



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:22 PM GMT

PDB ID : 3TQI
Title : Structure of the GMP synthase (guaA) from Coxiella burnetii
Authors : Franklin, M.C.; Cheung, J.; Rudolph, M.; Cassidy, M.; Gary, E.; Burshteyn, F.; Love, J.
Deposited on : 2011-09-09
Resolution : 2.84 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

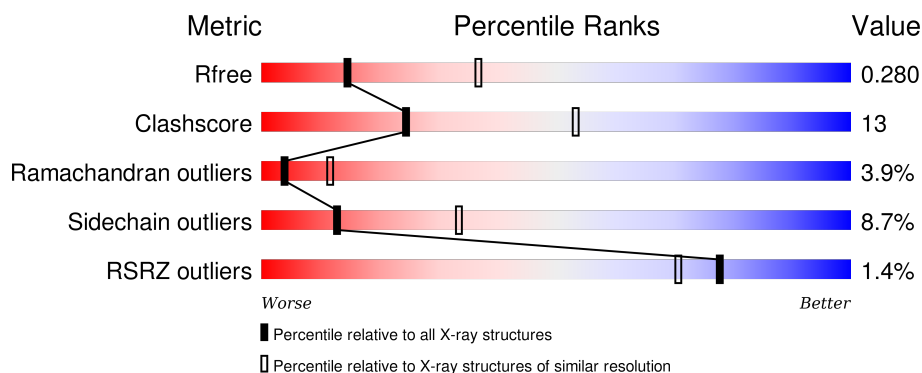
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.84 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	3170 (2.88-2.80)
Clashscore	102246	3658 (2.88-2.80)
Ramachandran outliers	100387	3591 (2.88-2.80)
Sidechain outliers	100360	3594 (2.88-2.80)
RSRZ outliers	91569	3184 (2.88-2.80)

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 $\leq 5\%$. 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	527	<div> <div>%</div> <div> <div></div> <div>63%</div> <div>19%</div> <div>5%</div> <div>12%</div> </div> </div>
1	B	527	<div> <div>%</div> <div> <div></div> <div>65%</div> <div>19%</div> <div>5%</div> <div>12%</div> </div> </div>
1	C	527	<div> <div>2%</div> <div> <div></div> <div>63%</div> <div>20%</div> <div>5%</div> <div>12%</div> </div> </div>
1	D	527	<div> <div>%</div> <div> <div></div> <div>58%</div> <div>25%</div> <div>• •</div> <div>12%</div> </div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 14708 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 GMP synthase [glutamine-hydrolyzing].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	464	Total	C	N	O	S	0	0	0
			3677	2371	626	663	17			
1	B	464	Total	C	N	O	S	0	0	0
			3677	2371	626	663	17			
1	C	464	Total	C	N	O	S	0	0	0
			3677	2371	626	663	17			
1	D	464	Total	C	N	O	S	0	0	0
			3677	2371	626	663	17			

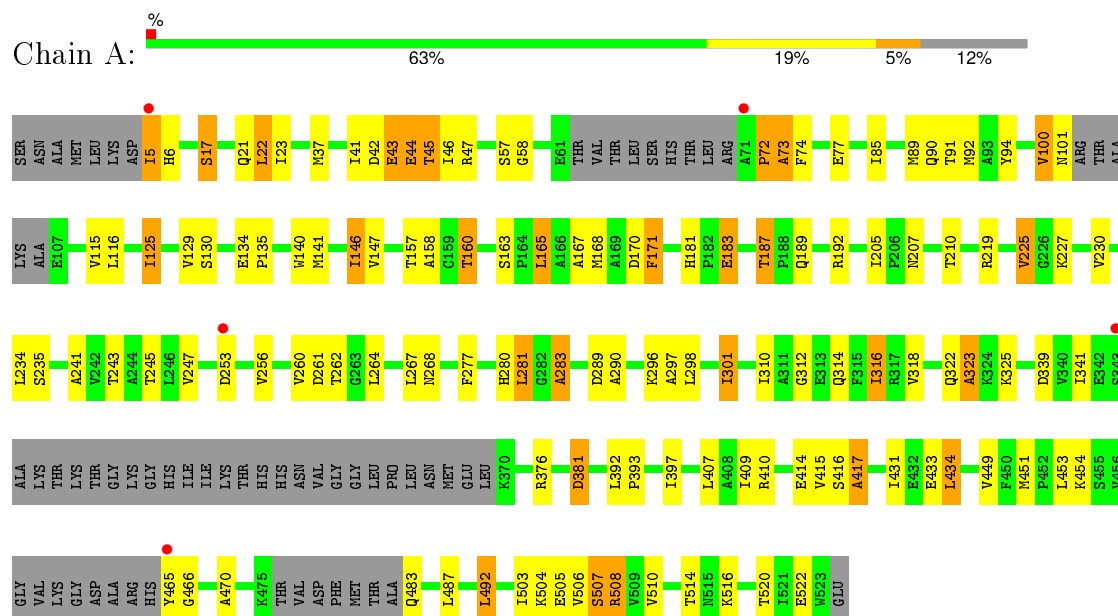
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	SER	-	EXPRESSION TAG	UNP Q83BZ6
C	-1	ASN	-	EXPRESSION TAG	UNP Q83BZ6
C	0	ALA	-	EXPRESSION TAG	UNP Q83BZ6
A	-2	SER	-	EXPRESSION TAG	UNP Q83BZ6
A	-1	ASN	-	EXPRESSION TAG	UNP Q83BZ6
A	0	ALA	-	EXPRESSION TAG	UNP Q83BZ6
D	-2	SER	-	EXPRESSION TAG	UNP Q83BZ6
D	-1	ASN	-	EXPRESSION TAG	UNP Q83BZ6
D	0	ALA	-	EXPRESSION TAG	UNP Q83BZ6
B	-2	SER	-	EXPRESSION TAG	UNP Q83BZ6
B	-1	ASN	-	EXPRESSION TAG	UNP Q83BZ6
B	0	ALA	-	EXPRESSION TAG	UNP Q83BZ6

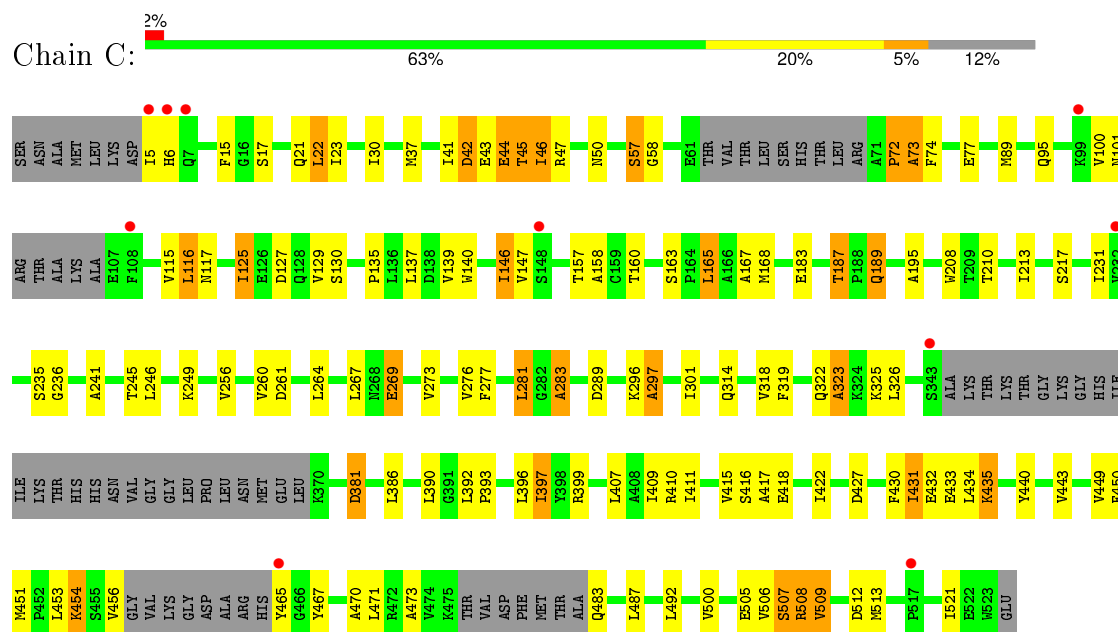
3 Residue-property plots

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.

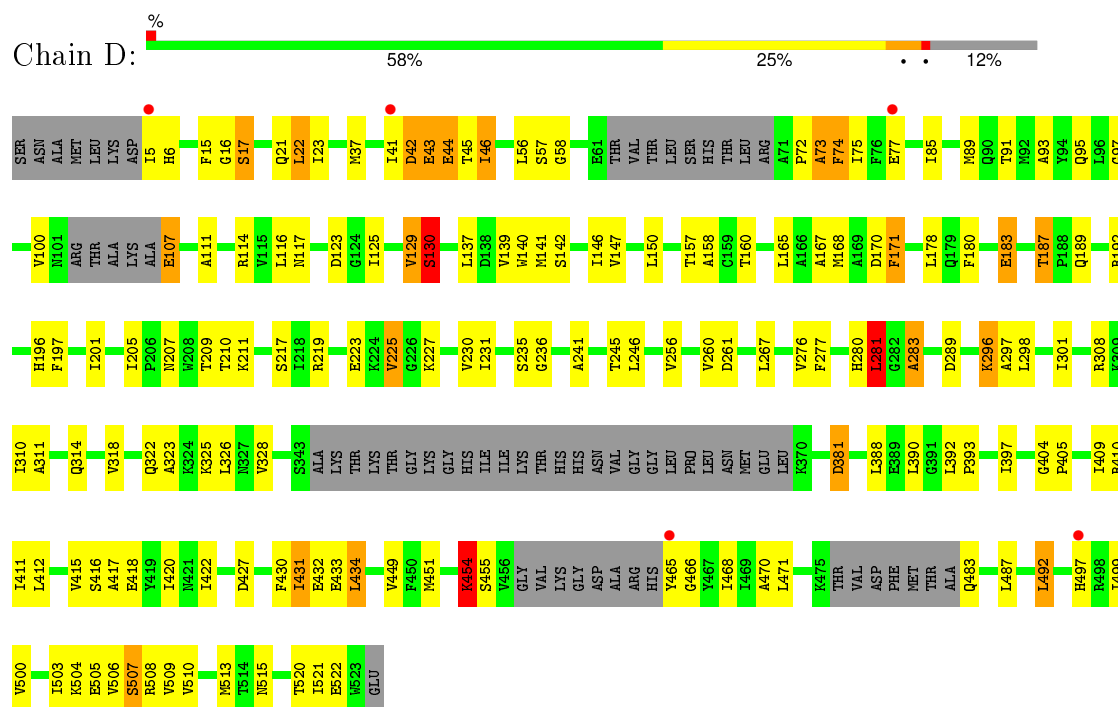
• Molecule 1: GMP synthase [glutamine-hydrolyzing]



- Molecule 1: GMP synthase [glutamine-hydrolyzing]



- Molecule 1: GMP synthase [glutamine-hydrolyzing]



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	74.91Å 143.95Å 107.89Å 90.00° 97.66° 90.00°	Depositor
Resolution (Å)	39.01 – 2.84 38.64 – 2.84	Depositor EDS
% Data completeness (in resolution range)	98.7 (39.01-2.84) 98.7 (38.64-2.84)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.58 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.245 , 0.281 0.242 , 0.280	Depositor DCC
R_{free} test set	2690 reflections (5.35%)	DCC
Wilson B-factor (Å ²)	59.1	Xtriage
Anisotropy	0.167	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 18.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 52999 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	14708	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.44% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	0.42	0/3758	0.60	0/5085
1	B	0.42	0/3758	0.59	0/5085
1	C	0.41	0/3758	0.59	0/5085
1	D	0.42	0/3758	0.60	0/5085
All	All	0.42	0/15032	0.60	0/20340

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	2
1	B	0	2
1	C	0	3
1	D	0	2
All	All	0	9

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	44	GLU	Peptide
1	A	57	SER	Peptide
1	B	44	GLU	Peptide
1	B	57	SER	Peptide
1	C	432	GLU	Peptide
1	C	44	GLU	Peptide
1	C	57	SER	Peptide

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Mol	Chain	Res	Type	Group
1	D	44	GLU	Peptide
1	D	57	SER	Peptide

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	3677	0	3699	90	0
1	B	3677	0	3699	94	0
1	C	3677	0	3699	102	0
1	D	3677	0	3699	107	0
All	All	14708	0	14796	380	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (380) 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:D:449:VAL:HG13	1:D:470:ALA:HB3	1.39	1.00
1:B:451:MET:CE	1:B:470:ALA:HB2	1.93	0.98
1:D:205:ILE:O	1:D:205:ILE:HD12	1.68	0.93
1:B:451:MET:HE2	1:B:470:ALA:HB2	1.50	0.92
1:B:483:GLN:OE1	1:B:483:GLN:N	2.03	0.91
1:D:246:LEU:HD13	1:D:390:LEU:HD11	1.55	0.87
1:C:241:ALA:O	1:C:245:THR:HG23	1.77	0.85
1:B:147:VAL:O	1:B:165:LEU:HD11	1.78	0.83
1:A:147:VAL:O	1:A:165:LEU:HD11	1.77	0.83
1:D:23:ILE:HG12	1:D:183:GLU:HG2	1.60	0.83
1:B:449:VAL:CG2	1:B:470:ALA:HB3	2.09	0.83
1:A:483:GLN:OE1	1:A:483:GLN:N	2.12	0.83
1:A:158:ALA:HB3	1:A:167:ALA:HB3	1.61	0.81
1:B:147:VAL:HG23	1:B:165:LEU:HD13	1.62	0.81
1:C:411:ILE:HD11	1:C:415:VAL:HG22	1.62	0.80
1:D:520:THR:HG23	1:D:522:GLU:O	1.83	0.79
1:C:487:LEU:HB2	1:C:492:LEU:HD21	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:147:VAL:O	1:C:165:LEU:HD11	1.82	0.78
1:A:449:VAL:CG2	1:A:470:ALA:HB3	2.14	0.78
1:A:322:GLN:O	1:A:323:ALA:CB	2.31	0.78
1:C:277:PHE:O	1:C:283:ALA:HB3	1.84	0.77
1:B:520:THR:HG23	1:B:522:GLU:O	1.85	0.77
1:A:241:ALA:O	1:A:245:THR:HG23	1.84	0.77
1:C:483:GLN:OE1	1:C:483:GLN:N	2.19	0.76
1:B:322:GLN:O	1:B:323:ALA:HB3	1.86	0.75
1:B:23:ILE:HG12	1:B:183:GLU:HG2	1.69	0.75
1:A:277:PHE:O	1:A:283:ALA:HB3	1.86	0.74
1:A:23:ILE:HG12	1:A:183:GLU:HG2	1.70	0.74
1:C:15:PHE:HB2	1:C:58:GLY:HA3	1.69	0.74
1:C:322:GLN:O	1:C:323:ALA:HB3	1.88	0.73
1:B:322:GLN:O	1:B:323:ALA:CB	2.37	0.73
1:C:322:GLN:O	1:C:323:ALA:CB	2.36	0.73
1:B:231:ILE:HD12	1:B:323:ALA:HB2	1.71	0.73
1:A:89:MET:HE2	1:A:168:MET:HG3	1.72	0.72
1:A:147:VAL:O	1:A:165:LEU:CD1	2.37	0.72
1:D:15:PHE:HB2	1:D:58:GLY:HA3	1.72	0.72
1:D:322:GLN:O	1:D:323:ALA:HB3	1.90	0.71
1:C:42:ASP:OD1	1:C:42:ASP:N	2.23	0.71
1:B:15:PHE:HB2	1:B:58:GLY:HA3	1.73	0.71
1:D:231:ILE:HD12	1:D:323:ALA:HB2	1.73	0.70
1:A:322:GLN:O	1:A:323:ALA:HB3	1.90	0.70
1:A:409:ILE:HG22	1:A:410:ARG:H	1.57	0.69
1:A:261:ASP:O	1:A:289:ASP:O	2.11	0.69
1:D:225:VAL:HG21	1:D:230:VAL:CG2	2.23	0.69
1:C:296:LYS:O	1:C:297:ALA:HB3	1.90	0.69
1:D:483:GLN:OE1	1:D:483:GLN:N	2.26	0.68
1:C:157:THR:HG22	1:C:167:ALA:C	2.14	0.68
1:A:281:LEU:O	1:A:281:LEU:HD12	1.91	0.68
1:B:277:PHE:O	1:B:283:ALA:HB3	1.94	0.68
1:C:158:ALA:HB3	1:C:167:ALA:HB3	1.76	0.67
1:B:416:SER:O	1:B:417:ALA:HB3	1.95	0.67
1:C:89:MET:CE	1:C:168:MET:HG3	2.24	0.67
1:C:147:VAL:O	1:C:165:LEU:CD1	2.42	0.66
1:A:89:MET:HG3	1:A:168:MET:HE2	1.78	0.66
1:A:449:VAL:HG22	1:A:470:ALA:HB3	1.76	0.66
1:C:411:ILE:HD11	1:C:415:VAL:CG2	2.24	0.65
1:C:21:GLN:O	1:C:22:LEU:HB2	1.97	0.64
1:A:296:LYS:O	1:A:297:ALA:HB3	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:520:THR:HG23	1:A:522:GLU:O	1.97	0.64
1:D:141:MET:CE	1:D:160:THR:HG21	2.27	0.63
1:A:416:SER:O	1:A:417:ALA:CB	2.46	0.63
1:D:141:MET:HE1	1:D:160:THR:HG21	1.79	0.63
1:B:140:TRP:N	1:B:187:THR:HG22	2.13	0.63
1:A:407:LEU:O	1:A:409:ILE:O	2.16	0.63
1:C:21:GLN:O	1:C:22:LEU:CB	2.47	0.63
1:C:160:THR:HG23	1:C:163:SER:H	1.62	0.63
1:A:21:GLN:O	1:A:22:LEU:CB	2.46	0.63
1:A:21:GLN:NE2	1:A:341:ILE:HD11	2.14	0.63
1:B:449:VAL:HG22	1:B:470:ALA:HB3	1.81	0.62
1:B:23:ILE:HD13	1:B:85:ILE:HD12	1.82	0.62
1:C:231:ILE:HD12	1:C:323:ALA:HB2	1.82	0.62
1:B:129:VAL:HG21	1:D:276:VAL:HG22	1.81	0.62
1:A:416:SER:O	1:A:417:ALA:HB3	1.99	0.62
1:D:451:MET:HE2	1:D:470:ALA:HB2	1.81	0.61
1:D:241:ALA:O	1:D:245:THR:HG23	1.99	0.61
1:D:21:GLN:O	1:D:22:LEU:CB	2.48	0.61
1:D:487:LEU:HB2	1:D:492:LEU:HD21	1.82	0.61
1:A:225:VAL:HG21	1:A:230:VAL:CG2	2.30	0.61
1:B:16:GLY:O	1:B:17:SER:HB3	2.01	0.61
1:A:140:TRP:H	1:A:187:THR:HG22	1.65	0.61
1:D:323:ALA:H	1:D:326:LEU:HD12	1.66	0.60
1:B:100:VAL:HG13	1:B:101:ASN:N	2.16	0.60
1:C:409:ILE:HG22	1:C:410:ARG:H	1.67	0.60
1:B:276:VAL:HG13	1:B:277:PHE:CD2	2.36	0.60
1:A:205:ILE:HD12	1:A:205:ILE:O	2.00	0.60
1:B:431:ILE:HA	1:B:434:LEU:HD12	1.82	0.60
1:B:416:SER:O	1:B:417:ALA:CB	2.49	0.60
1:C:451:MET:HE2	1:C:470:ALA:HB2	1.84	0.60
1:C:319:PHE:O	1:C:322:GLN:O	2.20	0.60
1:A:21:GLN:O	1:A:22:LEU:HB2	2.02	0.59
1:A:392:LEU:HB2	1:A:397:ILE:HD11	1.83	0.59
1:D:16:GLY:O	1:D:17:SER:HB3	2.01	0.59
1:B:246:LEU:HD13	1:B:390:LEU:HD11	1.83	0.59
1:A:158:ALA:HB3	1:A:167:ALA:CB	2.32	0.59
1:D:427:ASP:O	1:D:431:ILE:HG22	2.03	0.59
1:D:449:VAL:CG1	1:D:470:ALA:HB3	2.25	0.59
1:A:314:GLN:O	1:A:318:VAL:HG23	2.03	0.58
1:B:451:MET:HE2	1:B:470:ALA:CB	2.29	0.58
1:B:300:GLY:C	1:B:301:ILE:HD12	2.24	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:178:LEU:HD22	1:D:180:PHE:CZ	2.39	0.58
1:C:261:ASP:O	1:C:289:ASP:O	2.21	0.58
1:D:433:GLU:O	1:D:434:LEU:HB2	2.04	0.58
1:D:409:ILE:HG22	1:D:410:ARG:H	1.68	0.58
1:A:41:ILE:HD11	1:A:45:THR:HG21	1.85	0.58
1:C:427:ASP:O	1:C:431:ILE:HG22	2.04	0.58
1:B:158:ALA:HB3	1:B:167:ALA:HB3	1.86	0.57
1:D:111:ALA:HB3	1:D:141:MET:HE2	1.86	0.57
1:B:129:VAL:HG12	1:B:130:SER:N	2.19	0.57
1:C:5:ILE:HG22	1:C:6:HIS:H	1.70	0.57
1:B:433:GLU:O	1:B:434:LEU:HB2	2.05	0.57
1:C:5:ILE:N	1:C:5:ILE:HD12	2.19	0.57
1:C:281:LEU:HD12	1:C:281:LEU:O	2.05	0.57
1:D:451:MET:CE	1:D:470:ALA:HB2	2.34	0.57
1:A:157:THR:HG22	1:A:167:ALA:C	2.25	0.56
1:C:381:ASP:N	1:C:381:ASP:OD1	2.37	0.56
1:A:260:VAL:HG23	1:A:262:THR:HG23	1.87	0.56
1:C:411:ILE:CD1	1:C:415:VAL:HG22	2.33	0.56
1:C:451:MET:CE	1:C:470:ALA:HB2	2.35	0.56
1:A:160:THR:HG22	1:A:163:SER:HB3	1.87	0.56
1:D:147:VAL:O	1:D:165:LEU:HD13	2.05	0.56
1:B:140:TRP:H	1:B:187:THR:HG22	1.69	0.56
1:B:454:LYS:HA	1:B:466:GLY:O	2.06	0.56
1:A:23:ILE:HD13	1:A:85:ILE:HD12	1.88	0.56
1:C:269:GLU:O	1:C:273:VAL:HG12	2.06	0.55
1:A:392:LEU:CB	1:A:397:ILE:HD11	2.35	0.55
1:A:503:ILE:HG22	1:A:504:LYS:O	2.07	0.55
1:D:107:GLU:N	1:D:107:GLU:OE1	2.39	0.55
1:A:433:GLU:O	1:A:434:LEU:HB2	2.06	0.55
1:B:449:VAL:HG23	1:B:470:ALA:HB3	1.85	0.55
1:C:296:LYS:O	1:C:297:ALA:CB	2.52	0.55
1:C:314:GLN:O	1:C:318:VAL:HG23	2.07	0.54
1:C:89:MET:HE2	1:C:168:MET:HG3	1.89	0.54
1:B:409:ILE:HG22	1:B:410:ARG:H	1.72	0.54
1:C:433:GLU:O	1:C:434:LEU:HB2	2.07	0.54
1:C:89:MET:HE3	1:C:168:MET:HG3	1.89	0.54
1:D:140:TRP:N	1:D:187:THR:HG22	2.22	0.54
1:C:411:ILE:HG22	1:C:450:PHE:HB3	1.90	0.54
1:D:21:GLN:O	1:D:22:LEU:HB2	2.07	0.54
1:D:140:TRP:H	1:D:187:THR:HG22	1.71	0.54
1:B:21:GLN:O	1:B:22:LEU:CB	2.54	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:VAL:HB	1:B:135:PRO:HG2	1.89	0.54
1:C:116:LEU:O	1:C:157:THR:O	2.25	0.53
1:B:111:ALA:HB3	1:B:141:MET:HG3	1.90	0.53
1:D:277:PHE:O	1:D:283:ALA:HB3	2.08	0.53
1:D:500:VAL:HG13	1:D:507:SER:HA	1.90	0.53
1:C:453:LEU:O	1:C:454:LYS:HB2	2.09	0.53
1:B:178:LEU:HD22	1:B:180:PHE:CE2	2.44	0.53
1:B:178:LEU:HD22	1:B:180:PHE:CZ	2.42	0.53
1:B:72:PRO:O	1:B:73:ALA:HB3	2.08	0.53
1:C:125:ILE:HG22	1:C:137:LEU:HD21	1.89	0.53
1:C:487:LEU:CB	1:C:492:LEU:HD21	2.36	0.53
1:D:322:GLN:O	1:D:323:ALA:CB	2.55	0.53
1:A:101:ASN:CB	1:A:146:ILE:HG22	2.39	0.53
1:C:410:ARG:HA	1:C:449:VAL:HG13	1.89	0.53
1:B:393:PRO:HG3	1:D:129:VAL:HG23	1.91	0.53
1:A:129:VAL:O	1:A:134:GLU:O	2.27	0.53
1:D:157:THR:HG22	1:D:167:ALA:C	2.29	0.53
1:B:263:GLY:O	1:B:420:ILE:HD12	2.09	0.53
1:B:147:VAL:O	1:B:165:LEU:CD1	2.52	0.53
1:D:261:ASP:O	1:D:289:ASP:O	2.27	0.53
1:C:246:LEU:HD13	1:C:390:LEU:HD11	1.91	0.53
1:D:392:LEU:HB2	1:D:397:ILE:HD11	1.91	0.53
1:B:319:PHE:O	1:B:322:GLN:O	2.27	0.53
1:A:90:GLN:HE21	1:A:100:VAL:HG22	1.74	0.52
1:B:225:VAL:HG21	1:B:230:VAL:CG2	2.39	0.52
1:D:72:PRO:HD2	1:D:95:GLN:OE1	2.08	0.52
1:D:381:ASP:N	1:D:381:ASP:OD1	2.32	0.52
1:D:205:ILE:HD12	1:D:205:ILE:C	2.29	0.52
1:B:23:ILE:CD1	1:B:85:ILE:HD12	2.40	0.52
1:A:189:GLN:NE2	1:A:192:ARG:HH11	2.08	0.52
1:C:431:ILE:HD13	1:C:440:TYR:CD1	2.44	0.52
1:B:32:VAL:HG21	1:B:198:VAL:CG1	2.40	0.52
1:D:430:PHE:O	1:D:433:GLU:O	2.27	0.52
1:B:157:THR:HG23	1:B:167:ALA:CB	2.40	0.52
1:A:451:MET:CE	1:A:470:ALA:HB2	2.40	0.52
1:A:297:ALA:O	1:A:310:ILE:HG21	2.10	0.52
1:C:507:SER:OG	1:C:507:SER:O	2.25	0.52
1:C:127:ASP:OD1	1:C:189:GLN:NE2	2.44	0.51
1:C:101:ASN:CB	1:C:146:ILE:HG22	2.40	0.51
1:A:409:ILE:HG22	1:A:410:ARG:N	2.25	0.51
1:C:507:SER:O	1:C:508:ARG:HB3	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:129:VAL:CG1	1:C:129:VAL:O	2.58	0.51
1:A:483:GLN:HE22	1:A:516:LYS:CD	2.23	0.51
1:A:520:THR:HG21	1:B:456:VAL:HB	1.92	0.51
1:D:158:ALA:HB3	1:D:167:ALA:HB3	1.92	0.50
1:C:512:ASP:HA	1:D:510:VAL:HG12	1.93	0.50
1:A:243:THR:O	1:A:247:VAL:HG23	2.11	0.50
1:A:510:VAL:HG12	1:B:512:ASP:HA	1.93	0.50
1:A:483:GLN:HE22	1:A:516:LYS:HD2	1.77	0.50
1:D:503:ILE:HG22	1:D:504:LYS:O	2.12	0.50
1:B:101:ASN:HB2	1:B:146:ILE:HG22	1.93	0.50
1:A:431:ILE:HA	1:A:434:LEU:HD12	1.93	0.50
1:C:430:PHE:CD2	1:C:471:LEU:HD22	2.47	0.50
1:D:45:THR:O	1:D:46:ILE:HB	2.12	0.50
1:C:409:ILE:HG22	1:C:410:ARG:N	2.27	0.49
1:A:506:VAL:HG12	1:A:507:SER:N	2.26	0.49
1:D:454:LYS:HA	1:D:466:GLY:O	2.12	0.49
1:D:219:ARG:O	1:D:223:GLU:HG3	2.13	0.49
1:C:392:LEU:HB2	1:C:397:ILE:HD11	1.94	0.49
1:D:276:VAL:O	1:D:280:HIS:O	2.29	0.49
1:C:30:ILE:HD13	1:C:195:ALA:HA	1.93	0.49
1:A:267:LEU:HD22	1:A:268:ASN:ND2	2.28	0.49
1:D:433:GLU:O	1:D:434:LEU:CB	2.59	0.49
1:A:298:LEU:HA	1:A:301:ILE:HD13	1.94	0.49
1:A:21:GLN:CD	1:A:341:ILE:HD11	2.33	0.49
1:B:22:LEU:HD13	1:B:25:ARG:HH21	1.78	0.49
1:A:101:ASN:HB2	1:A:146:ILE:HG22	1.94	0.49
1:A:17:SER:CB	1:A:58:GLY:HA2	2.43	0.49
1:A:72:PRO:O	1:A:73:ALA:HB3	2.11	0.49
1:B:433:GLU:O	1:B:434:LEU:CB	2.60	0.49
1:A:41:ILE:CD1	1:A:45:THR:HG21	2.43	0.49
1:D:308:ARG:O	1:D:311:ALA:O	2.31	0.49
1:C:276:VAL:HG23	1:C:277:PHE:CD2	2.48	0.48
1:A:90:GLN:NE2	1:A:100:VAL:HG22	2.28	0.48
1:D:411:ILE:HD11	1:D:420:ILE:HG22	1.95	0.48
1:D:455:SER:HB3	1:D:468:ILE:HD11	1.95	0.48
1:D:89:MET:HG3	1:D:168:MET:HE2	1.95	0.48
1:C:140:TRP:H	1:C:187:THR:HG22	1.78	0.48
1:B:506:VAL:HG12	1:B:507:SER:N	2.28	0.48
1:C:396:LEU:HD23	1:C:396:LEU:O	2.13	0.48
1:B:129:VAL:HG23	1:D:393:PRO:HG3	1.96	0.48
1:A:45:THR:O	1:A:46:ILE:HB	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:129:VAL:HG12	1:D:130:SER:N	2.28	0.48
1:D:157:THR:HG23	1:D:167:ALA:CB	2.44	0.48
1:C:45:THR:O	1:C:46:ILE:HB	2.14	0.48
1:B:16:GLY:O	1:B:17:SER:CB	2.61	0.47
1:D:23:ILE:HD13	1:D:85:ILE:HD12	1.95	0.47
1:D:392:LEU:CB	1:D:397:ILE:HD11	2.43	0.47
1:D:41:ILE:HD11	1:D:45:THR:HG21	1.95	0.47
1:D:197:PHE:HA	1:D:201:ILE:HD12	1.97	0.47
1:C:467:TYR:O	1:C:506:VAL:O	2.33	0.47
1:B:514:THR:HG21	1:B:519:ALA:HB2	1.96	0.47
1:A:170:ASP:O	1:A:171:PHE:HB2	2.14	0.47
1:D:506:VAL:O	1:D:507:SER:OG	2.28	0.47
1:C:509:VAL:HG22	1:D:513:MET:CE	2.44	0.47
1:D:45:THR:O	1:D:46:ILE:CB	2.63	0.47
1:D:506:VAL:HG12	1:D:507:SER:N	2.29	0.47
1:B:411:ILE:HD11	1:B:420:ILE:HG22	1.97	0.47
1:C:72:PRO:O	1:C:73:ALA:HB3	2.15	0.47
1:B:147:VAL:CG2	1:B:165:LEU:HD13	2.38	0.47
1:D:280:HIS:O	1:D:281:LEU:CG	2.63	0.47
1:A:160:THR:HG22	1:A:163:SER:CB	2.45	0.47
1:A:433:GLU:O	1:A:434:LEU:CB	2.63	0.47
1:B:72:PRO:O	1:B:73:ALA:CB	2.63	0.47
1:C:416:SER:O	1:C:418:GLU:N	2.47	0.47
1:C:5:ILE:HG22	1:C:6:HIS:N	2.30	0.46
1:D:72:PRO:O	1:D:73:ALA:HB3	2.14	0.46
1:C:396:LEU:C	1:C:396:LEU:HD23	2.36	0.46
1:C:260:VAL:O	1:C:260:VAL:HG23	2.15	0.46
1:D:170:ASP:O	1:D:171:PHE:HB2	2.15	0.46
1:B:125:ILE:HG23	1:B:189:GLN:CG	2.45	0.46
1:B:125:ILE:O	1:B:137:LEU:HD11	2.15	0.46
1:C:57:SER:OG	1:C:58:GLY:N	2.48	0.46
1:D:139:VAL:HA	1:D:187:THR:HB	1.98	0.46
1:C:411:ILE:CG1	1:C:415:VAL:HG22	2.45	0.46
1:D:298:LEU:HD13	1:D:415:VAL:HG11	1.97	0.46
1:B:45:THR:O	1:B:46:ILE:HB	2.14	0.46
1:B:430:PHE:CD2	1:B:471:LEU:HD22	2.51	0.46
1:B:100:VAL:CG1	1:B:101:ASN:N	2.78	0.46
1:C:158:ALA:HB3	1:C:167:ALA:CB	2.45	0.46
1:C:101:ASN:HB2	1:C:146:ILE:HG22	1.98	0.46
1:B:125:ILE:HG23	1:B:189:GLN:HG3	1.97	0.46
1:B:157:THR:HG22	1:B:167:ALA:C	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:139:VAL:HA	1:C:187:THR:HB	1.98	0.45
1:C:23:ILE:HG12	1:C:183:GLU:HG2	1.98	0.45
1:D:280:HIS:O	1:D:281:LEU:HG	2.17	0.45
1:B:289:ASP:O	1:B:291:LYS:N	2.50	0.45
1:C:140:TRP:N	1:C:187:THR:HG22	2.31	0.45
1:D:189:GLN:HE21	1:D:192:ARG:HD3	1.81	0.45
1:A:381:ASP:N	1:A:381:ASP:OD1	2.47	0.45
1:D:16:GLY:O	1:D:17:SER:CB	2.62	0.45
1:B:409:ILE:HG22	1:B:410:ARG:N	2.32	0.45
1:D:5:ILE:O	1:D:6:HIS:HB2	2.17	0.45
1:D:231:ILE:HG13	1:D:328:VAL:HG11	1.99	0.45
1:C:101:ASN:HB3	1:C:146:ILE:HG22	1.99	0.45
1:D:123:ASP:O	1:D:196:HIS:HE1	2.00	0.45
1:C:411:ILE:HD12	1:C:411:ILE:C	2.37	0.45
1:C:129:VAL:O	1:C:129:VAL:HG12	2.17	0.44
1:A:487:LEU:HB2	1:A:492:LEU:HD21	1.99	0.44
1:B:257:CYS:HB2	1:B:285:VAL:HG22	1.99	0.44
1:D:157:THR:HG23	1:D:167:ALA:HB3	1.99	0.44
1:A:507:SER:OG	1:A:507:SER:O	2.35	0.44
1:C:45:THR:O	1:C:46:ILE:CB	2.66	0.44
1:C:23:ILE:CG1	1:C:183:GLU:HG2	2.48	0.44
1:C:208:TRP:CE2	1:C:213:ILE:HD11	2.53	0.44
1:C:72:PRO:HD2	1:C:95:GLN:OE1	2.17	0.44
1:B:45:THR:O	1:B:46:ILE:CB	2.66	0.44
1:C:392:LEU:CB	1:C:397:ILE:HD11	2.48	0.44
1:D:507:SER:O	1:D:508:ARG:HB3	2.18	0.44
1:A:115:VAL:HB	1:A:135:PRO:HG2	1.99	0.44
1:C:115:VAL:HB	1:C:135:PRO:HG2	1.99	0.44
1:D:209:THR:HG22	1:D:211:LYS:H	1.83	0.44
1:A:451:MET:HE1	1:A:470:ALA:HB2	2.00	0.44
1:A:296:LYS:O	1:A:297:ALA:CB	2.63	0.44
1:B:129:VAL:HG12	1:B:130:SER:H	1.83	0.44
1:C:453:LEU:HD13	1:D:412:LEU:HD22	1.99	0.44
1:C:37:MET:SD	1:C:41:ILE:HD13	2.58	0.44
1:D:409:ILE:HG22	1:D:410:ARG:N	2.33	0.43
1:B:100:VAL:CG2	1:B:147:VAL:HG12	2.48	0.43
1:D:483:GLN:N	1:D:515:ASN:OD1	2.51	0.43
1:B:157:THR:HG23	1:B:167:ALA:HB1	2.00	0.43
1:A:514:THR:HG21	1:B:508:ARG:HA	1.99	0.43
1:A:187:THR:O	1:A:187:THR:OG1	2.33	0.43
1:D:93:ALA:O	1:D:97:GLY:O	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:74:PHE:C	1:D:74:PHE:CD2	2.90	0.43
1:A:89:MET:CE	1:A:168:MET:HG3	2.46	0.43
1:B:431:ILE:C	1:B:433:GLU:O	2.57	0.43
1:D:37:MET:SD	1:D:41:ILE:HD13	2.59	0.43
1:A:125:ILE:HD13	1:A:192:ARG:CZ	2.49	0.43
1:C:500:VAL:HG13	1:C:507:SER:HA	2.01	0.43
1:D:507:SER:OG	1:D:507:SER:O	2.35	0.43
1:C:393:PRO:O	1:C:397:ILE:HD13	2.19	0.43
1:B:396:LEU:C	1:B:396:LEU:HD23	2.39	0.43
1:B:323:ALA:H	1:B:326:LEU:HD12	1.84	0.42
1:B:140:TRP:H	1:B:187:THR:CG2	2.32	0.42
1:C:431:ILE:HD11	1:C:435:LYS:HD3	2.00	0.42
1:D:296:LYS:O	1:D:297:ALA:HB3	2.19	0.42
1:D:42:ASP:N	1:D:42:ASP:OD1	2.47	0.42
1:C:431:ILE:HD12	1:C:431:ILE:C	2.40	0.42
1:B:453:LEU:O	1:B:454:LYS:HB2	2.19	0.42
1:A:312:GLY:O	1:A:316:ILE:HG13	2.18	0.42
1:B:431:ILE:O	1:B:433:GLU:O	2.37	0.42
1:D:314:GLN:O	1:D:318:VAL:HG23	2.20	0.42
1:A:5:ILE:HG23	1:A:6:HIS:N	2.34	0.42
1:B:253:ASP:N	1:B:253:ASP:OD1	2.45	0.42
1:A:92:MET:CE	1:A:168:MET:HE3	2.49	0.42
1:D:178:LEU:HD22	1:D:180:PHE:CE2	2.55	0.42
1:D:499:ILE:HG23	1:D:503:ILE:HD12	2.02	0.42
1:D:416:SER:O	1:D:417:ALA:HB3	2.20	0.42
1:C:443:VAL:HG21	1:C:473:ALA:HB1	2.01	0.42
1:B:100:VAL:HG23	1:B:147:VAL:HG12	2.01	0.42
1:A:451:MET:HE2	1:A:470:ALA:HB2	2.02	0.42
1:A:205:ILE:CD1	1:A:207:ASN:ND2	2.83	0.42
1:A:101:ASN:HB3	1:A:146:ILE:HG22	2.00	0.42
1:D:521:ILE:HD12	1:D:521:ILE:H	1.84	0.42
1:C:456:VAL:HB	1:D:520:THR:HG21	2.02	0.42
1:C:276:VAL:CG2	1:C:277:PHE:CD2	3.03	0.42
1:B:21:GLN:O	1:B:22:LEU:HB2	2.20	0.42
1:C:453:LEU:O	1:C:454:LYS:CB	2.68	0.42
1:B:467:TYR:O	1:B:506:VAL:O	2.38	0.42
1:C:509:VAL:HG22	1:D:513:MET:HE2	2.02	0.42
1:B:209:THR:HG22	1:B:210:THR:N	2.35	0.42
1:D:56:LEU:HD21	1:D:75:ILE:CD1	2.50	0.41
1:C:245:THR:HG21	1:C:392:LEU:HD21	2.01	0.41
1:A:393:PRO:O	1:A:397:ILE:HD13	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:411:ILE:CD1	1:B:420:ILE:HG22	2.51	0.41
1:B:114:ARG:HA	1:B:136:LEU:HD23	2.03	0.41
1:A:453:LEU:HD13	1:B:412:LEU:HD12	2.01	0.41
1:B:72:PRO:HD2	1:B:95:GLN:OE1	2.20	0.41
1:B:451:MET:HE3	1:B:470:ALA:HB2	1.91	0.41
1:D:205:ILE:CD1	1:D:207:ASN:ND2	2.83	0.41
1:D:89:MET:HE3	1:D:168:MET:HG3	2.01	0.41
1:B:371:LEU:HD12	1:B:371:LEU:N	2.35	0.41
1:D:168:MET:HB2	1:D:168:MET:HE3	1.83	0.41
1:A:466:GLY:C	1:A:506:VAL:O	2.59	0.41
1:D:513:MET:HE2	1:D:513:MET:HB2	1.93	0.41
1:D:404:GLY:N	1:D:405:PRO:HD2	2.36	0.41
1:C:41:ILE:HD11	1:C:45:THR:HG21	2.03	0.41
1:C:513:MET:CE	1:D:471:LEU:HD12	2.50	0.41
1:A:43:GLU:O	1:A:44:GLU:CB	2.69	0.41
1:D:388:LEU:HA	1:D:388:LEU:HD12	1.96	0.41
1:D:43:GLU:O	1:D:44:GLU:HB3	2.21	0.41
1:C:411:ILE:HD12	1:C:411:ILE:O	2.21	0.41
1:C:323:ALA:H	1:C:326:LEU:HD12	1.85	0.41
1:D:150:LEU:HG	1:D:165:LEU:HD23	2.02	0.41
1:A:17:SER:HB2	1:A:58:GLY:HA2	2.02	0.41
1:B:130:SER:HB3	1:B:134:GLU:O	2.22	0.40
1:D:411:ILE:HD11	1:D:420:ILE:CG2	2.51	0.40
1:C:513:MET:HE2	1:C:513:MET:HB2	1.95	0.40
1:A:181:HIS:O	1:A:187:THR:CG2	2.69	0.40
1:A:37:MET:SD	1:A:41:ILE:HD13	2.62	0.40
1:D:141:MET:HE3	1:D:160:THR:HG21	2.01	0.40
1:A:205:ILE:HD12	1:A:205:ILE:C	2.41	0.40
1:B:242:VAL:HG12	1:B:375:LEU:HD21	2.03	0.40
1:A:234:LEU:HD23	1:A:234:LEU:HA	1.94	0.40
1:C:43:GLU:O	1:C:44:GLU:CB	2.69	0.40
1:C:396:LEU:HD22	1:C:397:ILE:HD12	2.03	0.40
1:A:280:HIS:O	1:A:281:LEU:HG	2.22	0.40
1:C:125:ILE:HG23	1:C:189:GLN:HG3	2.03	0.40
1:B:281:LEU:O	1:B:281:LEU:CG	2.69	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	452/527 (86%)	401 (89%)	34 (8%)	17 (4%)	4	12
1	B	452/527 (86%)	405 (90%)	29 (6%)	18 (4%)	4	11
1	C	452/527 (86%)	398 (88%)	37 (8%)	17 (4%)	4	12
1	D	452/527 (86%)	394 (87%)	40 (9%)	18 (4%)	4	11
All	All	1808/2108 (86%)	1598 (88%)	140 (8%)	70 (4%)	4	12

All (70) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	17	SER
1	A	73	ALA
1	A	210	THR
1	A	323	ALA
1	A	417	ALA
1	B	22	LEU
1	B	73	ALA
1	B	129	VAL
1	B	323	ALA
1	C	73	ALA
1	C	125	ILE
1	C	323	ALA
1	C	417	ALA
1	D	46	ILE
1	D	73	ALA
1	D	434	LEU
1	A	22	LEU
1	A	283	ALA
1	A	325	LYS
1	B	125	ILE
1	B	325	LYS
1	B	417	ALA

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Mol	Chain	Res	Type
1	C	22	LEU
1	C	325	LYS
1	D	22	LEU
1	D	129	VAL
1	A	507	SER
1	B	17	SER
1	B	282	GLY
1	B	290	ALA
1	B	434	LEU
1	B	507	SER
1	C	17	SER
1	C	236	GLY
1	D	171	PHE
1	D	281	LEU
1	D	325	LYS
1	A	171	PHE
1	A	290	ALA
1	A	434	LEU
1	B	45	THR
1	C	297	ALA
1	C	454	LYS
1	C	507	SER
1	D	130	SER
1	D	236	GLY
1	A	45	THR
1	A	72	PRO
1	A	508	ARG
1	B	46	ILE
1	B	117	ASN
1	B	130	SER
1	B	283	ALA
1	C	45	THR
1	C	283	ALA
1	D	17	SER
1	D	283	ALA
1	D	432	GLU
1	D	507	SER
1	A	125	ILE
1	A	301	ILE
1	C	117	ASN
1	D	117	ASN
1	D	125	ILE

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Mol	Chain	Res	Type
1	D	454	LYS
1	C	46	ILE
1	C	301	ILE
1	D	301	ILE
1	B	301	ILE
1	C	72	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	398/449 (89%)	362 (91%)	36 (9%)	12	32
1	B	398/449 (89%)	366 (92%)	32 (8%)	15	38
1	C	398/449 (89%)	364 (92%)	34 (8%)	13	35
1	D	398/449 (89%)	362 (91%)	36 (9%)	12	32
All	All	1592/1796 (89%)	1454 (91%)	138 (9%)	13	33

All (138) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	A	42	ASP
1	A	43	GLU
1	A	47	ARG
1	A	74	PHE
1	A	77	GLU
1	A	91	THR
1	A	94	TYR
1	A	100	VAL
1	A	116	LEU
1	A	130	SER
1	A	141	MET
1	A	146	ILE
1	A	160	THR
1	A	165	LEU

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Mol	Chain	Res	Type
1	A	183	GLU
1	A	187	THR
1	A	219	ARG
1	A	225	VAL
1	A	227	LYS
1	A	235	SER
1	A	253	ASP
1	A	256	VAL
1	A	264	LEU
1	A	281	LEU
1	A	316	ILE
1	A	339	ASP
1	A	376	ARG
1	A	381	ASP
1	A	414	GLU
1	A	415	VAL
1	A	454	LYS
1	A	465	TYR
1	A	492	LEU
1	A	505	GLU
1	A	508	ARG
1	B	23	ILE
1	B	48	ASP
1	B	50	ASN
1	B	74	PHE
1	B	77	GLU
1	B	91	THR
1	B	99	LYS
1	B	100	VAL
1	B	116	LEU
1	B	130	SER
1	B	146	ILE
1	B	165	LEU
1	B	183	GLU
1	B	189	GLN
1	B	210	THR
1	B	225	VAL
1	B	227	LYS
1	B	235	SER
1	B	253	ASP
1	B	256	VAL
1	B	260	VAL

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Mol	Chain	Res	Type
1	B	264	LEU
1	B	269	GLU
1	B	281	LEU
1	B	418	GLU
1	B	435	LYS
1	B	465	TYR
1	B	492	LEU
1	B	505	GLU
1	B	508	ARG
1	B	509	VAL
1	B	521	ILE
1	C	42	ASP
1	C	47	ARG
1	C	50	ASN
1	C	74	PHE
1	C	77	GLU
1	C	100	VAL
1	C	116	LEU
1	C	130	SER
1	C	146	ILE
1	C	165	LEU
1	C	187	THR
1	C	189	GLN
1	C	210	THR
1	C	217	SER
1	C	235	SER
1	C	249	LYS
1	C	256	VAL
1	C	264	LEU
1	C	267	LEU
1	C	269	GLU
1	C	281	LEU
1	C	381	ASP
1	C	386	LEU
1	C	397	ILE
1	C	399	ARG
1	C	407	LEU
1	C	422	ILE
1	C	431	ILE
1	C	435	LYS
1	C	465	TYR
1	C	505	GLU

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Mol	Chain	Res	Type
1	C	508	ARG
1	C	509	VAL
1	C	521	ILE
1	D	42	ASP
1	D	43	GLU
1	D	74	PHE
1	D	77	GLU
1	D	91	THR
1	D	100	VAL
1	D	107	GLU
1	D	114	ARG
1	D	116	LEU
1	D	130	SER
1	D	137	LEU
1	D	142	SER
1	D	146	ILE
1	D	183	GLU
1	D	187	THR
1	D	210	THR
1	D	217	SER
1	D	225	VAL
1	D	227	LYS
1	D	235	SER
1	D	256	VAL
1	D	260	VAL
1	D	267	LEU
1	D	281	LEU
1	D	296	LYS
1	D	310	ILE
1	D	381	ASP
1	D	418	GLU
1	D	422	ILE
1	D	431	ILE
1	D	454	LYS
1	D	465	TYR
1	D	492	LEU
1	D	497	HIS
1	D	505	GLU
1	D	509	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	HIS
1	A	52	HIS
1	A	90	GLN
1	A	189	GLN
1	A	196	HIS
1	A	268	ASN
1	A	278	GLN
1	B	50	ASN
1	B	101	ASN
1	B	191	HIS
1	B	196	HIS
1	B	268	ASN
1	B	327	ASN
1	B	445	GLN
1	B	501	ASN
1	C	50	ASN
1	C	196	HIS
1	C	254	GLN
1	C	278	GLN
1	C	515	ASN
1	D	181	HIS
1	D	189	GLN
1	D	196	HIS
1	D	207	ASN
1	D	445	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	464/527 (88%)	0.02	5 (1%) 82 76	35, 55, 80, 98	0
1	B	464/527 (88%)	0.02	6 (1%) 79 72	35, 53, 80, 102	0
1	C	464/527 (88%)	0.08	10 (2%) 65 56	36, 56, 84, 96	0
1	D	464/527 (88%)	0.02	5 (1%) 82 76	33, 53, 80, 93	0
All	All	1856/2108 (88%)	0.03	26 (1%) 78 71	33, 54, 81, 102	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	465	TYR	4.6
1	D	465	TYR	4.0
1	C	5	ILE	3.9
1	A	465	TYR	3.9
1	B	497	HIS	3.7
1	C	517	PRO	3.2
1	B	5	ILE	3.1
1	B	465	TYR	3.0
1	C	6	HIS	2.9
1	C	232	VAL	2.7
1	C	108	PHE	2.6
1	A	5	ILE	2.4
1	A	343	SER	2.4
1	B	46	ILE	2.4
1	D	41	ILE	2.4
1	C	148	SER	2.3
1	C	343	SER	2.3
1	C	7	GLN	2.3
1	A	71	ALA	2.3
1	A	253	ASP	2.2
1	D	5	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	77	GLU	2.1
1	B	71	ALA	2.1
1	C	99	LYS	2.1
1	D	497	HIS	2.0
1	B	79	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.