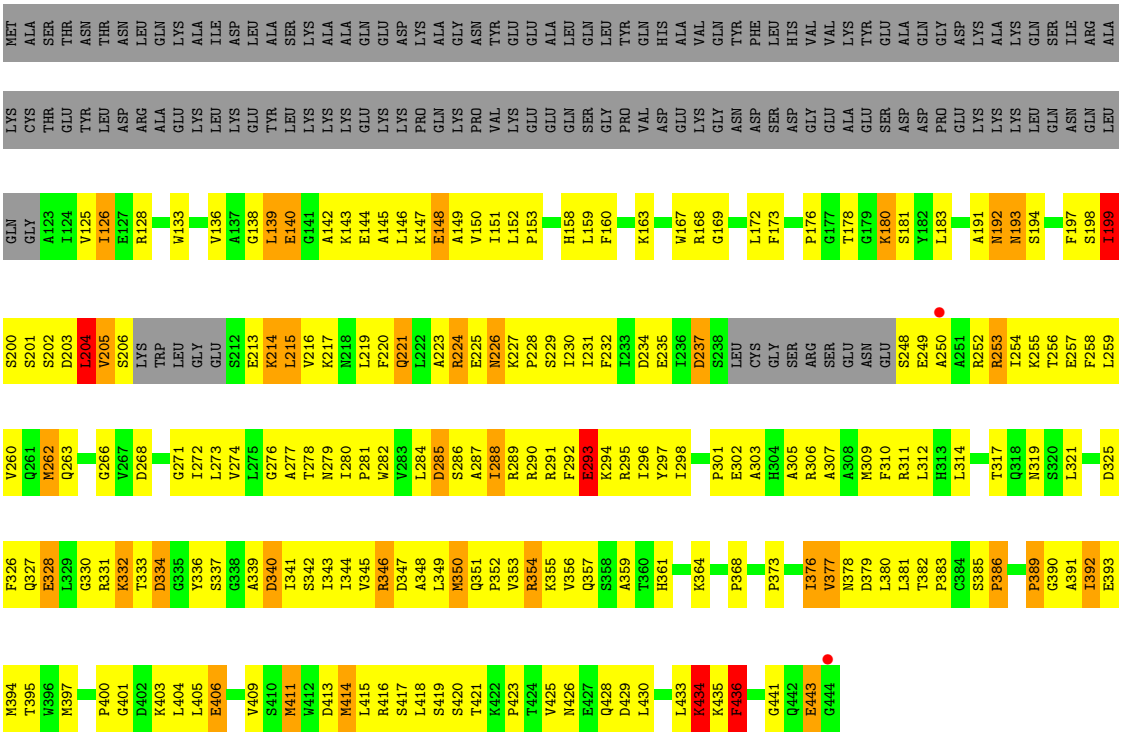
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	308	2396	1523	416	448	9	0	0	0

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: Vacuolar protein sorting-associating protein 4B

Chain A: 23% 38% 8% 31%



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α, β, γ	80.63Å 80.63Å 135.52Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 3.50 38.64 – 3.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-3.50) 90.0 (38.64-3.50)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.61 (at 3.48Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.250 , 0.304 0.253 , 0.303	Depositor DCC
R_{free} test set	251 reflections (4.42%)	wwPDB-VP
Wilson B-factor (Å^2)	105.2	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 85.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.097 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	2396	wwPDB-VP
Average B, all atoms (Å^2)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.24% 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

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	0.63	0/2443	0.83	1/3303 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	202	SER	N-CA-C	-5.33	96.59	111.00

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	2396	0	2434	239	2
All	All	2396	0	2434	239	2

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 49.

All (239) 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:328:GLU:HA	1:A:331:ARG:HE	1.24	1.01
1:A:140:GLU:CD	1:A:140:GLU:H	1.66	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:ASP:HA	1:A:277:ALA:HB3	1.48	0.96
1:A:351:GLN:HB2	1:A:352:PRO:HD3	1.50	0.93
1:A:126:ILE:HD12	1:A:126:ILE:H	1.37	0.90
1:A:285:ASP:OD2	1:A:287:ALA:HB3	1.73	0.88
1:A:361:HIS:CE1	1:A:386:PRO:HA	2.07	0.88
1:A:354:ARG:HA	1:A:357:GLN:HG2	1.56	0.88
1:A:377:VAL:HG12	1:A:378:ASN:H	1.39	0.86
1:A:152:LEU:HB2	1:A:153:PRO:HD3	1.58	0.85
1:A:385:SER:OG	1:A:386:PRO:HD2	1.83	0.79
1:A:140:GLU:CD	1:A:140:GLU:N	2.36	0.79
1:A:292:PHE:HB2	1:A:295:ARG:NH1	1.98	0.78
1:A:149:ALA:HB2	1:A:294:LYS:NZ	2.00	0.77
1:A:215:LEU:HD22	1:A:215:LEU:H	1.48	0.76
1:A:346:ARG:HG2	1:A:346:ARG:HH11	1.49	0.76
1:A:201:SER:C	1:A:203:ASP:H	1.89	0.76
1:A:125:VAL:HG22	1:A:198:SER:O	1.85	0.75
1:A:289:ARG:NH1	1:A:443:GLU:HG3	2.02	0.74
1:A:336:TYR:HD2	1:A:340:ASP:HB3	1.53	0.73
1:A:311:ARG:NH1	1:A:326:PHE:HB3	2.04	0.73
1:A:328:GLU:HA	1:A:331:ARG:NE	2.02	0.73
1:A:418:LEU:O	1:A:420:SER:N	2.22	0.73
1:A:198:SER:HG	1:A:232:PHE:HD2	1.37	0.72
1:A:325:ASP:HB3	1:A:411:MET:HE3	1.72	0.72
1:A:400:PRO:HB2	1:A:403:LYS:HB2	1.70	0.72
1:A:286:SER:O	1:A:289:ARG:HG2	1.90	0.71
1:A:354:ARG:HA	1:A:357:GLN:CG	2.19	0.71
1:A:201:SER:HB3	1:A:235:GLU:O	1.91	0.71
1:A:345:VAL:HA	1:A:414:MET:HE1	1.71	0.71
1:A:126:ILE:HD12	1:A:126:ILE:N	2.06	0.71
1:A:364:LYS:HD3	1:A:378:ASN:O	1.90	0.71
1:A:289:ARG:HH11	1:A:443:GLU:HG3	1.56	0.70
1:A:237:ASP:OD2	1:A:278:THR:OG1	2.06	0.70
1:A:252:ARG:HA	1:A:255:LYS:HB2	1.74	0.69
1:A:178:THR:HG23	1:A:180:LYS:HG3	1.74	0.69
1:A:168:ARG:CZ	1:A:271:GLY:H	2.06	0.69
1:A:203:ASP:OD1	1:A:206:SER:HB3	1.91	0.69
1:A:325:ASP:HB3	1:A:411:MET:CE	2.23	0.69
1:A:341:ILE:O	1:A:345:VAL:HG23	1.93	0.68
1:A:361:HIS:ND1	1:A:386:PRO:HA	2.08	0.68
1:A:149:ALA:HB2	1:A:294:LYS:HZ2	1.59	0.67
1:A:443:GLU:N	1:A:443:GLU:OE2	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:GLU:C	1:A:226:ASN:HD22	2.00	0.65
1:A:292:PHE:O	1:A:295:ARG:CZ	2.42	0.65
1:A:355:LYS:O	1:A:359:ALA:HB2	1.95	0.65
1:A:258:PHE:CZ	1:A:262:MET:HG3	2.32	0.65
1:A:307:ALA:HB2	1:A:330:GLY:HA3	1.79	0.65
1:A:418:LEU:C	1:A:420:SER:H	1.99	0.65
1:A:302:GLU:HB2	1:A:334:ASP:HB3	1.80	0.64
1:A:346:ARG:HG2	1:A:346:ARG:NH1	2.13	0.64
1:A:364:LYS:HG3	1:A:379:ASP:HA	1.80	0.64
1:A:230:ILE:CD1	1:A:273:LEU:HB2	2.28	0.63
1:A:286:SER:HA	1:A:289:ARG:NE	2.12	0.63
1:A:229:SER:OG	1:A:272:ILE:HD13	1.99	0.63
1:A:302:GLU:HA	1:A:306:ARG:HD2	1.80	0.63
1:A:203:ASP:O	1:A:204:LEU:HG	1.99	0.63
1:A:201:SER:C	1:A:203:ASP:N	2.53	0.62
1:A:203:ASP:C	1:A:204:LEU:HD23	2.20	0.62
1:A:230:ILE:HD13	1:A:273:LEU:HB2	1.80	0.62
1:A:280:ILE:HG22	1:A:282:TRP:CH2	2.34	0.62
1:A:434:LYS:HA	1:A:434:LYS:HE2	1.81	0.62
1:A:140:GLU:HA	1:A:143:LYS:HB2	1.82	0.62
1:A:192:ASN:O	1:A:193:ASN:HB2	1.98	0.62
1:A:280:ILE:HG13	1:A:280:ILE:O	2.00	0.62
1:A:306:ARG:NE	1:A:334:ASP:HA	2.15	0.61
1:A:290:ARG:HA	1:A:443:GLU:HG2	1.82	0.61
1:A:258:PHE:CE1	1:A:262:MET:HG3	2.36	0.61
1:A:213:GLU:HG2	1:A:254:ILE:HG13	1.82	0.61
1:A:292:PHE:HB2	1:A:295:ARG:HH11	1.66	0.60
1:A:151:ILE:CD1	1:A:151:ILE:N	2.65	0.60
1:A:133:TRP:NE1	1:A:147:LYS:HE3	2.16	0.60
1:A:229:SER:O	1:A:272:ILE:HD12	2.02	0.59
1:A:173:PHE:O	1:A:297:TYR:HA	2.02	0.59
1:A:306:ARG:HE	1:A:334:ASP:HA	1.66	0.59
1:A:191:ALA:C	1:A:193:ASN:H	2.05	0.59
1:A:178:THR:CG2	1:A:180:LYS:HG3	2.32	0.59
1:A:153:PRO:HG3	1:A:160:PHE:CZ	2.38	0.58
1:A:306:ARG:CZ	1:A:333:THR:O	2.51	0.58
1:A:286:SER:HA	1:A:289:ARG:HG2	1.85	0.58
1:A:426:ASN:ND2	1:A:429:ASP:HB2	2.18	0.58
1:A:345:VAL:O	1:A:349:LEU:HG	2.04	0.58
1:A:405:LEU:HD23	1:A:405:LEU:O	2.03	0.58
1:A:226:ASN:HD22	1:A:226:ASN:N	2.01	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:381:LEU:O	1:A:404:LEU:HD12	2.03	0.58
1:A:150:VAL:O	1:A:153:PRO:HD2	2.04	0.57
1:A:350:MET:O	1:A:351:GLN:C	2.39	0.57
1:A:151:ILE:N	1:A:151:ILE:HD12	2.17	0.57
1:A:214:LYS:HD2	1:A:217:LYS:HB2	1.86	0.57
1:A:198:SER:OG	1:A:232:PHE:HD2	1.88	0.57
1:A:295:ARG:HG3	1:A:441:GLY:O	2.04	0.57
1:A:292:PHE:C	1:A:295:ARG:CZ	2.74	0.56
1:A:220:PHE:O	1:A:223:ALA:HB3	2.06	0.56
1:A:351:GLN:HB2	1:A:352:PRO:CD	2.28	0.55
1:A:125:VAL:CG2	1:A:198:SER:HB3	2.37	0.55
1:A:138:GLY:O	1:A:140:GLU:N	2.39	0.55
1:A:252:ARG:HB3	1:A:255:LYS:HZ2	1.72	0.55
1:A:298:ILE:HG22	1:A:298:ILE:O	2.05	0.55
1:A:227:LYS:HA	1:A:228:PRO:C	2.26	0.55
1:A:234:ASP:O	1:A:235:GLU:HB2	2.07	0.55
1:A:168:ARG:NH2	1:A:271:GLY:H	2.05	0.55
1:A:138:GLY:O	1:A:143:LYS:HD2	2.07	0.55
1:A:377:VAL:HG12	1:A:378:ASN:N	2.17	0.55
1:A:150:VAL:C	1:A:153:PRO:HD2	2.28	0.54
1:A:152:LEU:HB2	1:A:153:PRO:CD	2.35	0.54
1:A:146:LEU:O	1:A:147:LYS:C	2.45	0.54
1:A:259:LEU:HA	1:A:262:MET:HB2	1.90	0.53
1:A:343:ILE:O	1:A:346:ARG:HB3	2.09	0.53
1:A:415:LEU:O	1:A:418:LEU:HB3	2.09	0.53
1:A:307:ALA:C	1:A:309:MET:N	2.61	0.53
1:A:231:ILE:HG12	1:A:272:ILE:HD11	1.91	0.52
1:A:172:LEU:HB2	1:A:276:GLY:O	2.10	0.52
1:A:237:ASP:OD1	1:A:237:ASP:N	2.41	0.52
1:A:392:ILE:HD13	1:A:392:ILE:N	2.25	0.52
1:A:204:LEU:HD23	1:A:204:LEU:N	2.25	0.52
1:A:149:ALA:HB2	1:A:294:LYS:HZ1	1.72	0.52
1:A:213:GLU:O	1:A:215:LEU:N	2.43	0.51
1:A:305:ALA:O	1:A:309:MET:HB2	2.10	0.51
1:A:292:PHE:O	1:A:293:GLU:C	2.48	0.51
1:A:180:LYS:HE2	1:A:180:LYS:H	1.75	0.51
1:A:426:ASN:CG	1:A:429:ASP:HB2	2.32	0.51
1:A:153:PRO:HG3	1:A:160:PHE:CE2	2.46	0.51
1:A:368:PRO:HB3	1:A:373:PRO:HA	1.93	0.51
1:A:201:SER:OG	1:A:235:GLU:HB3	2.10	0.50
1:A:216:VAL:O	1:A:219:LEU:HB3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:GLN:O	1:A:331:ARG:HG2	2.11	0.50
1:A:311:ARG:HH11	1:A:326:PHE:HB3	1.76	0.50
1:A:292:PHE:O	1:A:294:LYS:N	2.44	0.50
1:A:347:ASP:O	1:A:351:GLN:HG2	2.11	0.50
1:A:306:ARG:HG3	1:A:341:ILE:HD11	1.93	0.50
1:A:339:ALA:O	1:A:340:ASP:C	2.49	0.50
1:A:257:GLU:OE1	1:A:257:GLU:HA	2.12	0.49
1:A:259:LEU:HG	1:A:291:ARG:HD2	1.94	0.49
1:A:311:ARG:NH1	1:A:326:PHE:CB	2.75	0.49
1:A:307:ALA:HB1	1:A:326:PHE:O	2.13	0.49
1:A:334:ASP:N	1:A:334:ASP:OD2	2.46	0.49
1:A:418:LEU:C	1:A:420:SER:N	2.65	0.49
1:A:253:ARG:HB3	1:A:254:ILE:HD12	1.94	0.48
1:A:227:LYS:HA	1:A:228:PRO:O	2.13	0.48
1:A:197:PHE:CE1	1:A:223:ALA:HA	2.48	0.48
1:A:292:PHE:CB	1:A:295:ARG:NH1	2.72	0.48
1:A:430:LEU:O	1:A:430:LEU:HD23	2.13	0.48
1:A:382:THR:OG1	1:A:383:PRO:HD2	2.14	0.48
1:A:400:PRO:HG2	1:A:403:LYS:HD2	1.96	0.48
1:A:337:SER:H	1:A:340:ASP:HB2	1.79	0.47
1:A:400:PRO:HB2	1:A:403:LYS:CB	2.41	0.47
1:A:125:VAL:HG22	1:A:198:SER:C	2.34	0.47
1:A:391:ALA:C	1:A:392:ILE:HD13	2.34	0.47
1:A:307:ALA:O	1:A:309:MET:N	2.48	0.47
1:A:336:TYR:CD2	1:A:340:ASP:HB3	2.42	0.47
1:A:259:LEU:O	1:A:259:LEU:HD23	2.14	0.47
1:A:319:ASN:HB2	1:A:321:LEU:HD13	1.96	0.46
1:A:126:ILE:N	1:A:126:ILE:CD1	2.70	0.46
1:A:302:GLU:CB	1:A:334:ASP:HB3	2.45	0.46
1:A:311:ARG:HH11	1:A:326:PHE:CB	2.28	0.46
1:A:125:VAL:HG21	1:A:198:SER:HB3	1.97	0.46
1:A:352:PRO:O	1:A:356:VAL:HG23	2.15	0.46
1:A:319:ASN:HA	1:A:409:VAL:O	2.15	0.46
1:A:256:THR:O	1:A:260:VAL:HG23	2.16	0.46
1:A:292:PHE:CA	1:A:295:ARG:NH1	2.79	0.46
1:A:232:PHE:CZ	1:A:234:ASP:HB2	2.50	0.46
1:A:307:ALA:C	1:A:309:MET:H	2.20	0.46
1:A:221:GLN:O	1:A:225:GLU:HB2	2.15	0.46
1:A:287:ALA:O	1:A:288:ILE:C	2.54	0.45
1:A:259:LEU:O	1:A:263:GLN:N	2.40	0.45
1:A:176:PRO:HA	1:A:279:ASN:OD1	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:GLU:CG	1:A:145:ALA:N	2.79	0.45
1:A:380:LEU:HA	1:A:403:LYS:O	2.16	0.45
1:A:411:MET:O	1:A:415:LEU:HG	2.16	0.45
1:A:344:ILE:N	1:A:344:ILE:HD12	2.31	0.45
1:A:286:SER:HA	1:A:289:ARG:CD	2.46	0.45
1:A:394:MET:O	1:A:395:THR:HG23	2.17	0.45
1:A:232:PHE:CE2	1:A:234:ASP:HB2	2.53	0.44
1:A:191:ALA:C	1:A:193:ASN:N	2.70	0.44
1:A:339:ALA:O	1:A:343:ILE:HG13	2.17	0.44
1:A:348:ALA:HA	1:A:351:GLN:HG3	2.00	0.44
1:A:144:GLU:HG3	1:A:145:ALA:N	2.32	0.44
1:A:231:ILE:HB	1:A:274:VAL:HG22	1.97	0.44
1:A:146:LEU:HD22	1:A:296:ILE:HD13	1.99	0.44
1:A:339:ALA:O	1:A:342:SER:N	2.50	0.44
1:A:416:ARG:NH1	1:A:420:SER:OG	2.51	0.44
1:A:301:PRO:HG2	1:A:301:PRO:O	2.18	0.44
1:A:382:THR:HB	1:A:405:LEU:HB3	1.98	0.44
1:A:433:LEU:O	1:A:434:LYS:C	2.56	0.44
1:A:325:ASP:CB	1:A:411:MET:HE3	2.46	0.44
1:A:433:LEU:O	1:A:435:LYS:N	2.50	0.44
1:A:142:ALA:O	1:A:145:ALA:HB3	2.17	0.43
1:A:205:VAL:O	1:A:206:SER:O	2.36	0.43
1:A:286:SER:CA	1:A:289:ARG:HG2	2.47	0.43
1:A:281:PRO:HB2	1:A:436:PHE:CD2	2.54	0.43
1:A:321:LEU:N	1:A:321:LEU:HD12	2.34	0.43
1:A:191:ALA:O	1:A:193:ASN:N	2.52	0.43
1:A:203:ASP:CG	1:A:206:SER:HB3	2.39	0.43
1:A:305:ALA:O	1:A:309:MET:N	2.52	0.43
1:A:400:PRO:O	1:A:401:GLY:C	2.56	0.43
1:A:248:SER:OG	1:A:249:GLU:N	2.52	0.43
1:A:311:ARG:HH12	1:A:326:PHE:HB3	1.79	0.43
1:A:385:SER:HG	1:A:386:PRO:HD2	1.83	0.43
1:A:125:VAL:CG2	1:A:125:VAL:O	2.67	0.42
1:A:312:LEU:HD23	1:A:312:LEU:C	2.40	0.42
1:A:332:LYS:C	1:A:333:THR:HG1	2.20	0.42
1:A:346:ARG:O	1:A:350:MET:HE1	2.19	0.42
1:A:126:ILE:HG22	1:A:197:PHE:CD2	2.53	0.42
1:A:224:ARG:H	1:A:224:ARG:HD3	1.84	0.42
1:A:125:VAL:O	1:A:125:VAL:HG23	2.19	0.42
1:A:310:PHE:CZ	1:A:341:ILE:HG23	2.53	0.42
1:A:180:LYS:O	1:A:183:LEU:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:ARG:O	1:A:128:ARG:HG3	2.19	0.42
1:A:138:GLY:C	1:A:140:GLU:OE2	2.57	0.42
1:A:199:ILE:HB	1:A:200:SER:H	1.58	0.42
1:A:340:ASP:O	1:A:341:ILE:C	2.58	0.42
1:A:405:LEU:HD23	1:A:405:LEU:C	2.40	0.42
1:A:321:LEU:HD12	1:A:321:LEU:H	1.84	0.42
1:A:167:TRP:H	1:A:167:TRP:HE3	1.61	0.42
1:A:194:SER:HB3	1:A:229:SER:N	2.35	0.42
1:A:286:SER:OG	1:A:289:ARG:NH2	2.53	0.42
1:A:368:PRO:HA	1:A:376:ILE:HA	2.02	0.42
1:A:286:SER:C	1:A:289:ARG:HG2	2.39	0.41
1:A:136:VAL:HB	1:A:143:LYS:HE2	2.02	0.41
1:A:220:PHE:HB3	1:A:224:ARG:NH1	2.35	0.41
1:A:344:ILE:HG23	1:A:417:SER:OG	2.21	0.41
1:A:413:ASP:O	1:A:414:MET:C	2.57	0.41
1:A:423:PRO:C	1:A:425:VAL:H	2.23	0.41
1:A:169:GLY:N	1:A:293:GLU:OE1	2.42	0.41
1:A:314:LEU:HD23	1:A:314:LEU:HA	1.83	0.41
1:A:350:MET:O	1:A:353:VAL:N	2.52	0.41
1:A:237:ASP:HA	1:A:284:LEU:HD21	2.03	0.41
1:A:136:VAL:HG11	1:A:183:LEU:HD13	2.03	0.41
1:A:348:ALA:HA	1:A:351:GLN:CG	2.51	0.41
1:A:192:ASN:O	1:A:193:ASN:CB	2.64	0.40
1:A:197:PHE:CE1	1:A:229:SER:CB	3.05	0.40
1:A:259:LEU:HD23	1:A:259:LEU:C	2.42	0.40
1:A:346:ARG:O	1:A:350:MET:CE	2.69	0.40
1:A:411:MET:SD	1:A:415:LEU:HD11	2.60	0.40
1:A:213:GLU:C	1:A:213:GLU:CD	2.79	0.40
1:A:286:SER:HA	1:A:289:ARG:CG	2.50	0.40
1:A:168:ARG:NH1	1:A:272:ILE:N	2.68	0.40
1:A:205:VAL:O	1:A:205:VAL:HG12	2.21	0.40
1:A:292:PHE:CD1	1:A:292:PHE:N	2.90	0.40

All (2) 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:158:HIS:O	1:A:406:GLU:OE2[5_555]	1.96	0.24
1:A:148:GLU:OE2	1:A:357:GLN:OE1[5_555]	2.19	0.01

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	302/444 (68%)	222 (74%)	56 (18%)	24 (8%)	1 10

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	139	LEU
1	A	163	LYS
1	A	214	LYS
1	A	250	ALA
1	A	293	GLU
1	A	419	SER
1	A	193	ASN
1	A	199	ILE
1	A	204	LEU
1	A	386	PRO
1	A	434	LYS
1	A	192	ASN
1	A	340	ASP
1	A	389	PRO
1	A	414	MET
1	A	303	ALA
1	A	393	GLU
1	A	436	PHE
1	A	443	GLU
1	A	377	VAL
1	A	390	GLY
1	A	266	GLY
1	A	205	VAL
1	A	288	ILE

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	263/378 (70%)	227 (86%)	36 (14%)	3 20

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	126	ILE
1	A	139	LEU
1	A	140	GLU
1	A	148	GLU
1	A	159	LEU
1	A	180	LYS
1	A	181	SER
1	A	199	ILE
1	A	204	LEU
1	A	215	LEU
1	A	221	GLN
1	A	224	ARG
1	A	226	ASN
1	A	237	ASP
1	A	253	ARG
1	A	262	MET
1	A	268	ASP
1	A	285	ASP
1	A	293	GLU
1	A	317	THR
1	A	328	GLU
1	A	332	LYS
1	A	334	ASP
1	A	346	ARG
1	A	350	MET
1	A	354	ARG
1	A	376	ILE
1	A	389	PRO
1	A	392	ILE
1	A	397	MET

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Mol	Chain	Res	Type
1	A	406	GLU
1	A	411	MET
1	A	421	THR
1	A	428	GLN
1	A	434	LYS
1	A	436	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	221	GLN
1	A	226	ASN
1	A	304	HIS
1	A	327	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 monosaccharides 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	308/444 (69%)	-0.38	2 (0%)	89	86	42, 83, 121, 133	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	444	GLY	3.0
1	A	250	ALA	2.4

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no monosaccharides 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.