Full wwPDB X-ray Structure Validation Report ⓘ

Dec 16, 2023 – 01:53 pm GMT

PDB ID	:	4BI9
Title	:	Crystal structure of wild-type SCP2 thiolase from Trypanosoma brucei.
Authors	:	Harijan, R.K.; Kiema, T.-R.; Weiss, M.S.; Michels, P.A.M.; Wierenga, R.K.
Deposited on	:	2013-04-10
Resolution	:	2.45 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:

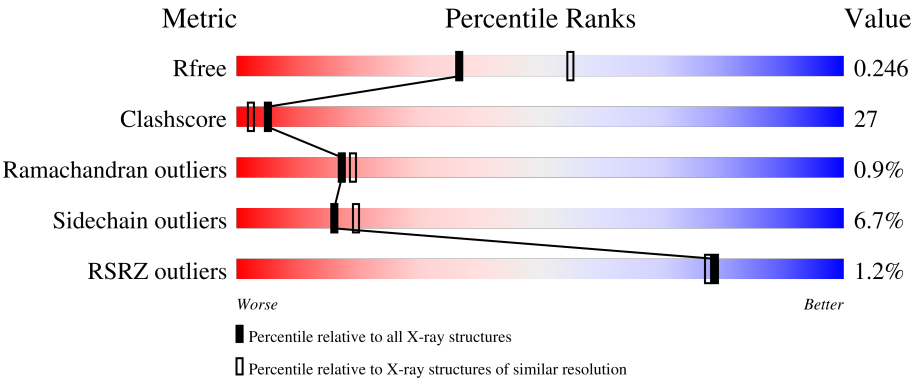
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.45 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	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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	454	2% 44% 44% • 8%
1	B	454	% 44% 45% • 8%
1	C	454	% 45% 44% • 8%
1	D	454	% 45% 43% • 8%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 12349 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 3-KETOACYL-COA THIOLASE, PUTATIVE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	418	Total	C	N	O	S	0	0	0
			3073	1924	540	592	17			
1	B	416	Total	C	N	O	S	0	0	0
			3069	1921	542	589	17			
1	C	419	Total	C	N	O	S	0	0	0
			3087	1931	545	594	17			
1	D	416	Total	C	N	O	S	0	0	0
			3066	1920	541	588	17			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	HIS	-	expression tag	UNP Q57XD5
A	-14	HIS	-	expression tag	UNP Q57XD5
A	-13	HIS	-	expression tag	UNP Q57XD5
A	-12	HIS	-	expression tag	UNP Q57XD5
A	-11	HIS	-	expression tag	UNP Q57XD5
A	-10	HIS	-	expression tag	UNP Q57XD5
A	-9	SER	-	expression tag	UNP Q57XD5
A	-8	SER	-	expression tag	UNP Q57XD5
A	-7	GLY	-	expression tag	UNP Q57XD5
A	-6	LEU	-	expression tag	UNP Q57XD5
A	-5	VAL	-	expression tag	UNP Q57XD5
A	-4	PRO	-	expression tag	UNP Q57XD5
A	-3	ARG	-	expression tag	UNP Q57XD5
A	-2	GLY	-	expression tag	UNP Q57XD5
A	-1	SER	-	expression tag	UNP Q57XD5
A	0	HIS	-	expression tag	UNP Q57XD5
B	-15	HIS	-	expression tag	UNP Q57XD5
B	-14	HIS	-	expression tag	UNP Q57XD5
B	-13	HIS	-	expression tag	UNP Q57XD5
B	-12	HIS	-	expression tag	UNP Q57XD5
B	-11	HIS	-	expression tag	UNP Q57XD5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-10	HIS	-	expression tag	UNP Q57XD5
B	-9	SER	-	expression tag	UNP Q57XD5
B	-8	SER	-	expression tag	UNP Q57XD5
B	-7	GLY	-	expression tag	UNP Q57XD5
B	-6	LEU	-	expression tag	UNP Q57XD5
B	-5	VAL	-	expression tag	UNP Q57XD5
B	-4	PRO	-	expression tag	UNP Q57XD5
B	-3	ARG	-	expression tag	UNP Q57XD5
B	-2	GLY	-	expression tag	UNP Q57XD5
B	-1	SER	-	expression tag	UNP Q57XD5
B	0	HIS	-	expression tag	UNP Q57XD5
C	-15	HIS	-	expression tag	UNP Q57XD5
C	-14	HIS	-	expression tag	UNP Q57XD5
C	-13	HIS	-	expression tag	UNP Q57XD5
C	-12	HIS	-	expression tag	UNP Q57XD5
C	-11	HIS	-	expression tag	UNP Q57XD5
C	-10	HIS	-	expression tag	UNP Q57XD5
C	-9	SER	-	expression tag	UNP Q57XD5
C	-8	SER	-	expression tag	UNP Q57XD5
C	-7	GLY	-	expression tag	UNP Q57XD5
C	-6	LEU	-	expression tag	UNP Q57XD5
C	-5	VAL	-	expression tag	UNP Q57XD5
C	-4	PRO	-	expression tag	UNP Q57XD5
C	-3	ARG	-	expression tag	UNP Q57XD5
C	-2	GLY	-	expression tag	UNP Q57XD5
C	-1	SER	-	expression tag	UNP Q57XD5
C	0	HIS	-	expression tag	UNP Q57XD5
D	-15	HIS	-	expression tag	UNP Q57XD5
D	-14	HIS	-	expression tag	UNP Q57XD5
D	-13	HIS	-	expression tag	UNP Q57XD5
D	-12	HIS	-	expression tag	UNP Q57XD5
D	-11	HIS	-	expression tag	UNP Q57XD5
D	-10	HIS	-	expression tag	UNP Q57XD5
D	-9	SER	-	expression tag	UNP Q57XD5
D	-8	SER	-	expression tag	UNP Q57XD5
D	-7	GLY	-	expression tag	UNP Q57XD5
D	-6	LEU	-	expression tag	UNP Q57XD5
D	-5	VAL	-	expression tag	UNP Q57XD5
D	-4	PRO	-	expression tag	UNP Q57XD5
D	-3	ARG	-	expression tag	UNP Q57XD5
D	-2	GLY	-	expression tag	UNP Q57XD5
D	-1	SER	-	expression tag	UNP Q57XD5

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Chain	Residue	Modelled	Actual	Comment	Reference
D	0	HIS	-	expression tag	UNP Q57XD5

- Molecule 2 is water.

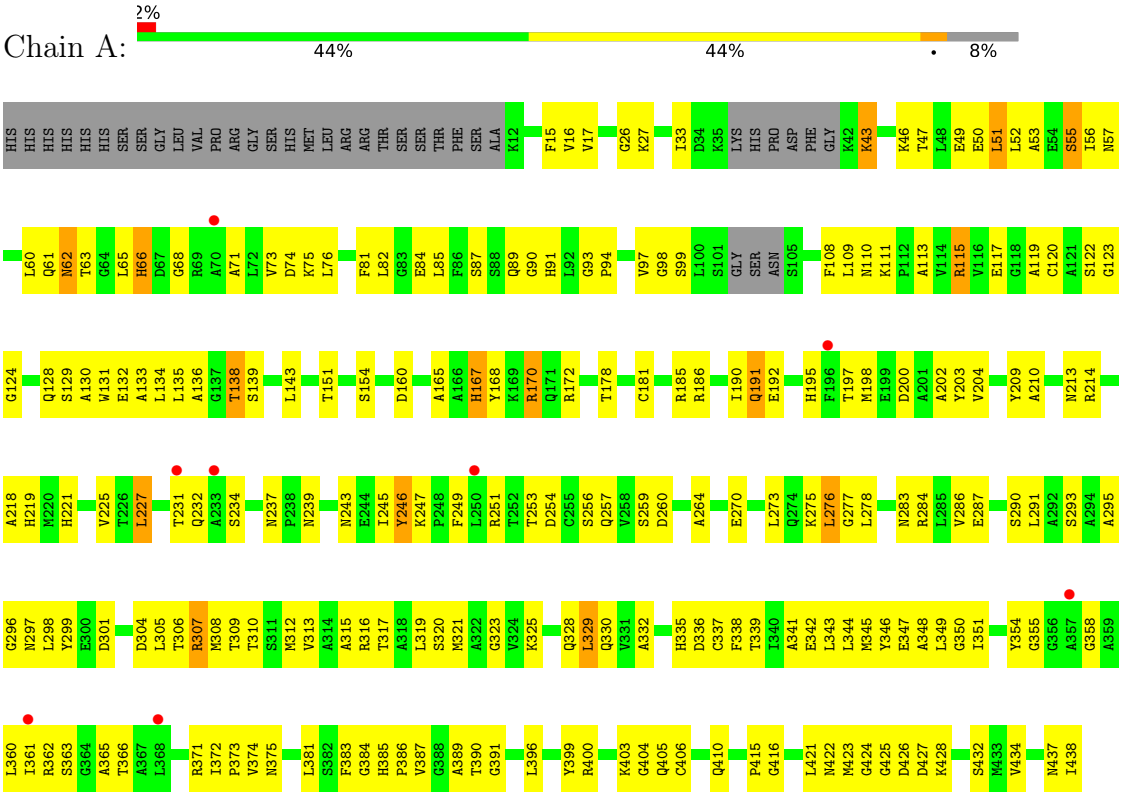
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	17	Total O 17 17	0	0
2	B	9	Total O 9 9	0	0
2	C	15	Total O 15 15	0	0
2	D	13	Total O 13 13	0	0

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.

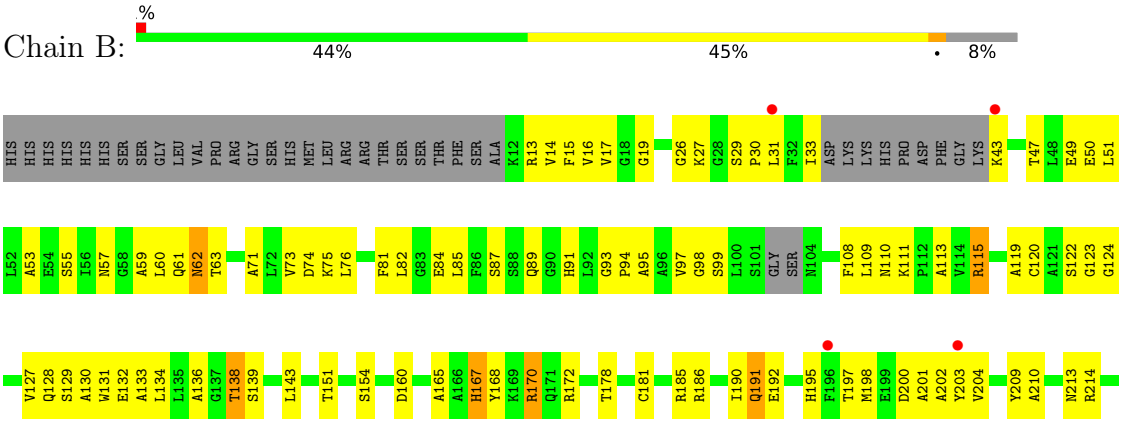
• Molecule 1: 3-KETOACYL-COA THIOLASE, PUTATIVE

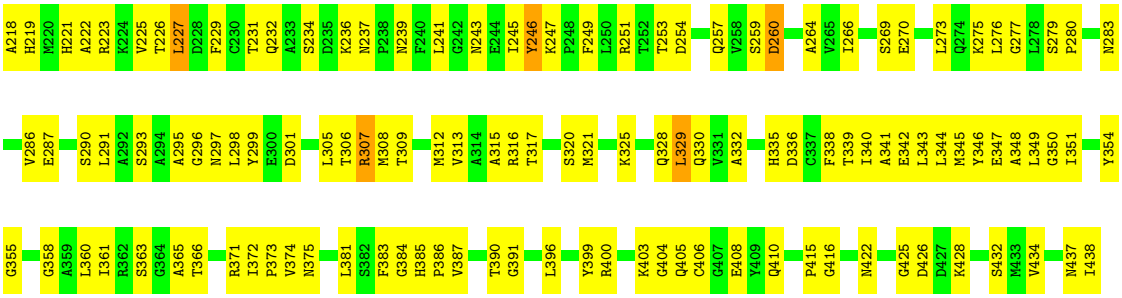
Chain A:

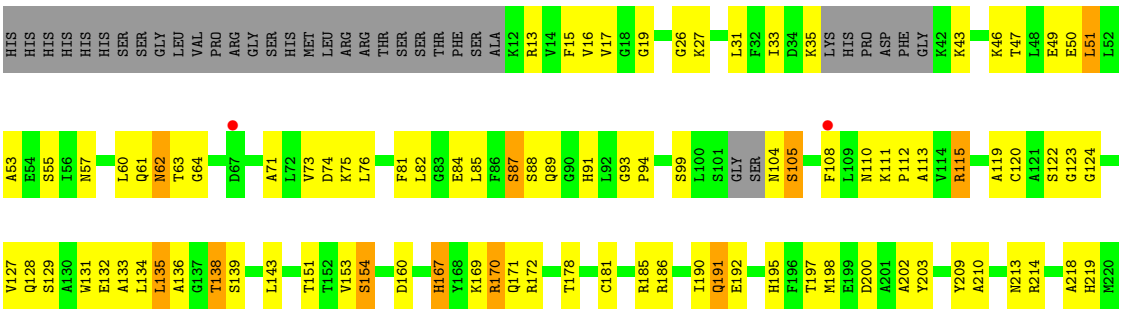


• Molecule 1: 3-KETOACYL-COA THIOLASE, PUTATIVE

Chain B:

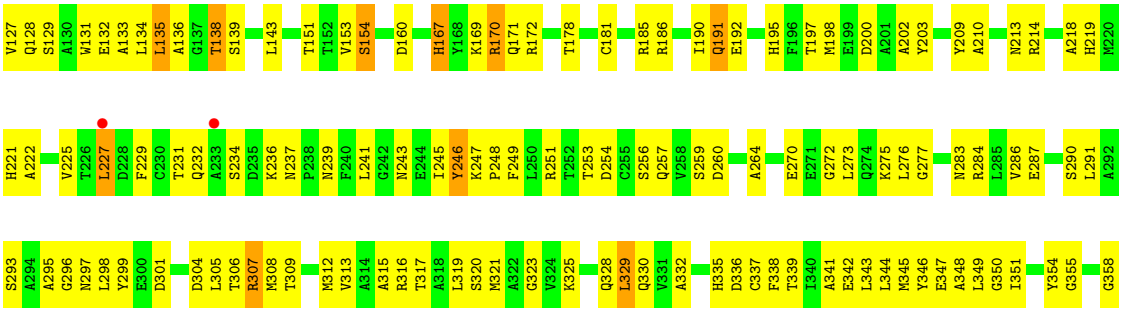


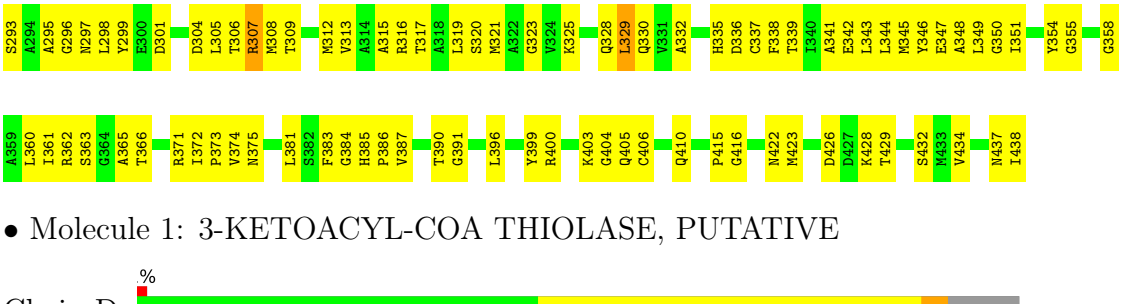


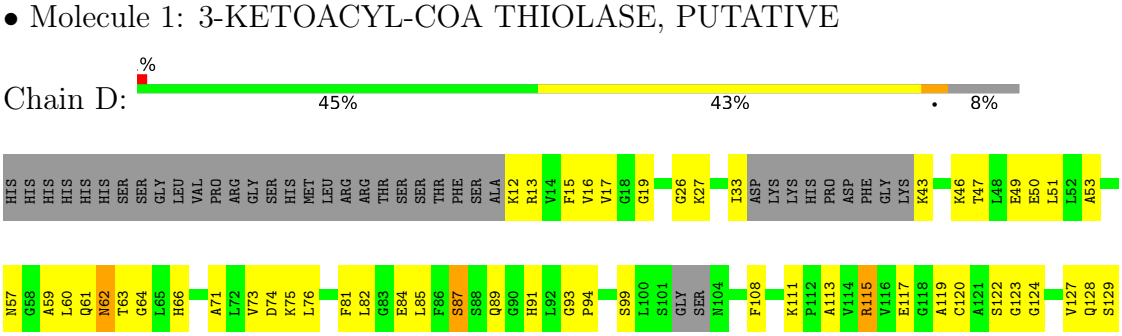


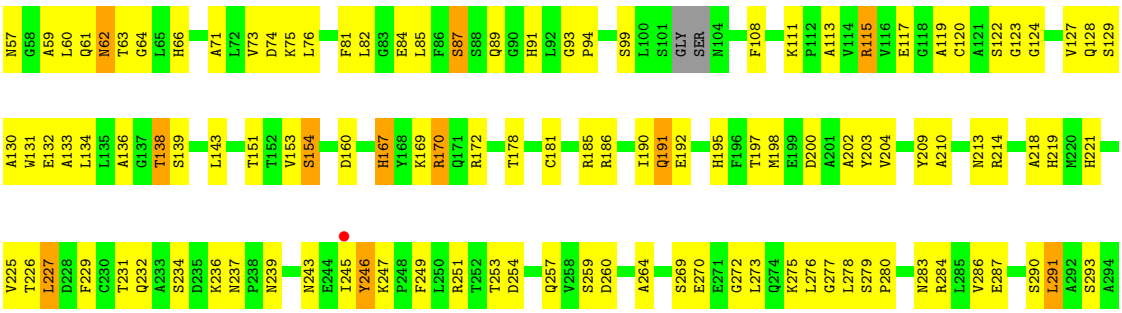
• Molecule 1: 3-KETOACYL-COA THIOLASE, PUTATIVE

Chain C:



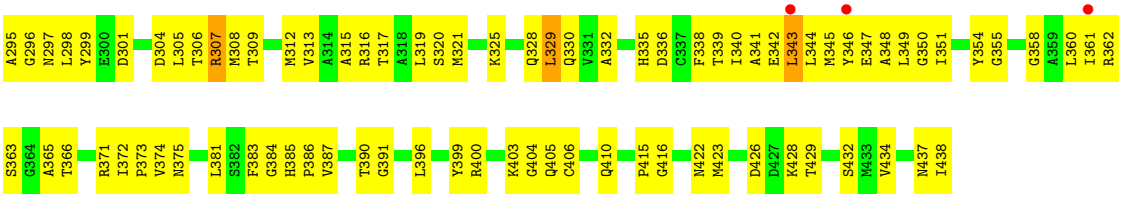






• Molecule 1: 3-KETOACYL-COA THIOLASE, PUTATIVE

Chain D:


A295 G296 N297 L298 Y299 E300 D301 D304 L305 T306 R307 M308 T309 M312 V313 A314 A315 R316 T317 A318 L319 S320 M321 K325 Q328 L329 Q330 V331 A332 H335 D336 C337 F338 T339 I340 A341 E342 L343 L344 M345 Y346 E347 A348 L349 G350 I351 Y354 G355 G358 A359 L360 I361 R362
S363 G364 A365 T366 R371 I372 P373 V374 M375 L381 S382 F383 G384 H385 P386 V387 T390 G391 L396 Y399 R400 K403 G404 Q405 C406 Q410 P415 G416 M422 M423 D426 D427 K428 T429 S432 M433 V434 M437 I438

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α, β, γ	59.14Å 59.14Å 377.57Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.75 – 2.45 50.75 – 2.45	Depositor EDS
% Data completeness (in resolution range)	91.5 (50.75-2.45) 88.5 (50.75-2.45)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.66 (at 2.45Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.224 , 0.242 0.224 , 0.246	Depositor DCC
R_{free} test set	2493 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	47.3	Xtriage
Anisotropy	0.553	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 82.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	0.449 for -h,-k,l 0.183 for h,-h-k,-l 0.177 for -k,-h,-l	Xtriage
Reported twinning fraction	0.500 for -h,-k,l	Depositor
Outliers	0 of 49663 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	12349	wwPDB-VP
Average B, all atoms (Å^2)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.80% 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	0.47	0/3119	0.67	3/4218 (0.1%)
1	B	0.46	0/3115	0.78	3/4211 (0.1%)
1	C	0.48	0/3133	0.66	2/4236 (0.0%)
1	D	0.47	0/3112	0.67	3/4207 (0.1%)
All	All	0.47	0/12479	0.70	11/16872 (0.1%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	307	ARG	NE-CZ-NH1	19.74	130.17	120.30
1	B	307	ARG	NE-CZ-NH2	-19.42	110.59	120.30
1	B	307	ARG	CD-NE-CZ	8.57	135.60	123.60
1	D	307	ARG	NE-CZ-NH2	-6.90	116.85	120.30
1	C	307	ARG	NE-CZ-NH2	-6.85	116.88	120.30
1	A	307	ARG	NE-CZ-NH2	-6.66	116.97	120.30
1	D	307	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	C	307	ARG	NE-CZ-NH1	6.26	123.43	120.30
1	A	307	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	D	66	HIS	C-N-CA	5.91	136.47	121.70
1	A	329	LEU	CB-CG-CD1	5.30	120.00	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	3073	0	3058	177	0
1	B	3069	0	3067	171	0
1	C	3087	0	3075	190	0
1	D	3066	0	3063	181	0
2	A	17	0	0	3	0
2	B	9	0	0	1	0
2	C	15	0	0	3	0
2	D	13	0	0	1	0
All	All	12349	0	12263	658	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 27.

All (658) 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:C:94:PRO:HB3	1:D:295:ALA:HB1	1.46	0.97
1:A:306:THR:HG1	1:A:354:TYR:HH	1.07	0.94
1:C:306:THR:HG1	1:C:354:TYR:HH	1.07	0.92
1:C:138:THR:HG21	1:D:132:GLU:HG2	1.53	0.90
1:B:290:SER:HB2	1:B:434:VAL:HB	1.54	0.90
1:C:132:GLU:HG2	1:D:138:THR:HG21	1.51	0.90
1:C:290:SER:HB2	1:C:434:VAL:HB	1.54	0.89
1:D:290:SER:HB2	1:D:434:VAL:HB	1.55	0.89
1:A:290:SER:HB2	1:A:434:VAL:HB	1.53	0.88
1:A:26:GLY:O	1:A:219:HIS:NE2	2.10	0.85
1:D:259:SER:HB2	1:D:386:PRO:HD3	1.57	0.85
1:C:259:SER:HB2	1:C:386:PRO:HD3	1.60	0.83
1:C:49:GLU:HG2	1:D:299:TYR:HE2	1.43	0.82
1:C:26:GLY:O	1:C:219:HIS:NE2	2.12	0.82
1:B:259:SER:HB2	1:B:386:PRO:HD3	1.60	0.81
1:A:426:ASP:H	1:A:428:LYS:HG2	1.47	0.80
1:A:259:SER:HB2	1:A:386:PRO:HD3	1.64	0.80
1:B:26:GLY:O	1:B:219:HIS:NE2	2.14	0.80
1:C:13:ARG:NE	1:C:287:GLU:OE2	2.15	0.79
1:A:132:GLU:HB3	1:B:132:GLU:HB3	1.65	0.79
1:D:426:ASP:H	1:D:428:LYS:HG2	1.49	0.77
1:A:365:ALA:HB1	1:A:371:ARG:HG2	1.67	0.76
1:C:104:ASN:OD1	1:C:105:SER:OG	2.03	0.76
1:B:426:ASP:H	1:B:428:LYS:HG2	1.52	0.75
1:C:426:ASP:H	1:C:428:LYS:HG2	1.52	0.75
1:D:336:ASP:OD1	1:D:375:ASN:ND2	2.20	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:360:LEU:HA	1:B:363:SER:HB3	1.68	0.75
1:D:26:GLY:O	1:D:219:HIS:NE2	2.17	0.74
1:C:203:TYR:HB3	1:C:361:ILE:HG13	1.70	0.74
1:C:360:LEU:HA	1:C:363:SER:HB3	1.68	0.74
1:D:315:ALA:HB1	1:D:349:LEU:HD13	1.69	0.74
1:B:336:ASP:OD1	1:B:375:ASN:ND2	2.20	0.74
1:A:336:ASP:OD1	1:A:375:ASN:ND2	2.21	0.73
1:C:306:THR:OG1	1:C:354:TYR:OH	2.02	0.73
1:C:336:ASP:OD1	1:C:375:ASN:ND2	2.22	0.73
1:D:13:ARG:NE	1:D:287:GLU:OE2	2.22	0.73
1:A:198:MET:O	1:A:251:ARG:NH2	2.20	0.73
1:C:365:ALA:HB1	1:C:371:ARG:HG2	1.70	0.72
1:C:91:HIS:NE2	1:D:429:THR:OG1	1.87	0.72
1:A:360:LEU:HA	1:A:363:SER:HB3	1.70	0.72
1:C:315:ALA:HB1	1:C:349:LEU:HD13	1.70	0.72
1:C:198:MET:O	1:C:251:ARG:NH2	2.21	0.71
1:A:203:TYR:HB3	1:A:361:ILE:HG13	1.72	0.71
1:D:198:MET:O	1:D:251:ARG:NH2	2.20	0.71
1:D:203:TYR:HB3	1:D:361:ILE:HG13	1.72	0.71
1:D:360:LEU:HA	1:D:363:SER:HB3	1.71	0.71
1:D:365:ALA:HB1	1:D:371:ARG:HG2	1.72	0.71
1:A:115:ARG:NH1	2:A:2003:HOH:O	2.23	0.71
1:B:53:ALA:HA	1:B:99:SER:HB3	1.72	0.70
1:B:365:ALA:HB1	1:B:371:ARG:HG2	1.73	0.70
1:A:53:ALA:O	1:A:57:ASN:ND2	2.24	0.69
1:B:203:TYR:HB3	1:B:361:ILE:HG13	1.72	0.69
2:B:2003:HOH:O	1:C:35:LYS:O	2.10	0.69
1:C:169:LYS:HE2	1:D:87:SER:O	1.92	0.69
1:B:198:MET:O	1:B:251:ARG:NH2	2.22	0.69
1:A:321:MET:O	2:A:2012:HOH:O	2.10	0.69
1:B:222:ALA:HB2	1:C:222:ALA:HB1	1.74	0.69
1:B:315:ALA:HB1	1:B:349:LEU:HD13	1.72	0.69
1:A:53:ALA:HA	1:A:99:SER:HB3	1.74	0.69
1:C:426:ASP:HB3	1:C:428:LYS:HE2	1.74	0.69
1:D:426:ASP:HB3	1:D:428:LYS:HE2	1.75	0.68
1:C:49:GLU:HG2	1:D:299:TYR:CE2	2.26	0.68
1:D:53:ALA:O	1:D:57:ASN:ND2	2.26	0.68
1:B:53:ALA:O	1:B:57:ASN:ND2	2.26	0.68
1:A:426:ASP:HB3	1:A:428:LYS:HE2	1.74	0.68
1:B:316:ARG:O	1:B:320:SER:OG	2.10	0.68
1:B:426:ASP:HB3	1:B:428:LYS:HE2	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:53:ALA:HA	1:D:99:SER:HB3	1.75	0.67
1:C:53:ALA:O	1:C:57:ASN:ND2	2.27	0.67
1:C:295:ALA:HB1	1:D:94:PRO:HB3	1.76	0.67
1:A:315:ALA:HB1	1:A:349:LEU:HD13	1.75	0.67
1:C:53:ALA:HA	1:C:99:SER:HB3	1.76	0.66
1:C:429:THR:OG1	1:D:91:HIS:NE2	1.96	0.66
1:B:257:GLN:HB2	1:B:384:GLY:HA2	1.76	0.66
1:C:13:ARG:NH2	1:C:287:GLU:OE1	2.29	0.65
1:A:57:ASN:HA	1:A:60:LEU:HD12	1.79	0.65
1:D:325:LYS:HG2	1:D:328:GLN:HB2	1.79	0.65
1:C:91:HIS:HE2	1:D:429:THR:CB	2.10	0.65
1:D:257:GLN:HB2	1:D:384:GLY:HA2	1.78	0.64
1:C:110:ASN:HB3	1:D:313:VAL:HG11	1.79	0.64
1:C:257:GLN:HB2	1:C:384:GLY:HA2	1.79	0.64
1:C:316:ARG:O	1:C:320:SER:OG	2.14	0.64
1:C:248:PRO:O	2:C:2008:HOH:O	2.14	0.64
1:A:309:THR:O	1:A:313:VAL:HG23	1.98	0.64
1:B:325:LYS:HG2	1:B:328:GLN:HB2	1.79	0.64
1:A:91:HIS:ND1	1:B:165:ALA:O	2.26	0.64
1:C:325:LYS:HG2	1:C:328:GLN:HB2	1.79	0.64
1:B:312:MET:O	1:B:316:ARG:HG2	1.98	0.63
1:A:165:ALA:O	1:B:91:HIS:ND1	2.31	0.63
1:C:344:LEU:O	1:C:348:ALA:N	2.29	0.63
1:A:257:GLN:HB2	1:A:384:GLY:HA2	1.81	0.63
1:A:325:LYS:HG2	1:A:328:GLN:HB2	1.79	0.63
1:D:316:ARG:O	1:D:320:SER:OG	2.15	0.63
1:C:254:ASP:HA	1:C:339:THR:HG23	1.79	0.62
1:B:408:GLU:HG3	1:C:31:LEU:HD11	1.81	0.62
1:A:73:VAL:O	1:A:111:LYS:NZ	2.24	0.62
1:A:170:ARG:NH2	1:A:301:ASP:OD1	2.32	0.62
1:A:344:LEU:O	1:A:348:ALA:N	2.28	0.62
1:A:151:THR:OG1	1:A:260:ASP:OD2	2.18	0.62
1:C:170:ARG:NH2	1:C:301:ASP:OD1	2.33	0.62
1:D:12:LYS:O	2:D:2001:HOH:O	2.16	0.62
1:B:57:ASN:HA	1:B:60:LEU:HD12	1.80	0.62
1:B:306:THR:OG1	1:B:354:TYR:OH	2.08	0.62
1:B:213:ASN:ND2	1:B:221:HIS:O	2.31	0.62
1:A:254:ASP:HA	1:A:339:THR:HG23	1.81	0.61
1:B:308:MET:O	1:B:312:MET:N	2.33	0.61
1:B:408:GLU:HG3	1:C:31:LEU:CD1	2.30	0.61
1:D:49:GLU:OE1	1:D:49:GLU:N	2.29	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:308:MET:O	1:D:312:MET:N	2.32	0.61
1:A:276:LEU:HB3	1:A:278:LEU:HD23	1.81	0.61
1:A:49:GLU:OE1	1:A:49:GLU:N	2.31	0.61
1:C:57:ASN:HA	1:C:60:LEU:HD12	1.83	0.61
1:B:49:GLU:OE1	1:B:49:GLU:N	2.29	0.60
1:C:218:ALA:HB3	1:C:221:HIS:HB2	1.83	0.60
1:A:81:PHE:O	1:A:115:ARG:NH2	2.35	0.60
1:A:143:LEU:HD11	1:A:264:ALA:HB1	1.84	0.60
1:A:347:GLU:OE2	1:A:355:GLY:N	2.32	0.60
1:C:160:ASP:OD1	1:C:172:ARG:NH1	2.35	0.60
1:B:81:PHE:O	1:B:115:ARG:NH2	2.34	0.60
1:D:81:PHE:O	1:D:115:ARG:NH2	2.35	0.60
1:B:143:LEU:HD11	1:B:264:ALA:HB1	1.83	0.60
1:A:312:MET:O	1:A:316:ARG:HG2	2.02	0.60
1:B:151:THR:OG1	1:B:260:ASP:OD2	2.20	0.60
1:D:213:ASN:ND2	1:D:221:HIS:O	2.30	0.60
1:D:306:THR:OG1	1:D:354:TYR:OH	2.10	0.60
1:D:312:MET:O	1:D:316:ARG:HG2	2.01	0.60
1:D:347:GLU:OE2	1:D:355:GLY:N	2.33	0.60
1:C:309:THR:O	1:C:313:VAL:HG23	2.02	0.59
1:D:151:THR:OG1	1:D:260:ASP:OD2	2.20	0.59
1:A:296:GLY:HA2	1:B:110:ASN:H	1.67	0.59
1:C:81:PHE:O	1:C:115:ARG:NH2	2.36	0.59
1:B:309:THR:O	1:B:313:VAL:HG23	2.02	0.59
1:D:186:ARG:HG2	1:D:305:LEU:HD22	1.85	0.59
1:A:119:ALA:O	1:A:122:SER:OG	2.21	0.59
1:C:346:TYR:HA	1:C:351:ILE:HD11	1.86	0.58
1:C:347:GLU:OE2	1:C:355:GLY:N	2.33	0.58
1:B:347:GLU:OE2	1:B:355:GLY:N	2.35	0.58
1:C:135:LEU:HB3	1:D:136:ALA:HB1	1.85	0.58
1:A:160:ASP:OD1	1:A:172:ARG:NH1	2.36	0.58
1:B:283:ASN:O	1:B:403:LYS:NZ	2.30	0.58
1:D:309:THR:O	1:D:313:VAL:HG23	2.03	0.58
1:A:218:ALA:HB3	1:A:221:HIS:HB2	1.85	0.58
1:A:308:MET:O	1:A:312:MET:N	2.32	0.58
1:D:210:ALA:O	1:D:214:ARG:NE	2.37	0.58
1:B:254:ASP:HA	1:B:339:THR:HG23	1.86	0.57
1:C:143:LEU:HD11	1:C:264:ALA:HB1	1.85	0.57
1:A:134:LEU:HA	1:A:139:SER:O	2.04	0.57
1:D:170:ARG:NH2	1:D:301:ASP:OD1	2.36	0.57
1:D:254:ASP:HA	1:D:339:THR:HG23	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:151:THR:OG1	1:C:260:ASP:OD2	2.22	0.57
1:C:87:SER:O	1:D:169:LYS:HE2	2.04	0.57
1:C:312:MET:O	1:C:316:ARG:HG2	2.05	0.57
1:B:170:ARG:NH2	1:B:301:ASP:OD1	2.37	0.57
1:D:57:ASN:HA	1:D:60:LEU:HD12	1.85	0.57
1:B:312:MET:HG2	1:B:348:ALA:HA	1.86	0.57
1:B:186:ARG:HG2	1:B:305:LEU:HD22	1.87	0.57
1:B:406:CYS:HB2	1:B:410:GLN:HA	1.86	0.57
1:C:49:GLU:OE1	1:C:49:GLU:N	2.32	0.57
1:D:312:MET:HG2	1:D:348:ALA:HA	1.86	0.57
1:A:243:ASN:OD1	1:A:246:TYR:N	2.30	0.56
1:C:243:ASN:OD1	1:C:246:TYR:N	2.29	0.56
1:D:143:LEU:HD11	1:D:264:ALA:HB1	1.86	0.56
1:A:349:LEU:HD12	1:A:350:GLY:H	1.71	0.56
1:D:191:GLN:HE22	1:D:249:PHE:HE1	1.52	0.56
1:C:75:LYS:HZ3	1:C:133:ALA:HB2	1.71	0.56
1:A:283:ASN:O	1:A:403:LYS:NZ	2.30	0.56
1:D:190:ILE:HG12	1:D:195:HIS:HB3	1.88	0.56
1:B:218:ALA:HB3	1:B:221:HIS:HB2	1.87	0.56
1:C:89:GLN:NE2	1:D:298:LEU:HD21	2.20	0.56
1:B:243:ASN:OD1	1:B:246:TYR:N	2.32	0.56
1:B:341:ALA:O	1:B:345:MET:N	2.33	0.56
1:B:349:LEU:HD12	1:B:350:GLY:H	1.70	0.56
1:C:136:ALA:HB3	1:C:138:THR:HG23	1.86	0.56
1:C:273:LEU:O	1:C:277:GLY:N	2.39	0.55
1:D:243:ASN:OD1	1:D:246:TYR:N	2.30	0.55
1:D:273:LEU:O	1:D:277:GLY:N	2.39	0.55
1:C:213:ASN:ND2	1:C:221:HIS:O	2.34	0.55
1:A:110:ASN:H	1:B:296:GLY:HA2	1.71	0.55
1:B:136:ALA:HB3	1:B:138:THR:HG23	1.88	0.55
1:B:344:LEU:O	1:B:348:ALA:N	2.32	0.55
1:C:296:GLY:O	1:D:94:PRO:HB2	2.05	0.55
1:A:109:LEU:HD11	1:B:297:ASN:HD22	1.71	0.55
1:B:191:GLN:HG2	1:B:192:GLU:N	2.21	0.55
1:B:399:TYR:O	1:B:403:LYS:HG2	2.07	0.55
1:A:66:HIS:O	1:A:68:GLY:N	2.39	0.55
1:C:308:MET:O	1:C:312:MET:N	2.33	0.55
1:D:344:LEU:O	1:D:348:ALA:N	2.31	0.55
1:B:190:ILE:HG12	1:B:195:HIS:HB3	1.90	0.54
1:C:197:THR:OG1	1:C:200:ASP:N	2.40	0.54
1:C:298:LEU:HD21	1:D:89:GLN:NE2	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:312:MET:HG2	1:C:348:ALA:HA	1.88	0.54
1:A:190:ILE:HG12	1:A:195:HIS:HB3	1.89	0.54
1:A:346:TYR:HA	1:A:351:ILE:HD11	1.89	0.54
1:B:198:MET:HG2	1:B:251:ARG:NH2	2.22	0.54
1:B:16:VAL:N	1:B:286:VAL:O	2.41	0.54
1:C:16:VAL:N	1:C:286:VAL:O	2.41	0.54
1:C:264:ALA:O	1:C:396:LEU:HD11	2.08	0.54
1:D:341:ALA:O	1:D:345:MET:N	2.37	0.54
1:B:185:ARG:HD3	1:B:246:TYR:CE1	2.43	0.54
1:A:136:ALA:HB3	1:A:138:THR:HG23	1.89	0.54
1:C:185:ARG:HD3	1:C:246:TYR:CE1	2.43	0.54
1:C:428:LYS:HB2	1:D:91:HIS:HE1	1.73	0.54
1:B:134:LEU:HA	1:B:139:SER:O	2.07	0.54
1:B:197:THR:OG1	1:B:200:ASP:N	2.40	0.54
1:C:186:ARG:HG2	1:C:305:LEU:HD22	1.90	0.54
1:C:190:ILE:HG12	1:C:195:HIS:HB3	1.90	0.54
1:C:191:GLN:HG2	1:C:192:GLU:N	2.22	0.54
1:C:210:ALA:O	1:C:214:ARG:NE	2.41	0.54
1:A:335:HIS:H	1:A:345:MET:HE3	1.73	0.53
1:D:186:ARG:HA	1:D:305:LEU:HD13	1.90	0.53
1:A:299:TYR:CD1	1:B:98:GLY:HA3	2.43	0.53
1:A:316:ARG:O	1:A:320:SER:OG	2.16	0.53
1:D:62:ASN:N	1:D:62:ASN:OD1	2.41	0.53
1:D:191:GLN:HG2	1:D:192:GLU:N	2.22	0.53
1:A:191:GLN:HE22	1:A:249:PHE:HE1	1.56	0.53
1:A:213:ASN:ND2	1:A:221:HIS:O	2.36	0.53
1:B:123:GLY:HA3	1:B:391:GLY:HA3	1.90	0.53
1:C:47:THR:N	1:C:50:GLU:OE1	2.41	0.53
1:A:191:GLN:HG2	1:A:192:GLU:N	2.24	0.53
1:C:186:ARG:HA	1:C:305:LEU:HD13	1.89	0.53
1:D:264:ALA:O	1:D:396:LEU:HD11	2.09	0.53
1:A:123:GLY:HA3	1:A:391:GLY:HA3	1.90	0.53
1:B:366:THR:HA	1:B:372:ILE:O	2.09	0.53
1:D:46:LYS:HD3	1:D:51:LEU:HD13	1.91	0.53
1:D:197:THR:OG1	1:D:200:ASP:N	2.41	0.53
1:B:191:GLN:HE22	1:B:249:PHE:HE1	1.57	0.53
1:B:210:ALA:O	1:B:214:ARG:NE	2.42	0.53
1:D:136:ALA:HB3	1:D:138:THR:HG23	1.89	0.53
1:A:185:ARG:HD3	1:A:246:TYR:CE1	2.43	0.52
1:B:332:ALA:HB3	1:B:374:VAL:HG22	1.91	0.52
1:C:132:GLU:O	1:D:136:ALA:HB2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:185:ARG:HD3	1:D:246:TYR:CE1	2.44	0.52
1:D:198:MET:HG2	1:D:251:ARG:NH2	2.24	0.52
1:D:218:ALA:HB3	1:D:221:HIS:HB2	1.91	0.52
1:A:399:TYR:O	1:A:403:LYS:HG2	2.08	0.52
1:D:134:LEU:HA	1:D:139:SER:O	2.09	0.52
1:A:197:THR:OG1	1:A:200:ASP:N	2.43	0.52
1:A:264:ALA:O	1:A:396:LEU:HD11	2.09	0.52
1:A:341:ALA:O	1:A:345:MET:N	2.37	0.52
1:B:408:GLU:HB3	1:C:31:LEU:HD21	1.92	0.52
1:A:186:ARG:HG2	1:A:305:LEU:HD22	1.92	0.52
1:B:73:VAL:O	1:B:111:LYS:NZ	2.26	0.52
1:C:62:ASN:OD1	1:C:62:ASN:N	2.41	0.52
1:B:404:GLY:HA2	1:B:410:GLN:CD	2.30	0.52
1:C:136:ALA:HB2	1:D:132:GLU:O	2.10	0.52
1:C:170:ARG:NH1	1:C:299:TYR:O	2.43	0.52
1:B:264:ALA:O	1:B:396:LEU:HD11	2.08	0.52
1:B:330:GLN:O	1:B:373:PRO:HD2	2.10	0.52
1:C:406:CYS:HB2	1:C:410:GLN:HA	1.91	0.52
1:A:124:GLY:H	1:A:422:ASN:HD22	1.58	0.52
1:A:273:LEU:O	1:A:277:GLY:N	2.43	0.52
1:D:399:TYR:O	1:D:403:LYS:HG2	2.10	0.52
1:A:297:ASN:HD22	1:B:109:LEU:HD11	1.75	0.51
1:C:169:LYS:NZ	2:C:2006:HOH:O	2.20	0.51
1:D:349:LEU:HD12	1:D:350:GLY:H	1.76	0.51
1:D:170:ARG:NH1	1:D:299:TYR:O	2.43	0.51
1:A:237:ASN:HD21	1:A:251:ARG:HB3	1.74	0.51
1:D:330:GLN:HB2	1:D:415:PRO:HB3	1.91	0.51
1:A:406:CYS:HB2	1:A:410:GLN:HA	1.92	0.51
1:B:251:ARG:HB2	1:B:253:THR:HG23	1.92	0.51
1:C:120:CYS:HA	1:C:387:VAL:HG13	1.92	0.51
1:D:283:ASN:O	1:D:403:LYS:NZ	2.29	0.51
1:B:273:LEU:O	1:B:277:GLY:N	2.43	0.51
1:C:134:LEU:HA	1:C:139:SER:O	2.11	0.51
1:C:399:TYR:O	1:C:403:LYS:HG2	2.10	0.51
1:D:160:ASP:OD1	1:D:172:ARG:NH1	2.42	0.51
1:A:94:PRO:HB2	1:B:298:LEU:HB2	1.91	0.51
1:B:260:ASP:N	1:B:260:ASP:OD1	2.44	0.51
1:B:330:GLN:HB2	1:B:415:PRO:HB3	1.92	0.51
1:A:298:LEU:HB2	1:B:94:PRO:HB2	1.92	0.51
1:C:110:ASN:ND2	1:D:313:VAL:HG21	2.26	0.51
1:B:186:ARG:HA	1:B:305:LEU:HD13	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:404:GLY:HA2	1:C:410:GLN:CD	2.30	0.51
1:C:15:PHE:HA	1:C:287:GLU:HA	1.92	0.51
1:C:75:LYS:NZ	1:D:132:GLU:OE1	2.29	0.51
1:A:404:GLY:HA2	1:A:410:GLN:CD	2.30	0.51
1:C:349:LEU:HD12	1:C:350:GLY:H	1.76	0.51
1:C:429:THR:HG1	1:D:91:HIS:HE2	0.52	0.50
1:D:406:CYS:HB2	1:D:410:GLN:HA	1.92	0.50
1:A:170:ARG:NH1	1:A:299:TYR:O	2.42	0.50
1:D:257:GLN:HG2	1:D:381:LEU:O	2.11	0.50
1:A:165:ALA:C	1:B:91:HIS:HD1	2.13	0.50
1:B:62:ASN:N	1:B:62:ASN:OD1	2.44	0.50
1:A:16:VAL:N	1:A:286:VAL:O	2.43	0.50
1:A:312:MET:HG2	1:A:348:ALA:HA	1.91	0.50
1:C:341:ALA:O	1:C:345:MET:N	2.38	0.50
1:A:251:ARG:HB2	1:A:253:THR:HG23	1.94	0.50
1:D:120:CYS:HA	1:D:387:VAL:HG13	1.93	0.50
1:D:416:GLY:HA2	1:D:437:ASN:HB3	1.94	0.50
1:A:15:PHE:HA	1:A:287:GLU:HA	1.93	0.50
1:A:198:MET:HG2	1:A:251:ARG:NH2	2.27	0.50
1:A:231:THR:O	1:A:251:ARG:NE	2.45	0.50
1:A:332:ALA:HB3	1:A:374:VAL:HG22	1.93	0.50
1:C:191:GLN:HE22	1:C:249:PHE:HE1	1.57	0.50
1:D:16:VAL:N	1:D:286:VAL:O	2.45	0.50
1:A:239:ASN:HB3	1:A:247:LYS:HG2	1.94	0.50
1:A:256:SER:OG	1:A:337:CYS:O	2.29	0.50
1:A:186:ARG:HA	1:A:305:LEU:HD13	1.93	0.50
1:A:366:THR:HA	1:A:372:ILE:O	2.11	0.50
1:B:47:THR:N	1:B:50:GLU:OE1	2.41	0.50
1:C:366:THR:HA	1:C:372:ILE:O	2.12	0.50
1:C:400:ARG:HB3	1:C:405:GLN:HB2	1.94	0.49
1:D:404:GLY:HA2	1:D:410:GLN:CD	2.32	0.49
1:D:308:MET:O	1:D:312:MET:HG3	2.11	0.49
1:C:73:VAL:O	1:C:111:LYS:NZ	2.27	0.49
1:C:330:GLN:HB2	1:C:415:PRO:HB3	1.93	0.49
1:A:120:CYS:HA	1:A:387:VAL:HG13	1.94	0.49
1:B:124:GLY:H	1:B:422:ASN:HD22	1.60	0.49
1:A:330:GLN:HB2	1:A:415:PRO:HB3	1.93	0.49
1:B:119:ALA:O	1:B:122:SER:OG	2.27	0.49
1:C:198:MET:HG2	1:C:251:ARG:NH2	2.27	0.49
1:A:91:HIS:HD1	1:B:165:ALA:C	2.12	0.49
1:D:329:LEU:HD23	1:D:329:LEU:H	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:416:GLY:HA2	1:C:437:ASN:HB3	1.95	0.49
1:C:94:PRO:CB	1:D:295:ALA:HB1	2.32	0.49
1:C:123:GLY:HA3	1:C:391:GLY:HA3	1.94	0.49
1:C:343:LEU:O	1:C:346:TYR:HB2	2.13	0.49
1:A:210:ALA:O	1:A:214:ARG:NE	2.45	0.49
1:A:295:ALA:N	1:B:111:LYS:O	2.46	0.49
1:C:330:GLN:O	1:C:373:PRO:HD2	2.13	0.49
1:C:332:ALA:HB3	1:C:374:VAL:HG22	1.94	0.49
1:A:46:LYS:HD3	1:A:51:LEU:HD13	1.94	0.48
1:A:310:THR:OG1	1:A:427:ASP:O	2.21	0.48
1:A:343:LEU:O	1:A:346:TYR:HB2	2.13	0.48
1:C:231:THR:O	1:C:251:ARG:NE	2.46	0.48
1:D:330:GLN:O	1:D:373:PRO:HD2	2.12	0.48
1:D:343:LEU:O	1:D:346:TYR:HB2	2.13	0.48
1:A:304:ASP:OD2	1:A:307:ARG:HD2	2.12	0.48
1:B:416:GLY:HA2	1:B:437:ASN:HB3	1.95	0.48
1:B:346:TYR:HA	1:B:351:ILE:HD11	1.95	0.48
1:C:260:ASP:OD1	1:C:260:ASP:N	2.45	0.48
1:D:332:ALA:HB3	1:D:374:VAL:HG22	1.94	0.48
1:B:160:ASP:OD1	1:B:172:ARG:NH1	2.46	0.48
1:C:254:ASP:O	1:C:338:PHE:HA	2.14	0.48
1:D:239:ASN:HB3	1:D:247:LYS:HG2	1.94	0.48
1:A:297:ASN:HA	1:B:97:VAL:HB	1.94	0.48
1:B:15:PHE:HA	1:B:287:GLU:HA	1.94	0.48
1:C:110:ASN:CB	1:D:313:VAL:HG11	2.44	0.48
1:C:237:ASN:HD21	1:C:251:ARG:HB3	1.78	0.48
1:D:346:TYR:HA	1:D:351:ILE:HD11	1.95	0.48
1:A:98:GLY:HA3	1:B:299:TYR:CD1	2.49	0.48
1:A:425:GLY:HA3	1:B:91:HIS:HE1	1.79	0.48
1:D:251:ARG:HB2	1:D:253:THR:HG23	1.96	0.48
1:B:257:GLN:HG2	1:B:381:LEU:O	2.12	0.48
1:D:277:GLY:O	1:D:278:LEU:HD22	2.14	0.48
1:A:120:CYS:HA	1:A:387:VAL:CG1	2.44	0.48
1:C:33:ILE:HG21	1:C:43:LYS:O	2.13	0.48
1:C:251:ARG:HB2	1:C:253:THR:HG23	1.95	0.48
1:C:115:ARG:HD2	1:D:117:GLU:HB3	1.94	0.48
1:A:257:GLN:HG2	1:A:381:LEU:O	2.14	0.48
1:D:73:VAL:O	1:D:111:LYS:NZ	2.28	0.48
1:A:330:GLN:O	1:A:372:ILE:HD12	2.14	0.47
1:C:120:CYS:HB3	1:C:335:HIS:CE1	2.49	0.47
1:D:342:GLU:O	1:D:345:MET:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:239:ASN:HB3	1:B:247:LYS:HG2	1.96	0.47
1:B:343:LEU:O	1:B:346:TYR:HB2	2.14	0.47
1:A:97:VAL:HB	1:B:297:ASN:HA	1.96	0.47
1:C:75:LYS:NZ	1:C:133:ALA:HB2	2.29	0.47
1:C:275:LYS:HB2	1:C:275:LYS:HE3	1.65	0.47
1:A:17:VAL:HG12	1:A:63:THR:HG22	1.95	0.47
1:A:400:ARG:HB3	1:A:405:GLN:HB2	1.97	0.47
1:C:428:LYS:HB2	1:D:91:HIS:CE1	2.49	0.47
1:D:15:PHE:HA	1:D:287:GLU:HA	1.95	0.47
1:D:75:LYS:NZ	1:D:133:ALA:HB2	2.30	0.47
1:A:33:ILE:HG21	1:A:43:LYS:O	2.13	0.47
1:B:13:ARG:HB3	1:B:287:GLU:OE2	2.15	0.47
1:B:74:ASP:HB2	1:B:139:SER:HB3	1.97	0.47
1:B:120:CYS:HA	1:B:387:VAL:HG13	1.95	0.47
1:D:120:CYS:HA	1:D:387:VAL:CG1	2.45	0.47
1:D:237:ASN:HD21	1:D:253:THR:HG23	1.80	0.47
1:B:231:THR:O	1:B:251:ARG:NE	2.48	0.47
1:C:46:LYS:HD3	1:C:51:LEU:HD13	1.97	0.47
1:C:120:CYS:HA	1:C:387:VAL:CG1	2.45	0.47
1:B:17:VAL:HG12	1:B:63:THR:HG22	1.97	0.47
1:A:202:ALA:HB2	1:A:231:THR:HA	1.97	0.47
1:A:330:GLN:O	1:A:373:PRO:HD2	2.15	0.47
1:B:275:LYS:HB2	1:B:275:LYS:HE3	1.66	0.47
1:C:257:GLN:HG2	1:C:381:LEU:O	2.15	0.47
1:A:254:ASP:O	1:A:338:PHE:HA	2.15	0.46
1:A:260:ASP:OD1	1:A:260:ASP:N	2.47	0.46
1:D:304:ASP:OD2	1:D:307:ARG:HD2	2.15	0.46
1:D:366:THR:HA	1:D:372:ILE:O	2.16	0.46
1:D:82:LEU:HD22	1:D:85:LEU:HD12	1.97	0.46
1:B:33:ILE:HG21	1:B:43:LYS:O	2.15	0.46
1:C:82:LEU:HD22	1:C:85:LEU:HD12	1.96	0.46
1:B:309:THR:O	1:B:313:VAL:N	2.35	0.46
1:C:51:LEU:HD12	1:C:51:LEU:HA	1.77	0.46
1:C:74:ASP:HB2	1:C:139:SER:HB3	1.98	0.46
1:C:136:ALA:HA	1:D:136:ALA:HA	1.98	0.46
1:D:272:GLY:O	1:D:276:LEU:HG	2.16	0.46
1:D:297:ASN:OD1	1:D:299:TYR:HD1	1.99	0.46
1:A:47:THR:N	1:A:50:GLU:OE1	2.43	0.46
1:A:385:HIS:ND1	1:A:390:THR:OG1	2.47	0.46
1:B:237:ASN:HD21	1:B:251:ARG:HB3	1.81	0.46
1:B:308:MET:O	1:B:312:MET:HG3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:119:ALA:O	1:C:122:SER:OG	2.29	0.46
1:D:123:GLY:HA3	1:D:391:GLY:HA3	1.96	0.46
1:D:210:ALA:HB1	1:D:214:ARG:HH21	1.80	0.46
1:C:256:SER:OG	1:C:337:CYS:O	2.33	0.46
1:A:62:ASN:OD1	1:A:62:ASN:N	2.46	0.46
1:B:74:ASP:HB2	1:B:139:SER:CB	2.45	0.46
1:C:124:GLY:H	1:C:422:ASN:HD22	1.62	0.46
1:C:202:ALA:HB2	1:C:231:THR:HA	1.98	0.46
1:C:335:HIS:H	1:C:345:MET:CE	2.28	0.46
1:D:47:THR:N	1:D:50:GLU:OE1	2.44	0.46
1:D:74:ASP:HB2	1:D:139:SER:HB3	1.98	0.46
1:D:119:ALA:O	1:D:122:SER:OG	2.30	0.46
1:D:317:THR:O	1:D:321:MET:HG3	2.16	0.46
1:A:243:ASN:O	1:A:247:LYS:HB2	2.16	0.46
1:A:426:ASP:N	1:A:428:LYS:HG2	2.25	0.46
1:B:82:LEU:HD22	1:B:85:LEU:HD12	1.98	0.46
1:C:272:GLY:O	1:C:276:LEU:HG	2.16	0.46
1:C:309:THR:O	1:C:313:VAL:N	2.34	0.46
1:D:275:LYS:HB2	1:D:275:LYS:HE3	1.66	0.46
1:B:51:LEU:HD23	1:B:51:LEU:HA	1.78	0.45
1:B:202:ALA:HB2	1:B:231:THR:HA	1.97	0.45
1:C:76:LEU:O	1:C:113:ALA:HA	2.16	0.45
1:A:120:CYS:HB3	1:A:335:HIS:CE1	2.51	0.45
1:A:416:GLY:HA2	1:A:437:ASN:HB3	1.99	0.45
1:C:304:ASP:OD2	1:C:307:ARG:HD2	2.16	0.45
1:D:17:VAL:HG12	1:D:63:THR:HG22	1.99	0.45
1:B:307:ARG:HG2	1:B:312:MET:SD	2.57	0.45
1:C:17:VAL:HG12	1:C:63:THR:HG22	1.98	0.45
1:D:237:ASN:HD21	1:D:251:ARG:HB3	1.81	0.45
1:A:74:ASP:HB2	1:A:139:SER:CB	2.47	0.45
1:B:204:VAL:HG23	1:B:361:ILE:HG12	1.99	0.45
1:D:120:CYS:HB3	1:D:335:HIS:CE1	2.51	0.45
1:A:74:ASP:HB2	1:A:139:SER:HB3	1.99	0.45
1:B:84:GLU:HA	1:B:89:GLN:N	2.32	0.45
1:C:13:ARG:HB3	1:C:287:GLU:OE2	2.17	0.45
1:C:61:GLN:C	1:C:63:THR:H	2.19	0.45
1:C:74:ASP:HB2	1:C:139:SER:CB	2.47	0.45
1:C:172:ARG:HD2	1:C:178:THR:OG1	2.16	0.45
1:C:200:ASP:OD1	1:C:358:GLY:HA2	2.17	0.45
1:A:342:GLU:O	1:A:345:MET:HB2	2.17	0.45
1:C:329:LEU:H	1:C:329:LEU:HD23	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:231:THR:O	1:D:251:ARG:NE	2.49	0.45
1:A:200:ASP:OD1	1:A:358:GLY:HA2	2.15	0.45
1:A:243:ASN:CG	1:A:245:ILE:H	2.19	0.45
1:A:386:PRO:HG2	1:A:389:ALA:HB3	1.99	0.45
1:B:237:ASN:HD21	1:B:253:THR:HG23	1.80	0.45
1:D:74:ASP:HB2	1:D:139:SER:CB	2.47	0.45
1:B:254:ASP:O	1:B:338:PHE:HA	2.16	0.45
1:C:227:LEU:O	1:C:231:THR:N	2.49	0.45
1:D:124:GLY:H	1:D:422:ASN:HD22	1.63	0.45
1:D:167:HIS:HD2	1:D:299:TYR:HA	1.82	0.45
1:D:259:SER:HB2	1:D:386:PRO:CD	2.38	0.45
1:D:400:ARG:HB3	1:D:405:GLN:HB2	1.98	0.45
1:A:52:LEU:O	1:A:56:ILE:HG13	2.17	0.45
1:A:298:LEU:HD13	1:B:94:PRO:HG2	1.98	0.45
1:B:120:CYS:HA	1:B:387:VAL:CG1	2.47	0.45
1:C:84:GLU:HA	1:C:89:GLN:N	2.32	0.45
1:B:200:ASP:OD1	1:B:358:GLY:HA2	2.17	0.45
1:B:342:GLU:O	1:B:345:MET:HB2	2.17	0.45
1:A:227:LEU:O	1:A:231:THR:N	2.50	0.44
1:C:243:ASN:CG	1:C:245:ILE:H	2.21	0.44
1:C:317:THR:O	1:C:321:MET:HG3	2.18	0.44
1:D:202:ALA:HB2	1:D:231:THR:HA	1.99	0.44
1:A:51:LEU:O	1:A:55:SER:OG	2.34	0.44
1:B:76:LEU:O	1:B:113:ALA:HA	2.17	0.44
1:B:181:CYS:O	1:B:185:ARG:HG3	2.17	0.44
1:A:75:LYS:NZ	1:A:133:ALA:HB2	2.32	0.44
1:A:94:PRO:HG2	1:B:298:LEU:HD13	1.99	0.44
1:A:297:ASN:OD1	1:A:299:TYR:HD1	2.01	0.44
1:D:227:LEU:O	1:D:231:THR:N	2.50	0.44
1:A:124:GLY:H	1:A:422:ASN:ND2	2.15	0.44
1:A:204:VAL:HG23	1:A:361:ILE:HG12	1.99	0.44
1:C:120:CYS:HB2	1:C:423:MET:O	2.18	0.44
1:C:229:PHE:CZ	1:C:236:LYS:HB2	2.53	0.44
1:C:239:ASN:HB3	1:C:247:LYS:HG2	1.99	0.44
1:D:51:LEU:HD12	1:D:51:LEU:HA	1.83	0.44
1:D:291:LEU:HA	1:D:432:SER:O	2.17	0.44
1:A:82:LEU:HD22	1:A:85:LEU:HD12	1.99	0.44
1:A:257:GLN:O	1:A:385:HIS:HB3	2.18	0.44
1:C:210:ALA:HB1	1:C:214:ARG:HH21	1.83	0.44
1:C:342:GLU:O	1:C:345:MET:HB2	2.18	0.44
1:D:278:LEU:HB3	1:D:279:SER:H	1.67	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:385:HIS:ND1	1:D:390:THR:OG1	2.47	0.44
1:A:131:TRP:CE3	1:A:291:LEU:HD13	2.52	0.44
1:A:316:ARG:O	1:A:319:LEU:HG	2.17	0.44
1:C:243:ASN:O	1:C:247:LYS:HB2	2.17	0.44
1:C:291:LEU:HA	1:C:432:SER:O	2.17	0.44
1:B:400:ARG:HB3	1:B:405:GLN:HB2	1.99	0.44
1:D:76:LEU:O	1:D:113:ALA:HA	2.18	0.44
1:A:275:LYS:HB2	1:A:275:LYS:HE3	1.63	0.44
1:C:91:HIS:CE1	1:D:428:LYS:HB2	2.53	0.44
1:C:243:ASN:HD21	1:C:245:ILE:HB	1.82	0.44
1:D:84:GLU:HA	1:D:89:GLN:N	2.33	0.44
1:D:120:CYS:HB2	1:D:423:MET:O	2.18	0.44
1:D:130:ALA:O	1:D:134:LEU:HG	2.18	0.44
1:A:319:LEU:O	1:A:323:GLY:N	2.46	0.44
1:B:329:LEU:HD23	1:B:329:LEU:H	1.82	0.44
1:D:260:ASP:OD1	1:D:260:ASP:N	2.48	0.44
1:B:19:GLY:O	1:B:62:ASN:ND2	2.50	0.43
1:B:131:TRP:CE3	1:B:291:LEU:HD13	2.53	0.43
1:B:291:LEU:HA	1:B:432:SER:O	2.17	0.43
1:C:290:SER:HB2	1:C:434:VAL:CB	2.39	0.43
1:D:61:GLN:C	1:D:63:THR:H	2.21	0.43
1:D:128:GLN:HA	1:D:291:LEU:HD21	1.99	0.43
1:A:237:ASN:HD21	1:A:253:THR:HG23	1.83	0.43
1:C:426:ASP:N	1:C:428:LYS:HG2	2.28	0.43
1:D:426:ASP:N	1:D:428:LYS:HG2	2.27	0.43
1:C:257:GLN:O	1:C:385:HIS:HB3	2.18	0.43
1:D:33:ILE:HG21	1:D:43:LYS:O	2.17	0.43
1:B:170:ARG:NH1	1:B:299:TYR:O	2.45	0.43
1:D:59:ALA:HB2	1:D:264:ALA:HB3	2.00	0.43
1:D:131:TRP:CG	1:D:291:LEU:HD23	2.54	0.43
1:D:197:THR:O	1:D:200:ASP:HB2	2.19	0.43
1:A:284:ARG:O	1:A:399:TYR:OH	2.35	0.43
1:B:75:LYS:NZ	1:B:133:ALA:HB2	2.33	0.43
1:B:172:ARG:HD2	1:B:178:THR:OG1	2.17	0.43
1:B:346:TYR:CZ	1:B:366:THR:HG21	2.54	0.43
1:B:385:HIS:ND1	1:B:390:THR:OG1	2.47	0.43
1:C:19:GLY:O	1:C:62:ASN:ND2	2.51	0.43
1:C:181:CYS:O	1:C:185:ARG:HG3	2.19	0.43
1:B:195:HIS:HD2	1:B:354:TYR:CE2	2.36	0.43
1:B:269:SER:O	1:B:273:LEU:HG	2.17	0.43
1:C:297:ASN:OD1	1:C:299:TYR:HD1	2.02	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:204:VAL:HG23	1:D:361:ILE:HG12	2.01	0.43
1:D:243:ASN:CG	1:D:245:ILE:H	2.22	0.43
1:A:291:LEU:HA	1:A:432:SER:O	2.18	0.43
1:A:295:ALA:O	1:B:111:LYS:N	2.51	0.43
1:B:59:ALA:HB2	1:B:264:ALA:HB3	2.00	0.43
1:C:195:HIS:HD2	1:C:354:TYR:CE2	2.37	0.43
1:A:317:THR:O	1:A:321:MET:HG3	2.19	0.43
1:B:229:PHE:CZ	1:B:236:LYS:HB2	2.53	0.43
1:C:35:LYS:O	2:C:2001:HOH:O	2.21	0.43
1:D:61:GLN:O	1:D:64:GLY:N	2.40	0.43
1:A:51:LEU:HD12	1:A:51:LEU:HA	1.80	0.43
1:A:61:GLN:C	1:A:63:THR:H	2.19	0.43
1:A:342:GLU:HA	1:A:345:MET:HB2	2.01	0.43
1:B:226:THR:OG1	1:B:229:PHE:N	2.47	0.43
1:C:94:PRO:HB2	1:D:296:GLY:O	2.19	0.43
1:C:203:TYR:CE2	1:C:362:ARG:HG2	2.54	0.43
1:B:31:LEU:HD23	1:B:31:LEU:HA	1.90	0.42
1:B:120:CYS:HB3	1:B:335:HIS:CE1	2.54	0.42
1:B:227:LEU:O	1:B:231:THR:N	2.52	0.42
1:C:131:TRP:CE3	1:C:291:LEU:HD13	2.53	0.42
1:C:308:MET:O	1:C:312:MET:HG3	2.19	0.42
1:B:360:LEU:HD22	1:B:365:ALA:HB3	2.00	0.42
1:C:61:GLN:O	1:C:64:GLY:N	2.43	0.42
1:C:167:HIS:HD2	1:C:299:TYR:HA	1.84	0.42
1:D:226:THR:OG1	1:D:229:PHE:N	2.44	0.42
1:D:254:ASP:O	1:D:338:PHE:HA	2.19	0.42
1:A:76:LEU:O	1:A:113:ALA:HA	2.18	0.42
1:B:259:SER:HB2	1:B:386:PRO:CD	2.41	0.42
1:C:284:ARG:O	1:C:399:TYR:OH	2.37	0.42
1:C:283:ASN:O	1:C:403:LYS:NZ	2.35	0.42
1:C:385:HIS:ND1	1:C:390:THR:OG1	2.49	0.42
1:D:316:ARG:O	1:D:319:LEU:HG	2.20	0.42
1:A:172:ARG:HD2	1:A:178:THR:OG1	2.20	0.42
1:A:335:HIS:HB3	1:A:345:MET:HE2	2.01	0.42
1:B:167:HIS:HD2	1:B:299:TYR:HA	1.85	0.42
1:C:197:THR:O	1:C:200:ASP:HB2	2.20	0.42
1:A:93:GLY:N	1:A:94:PRO:HD2	2.35	0.42
1:C:93:GLY:N	1:C:94:PRO:HD2	2.35	0.42
1:D:19:GLY:O	1:D:62:ASN:ND2	2.53	0.42
1:D:279:SER:HA	1:D:280:PRO:HD3	1.92	0.42
1:C:61:GLN:C	1:C:63:THR:N	2.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:110:ASN:CG	1:D:313:VAL:HG21	2.40	0.42
1:C:234:SER:CB	1:C:237:ASN:HB3	2.49	0.42
1:D:200:ASP:OD1	1:D:362:ARG:NH1	2.52	0.42
1:A:91:HIS:HE1	1:B:425:GLY:HA3	1.84	0.42
1:A:243:ASN:HD21	1:A:245:ILE:HB	1.84	0.42
1:A:308:MET:O	1:A:312:MET:HG3	2.20	0.42
1:D:290:SER:HB2	1:D:434:VAL:CB	2.39	0.42
1:B:198:MET:O	1:B:201:ALA:HB3	2.20	0.42
1:C:342:GLU:HA	1:C:345:MET:HB2	2.02	0.42
1:A:128:GLN:HE22	1:A:293:SER:HB2	1.85	0.41
1:A:168:TYR:HB2	1:B:89:GLN:OE1	2.20	0.41
1:B:243:ASN:O	1:B:247:LYS:HB2	2.20	0.41
1:C:241:LEU:HD23	1:C:241:LEU:HA	1.87	0.41
1:C:330:GLN:O	1:C:372:ILE:HD12	2.20	0.41
1:D:172:ARG:HD2	1:D:178:THR:OG1	2.20	0.41
1:D:229:PHE:CZ	1:D:236:LYS:HB2	2.54	0.41
1:A:120:CYS:HB2	1:A:423:MET:O	2.20	0.41
1:A:167:HIS:HD2	1:A:299:TYR:HA	1.84	0.41
1:A:181:CYS:O	1:A:185:ARG:HG3	2.20	0.41
1:A:277:GLY:O	1:A:278:LEU:HD22	2.20	0.41
1:D:284:ARG:O	1:D:399:TYR:OH	2.35	0.41
1:A:330:GLN:C	1:A:372:ILE:HD12	2.41	0.41
1:B:241:LEU:HD23	1:B:241:LEU:HA	1.92	0.41
1:C:124:GLY:O	1:C:127:VAL:HB	2.19	0.41
1:C:335:HIS:H	1:C:345:MET:HE3	1.85	0.41
1:D:309:THR:O	1:D:313:VAL:N	2.37	0.41
1:C:84:GLU:O	1:C:88:SER:HA	2.21	0.41
1:C:112:PRO:HA	1:D:293:SER:HB3	2.02	0.41
1:D:124:GLY:O	1:D:127:VAL:HB	2.20	0.41
1:D:360:LEU:HA	1:D:360:LEU:HD23	1.81	0.41
1:B:29:SER:HA	1:B:30:PRO:HD3	1.90	0.41
1:B:61:GLN:C	1:B:63:THR:H	2.22	0.41
1:B:234:SER:CB	1:B:237:ASN:HB3	2.50	0.41
1:A:111:LYS:O	1:B:295:ALA:N	2.53	0.41
1:B:317:THR:O	1:B:321:MET:HG3	2.20	0.41
1:D:170:ARG:NH2	1:D:299:TYR:O	2.53	0.41
1:D:204:VAL:HG21	1:D:343:LEU:HD13	2.02	0.41
1:D:340:ILE:O	1:D:343:LEU:HB2	2.21	0.41
1:A:33:ILE:HD13	1:A:43:LYS:HB3	2.02	0.41
1:D:75:LYS:O	1:D:76:LEU:HD23	2.20	0.41
1:D:243:ASN:O	1:D:247:LYS:HB2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:GLN:C	1:A:63:THR:N	2.73	0.41
1:A:90:GLY:HA2	2:A:2003:HOH:O	2.20	0.41
1:A:404:GLY:HA2	1:A:410:GLN:NE2	2.35	0.41
1:D:346:TYR:CZ	1:D:366:THR:HG21	2.56	0.41
1:D:372:ILE:O	1:D:374:VAL:HG23	2.21	0.41
1:A:115:ARG:HE	1:A:117:GLU:HB2	1.85	0.41
1:A:203:TYR:CE2	1:A:362:ARG:HG2	2.56	0.41
1:A:234:SER:CB	1:A:237:ASN:HB3	2.51	0.41
1:A:299:TYR:OH	1:B:95:ALA:O	2.17	0.41
1:A:335:HIS:H	1:A:345:MET:CE	2.32	0.41
1:A:421:LEU:CD1	1:A:432:SER:HB2	2.51	0.41
1:B:33:ILE:HD13	1:B:43:LYS:HB3	2.01	0.41
1:B:128:GLN:HE22	1:B:293:SER:HB2	1.86	0.41
1:B:130:ALA:O	1:B:134:LEU:HG	2.20	0.41
1:B:143:LEU:HD13	1:B:266:ILE:HD12	2.01	0.41
1:B:197:THR:O	1:B:200:ASP:HB2	2.21	0.41
1:B:213:ASN:ND2	1:B:223:ARG:O	2.38	0.41
1:B:408:GLU:HG3	1:C:31:LEU:HD13	2.01	0.41
1:C:153:VAL:HG23	1:C:154:SER:O	2.21	0.41
1:C:170:ARG:HE	1:C:171:GLN:HG3	1.86	0.41
1:C:316:ARG:O	1:C:319:LEU:HG	2.20	0.41
1:C:335:HIS:HB3	1:C:345:MET:HE2	2.03	0.41
1:D:13:ARG:NH2	1:D:287:GLU:OE1	2.53	0.41
1:D:269:SER:O	1:D:273:LEU:HG	2.21	0.41
1:A:84:GLU:HA	1:A:89:GLN:N	2.36	0.41
1:A:345:MET:SD	1:A:421:LEU:HD23	2.61	0.41
1:B:93:GLY:N	1:B:94:PRO:HD2	2.36	0.41
1:C:319:LEU:O	1:C:323:GLY:N	2.44	0.41
1:A:89:GLN:OE1	1:B:168:TYR:HB2	2.21	0.40
1:A:253:THR:OG1	1:A:254:ASP:N	2.53	0.40
1:B:243:ASN:CG	1:B:245:ILE:H	2.22	0.40
1:B:340:ILE:O	1:B:343:LEU:HB2	2.21	0.40
1:D:360:LEU:HD22	1:D:365:ALA:HB3	2.02	0.40
1:A:372:ILE:O	1:A:372:ILE:HG23	2.21	0.40
1:B:257:GLN:O	1:B:385:HIS:HB3	2.21	0.40
1:B:279:SER:HA	1:B:280:PRO:HD3	1.92	0.40
1:D:200:ASP:OD1	1:D:358:GLY:HA2	2.21	0.40
1:A:130:ALA:O	1:A:134:LEU:HG	2.21	0.40
1:A:131:TRP:O	1:A:135:LEU:HG	2.22	0.40
1:B:124:GLY:O	1:B:127:VAL:HB	2.22	0.40
1:B:210:ALA:HB1	1:B:214:ARG:HH21	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:229:PHE:HZ	1:B:236:LYS:HB2	1.87	0.40
1:B:342:GLU:HA	1:B:345:MET:HB2	2.02	0.40
1:C:33:ILE:HD13	1:C:43:LYS:HB3	2.03	0.40
1:C:128:GLN:HE22	1:C:293:SER:HB2	1.86	0.40
1:D:61:GLN:C	1:D:63:THR:N	2.74	0.40
1:D:123:GLY:O	1:D:127:VAL:HG23	2.21	0.40
1:D:153:VAL:HG23	1:D:154:SER:O	2.21	0.40
1:D:234:SER:CB	1:D:237:ASN:HB3	2.51	0.40
1:A:120:CYS:HB2	1:A:424:GLY:HA2	2.04	0.40
1:A:195:HIS:HD2	1:A:354:TYR:CE2	2.40	0.40
1:B:124:GLY:H	1:B:422:ASN:ND2	2.18	0.40
1:C:124:GLY:H	1:C:422:ASN:ND2	2.19	0.40
1:D:93:GLY:N	1:D:94:PRO:HD2	2.36	0.40
1:D:181:CYS:O	1:D:185:ARG:HG3	2.22	0.40
1:A:309:THR:HA	1:A:312:MET:HB2	2.02	0.40
1:B:297:ASN:OD1	1:B:299:TYR:HD1	2.04	0.40
1:C:237:ASN:HD21	1:C:253:THR:HG23	1.87	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	412/454 (91%)	362 (88%)	45 (11%)	5 (1%)	13	12
1	B	410/454 (90%)	363 (88%)	44 (11%)	3 (1%)	22	25
1	C	413/454 (91%)	361 (87%)	48 (12%)	4 (1%)	15	16
1	D	410/454 (90%)	363 (88%)	44 (11%)	3 (1%)	22	25
All	All	1645/1816 (91%)	1449 (88%)	181 (11%)	15 (1%)	17	19

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	27	LYS
1	A	43	LYS
1	B	27	LYS
1	C	27	LYS
1	C	105	SER
1	D	27	LYS
1	A	66	HIS
1	A	71	ALA
1	A	232	GLN
1	B	71	ALA
1	B	232	GLN
1	C	71	ALA
1	C	232	GLN
1	D	71	ALA
1	D	232	GLN

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	315/350 (90%)	293 (93%)	22 (7%)	15	18
1	B	316/350 (90%)	294 (93%)	22 (7%)	15	18
1	C	317/350 (91%)	296 (93%)	21 (7%)	16	20
1	D	315/350 (90%)	295 (94%)	20 (6%)	18	22
All	All	1263/1400 (90%)	1178 (93%)	85 (7%)	16	20

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	LEU
1	A	55	SER
1	A	62	ASN
1	A	65	LEU
1	A	87	SER
1	A	108	PHE
1	A	115	ARG

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Mol	Chain	Res	Type
1	A	129	SER
1	A	138	THR
1	A	154	SER
1	A	167	HIS
1	A	170	ARG
1	A	191	GLN
1	A	209	TYR
1	A	225	VAL
1	A	227	LEU
1	A	246	TYR
1	A	270	GLU
1	A	276	LEU
1	A	329	LEU
1	A	383	PHE
1	A	438	ILE
1	B	14	VAL
1	B	55	SER
1	B	62	ASN
1	B	87	SER
1	B	108	PHE
1	B	115	ARG
1	B	129	SER
1	B	138	THR
1	B	154	SER
1	B	167	HIS
1	B	170	ARG
1	B	191	GLN
1	B	209	TYR
1	B	225	VAL
1	B	227	LEU
1	B	246	TYR
1	B	260	ASP
1	B	270	GLU
1	B	276	LEU
1	B	329	LEU
1	B	383	PHE
1	B	438	ILE
1	C	51	LEU
1	C	55	SER
1	C	62	ASN
1	C	87	SER
1	C	108	PHE

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Mol	Chain	Res	Type
1	C	115	ARG
1	C	129	SER
1	C	135	LEU
1	C	138	THR
1	C	154	SER
1	C	167	HIS
1	C	170	ARG
1	C	191	GLN
1	C	209	TYR
1	C	225	VAL
1	C	227	LEU
1	C	246	TYR
1	C	270	GLU
1	C	329	LEU
1	C	383	PHE
1	C	438	ILE
1	D	62	ASN
1	D	87	SER
1	D	108	PHE
1	D	115	ARG
1	D	129	SER
1	D	138	THR
1	D	154	SER
1	D	167	HIS
1	D	170	ARG
1	D	191	GLN
1	D	209	TYR
1	D	225	VAL
1	D	227	LEU
1	D	246	TYR
1	D	270	GLU
1	D	291	LEU
1	D	329	LEU
1	D	343	LEU
1	D	383	PHE
1	D	438	ILE

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	422	ASN
1	B	422	ASN

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Mol	Chain	Res	Type
1	C	422	ASN
1	D	422	ASN

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	418/454 (92%)	-0.11	8 (1%)	66	64	34, 65, 86, 105	0
1	B	416/454 (91%)	-0.18	4 (0%)	82	83	34, 65, 85, 104	0
1	C	419/454 (92%)	-0.18	4 (0%)	82	83	34, 65, 86, 108	0
1	D	416/454 (91%)	-0.21	4 (0%)	82	83	34, 64, 86, 105	0
All	All	1669/1816 (91%)	-0.17	20 (1%)	79	77	34, 65, 86, 108	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	233	ALA	10.2
1	B	203	TYR	4.8
1	A	233	ALA	4.7
1	A	361	ILE	4.4
1	A	231	THR	3.1
1	A	357	ALA	3.0
1	A	250	LEU	2.6
1	D	361	ILE	2.6
1	D	343	LEU	2.6
1	A	196	PHE	2.4
1	D	245	ILE	2.4
1	C	67	ASP	2.2
1	A	70	ALA	2.2
1	A	368	LEU	2.2
1	B	196	PHE	2.2
1	C	227	LEU	2.2
1	B	31	LEU	2.1
1	B	43	LYS	2.1
1	C	108	PHE	2.1
1	D	346	TYR	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.