



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:23 PM GMT

PDB ID : 3TTK
Title : Crystal structure of apo-SpuD
Authors : Wu, D.H.; Lim, S.C.; Song, H.W.
Deposited on : 2011-09-14
Resolution : 2.97 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

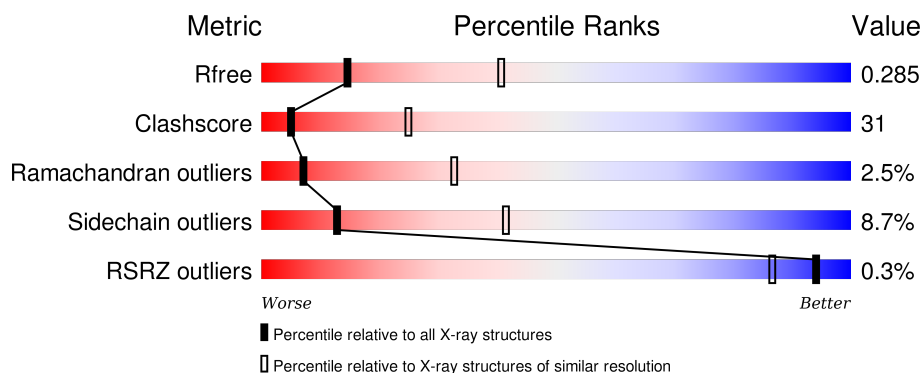
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.97 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	1992 (3.00-2.96)
Clashscore	102246	2349 (3.00-2.96)
Ramachandran outliers	100387	2274 (3.00-2.96)
Sidechain outliers	100360	2277 (3.00-2.96)
RSRZ outliers	91569	2007 (3.00-2.96)

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	345	<div> <div></div> <div>50%40%8% .</div> </div>
1	B	345	<div> <div></div> <div>52%41%6% .</div> </div>
1	C	345	<div> <div>%</div> <div>54%37%8% .</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8157 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 Polyamine transport protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	340	Total	C	N	O	S	0	0	0
			2675	1724	433	509	9			
1	B	340	Total	C	N	O	S	0	0	0
			2675	1724	433	509	9			
1	C	340	Total	C	N	O	S	0	0	0
			2675	1724	433	509	9			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	21	GLY	-	EXPRESSION TAG	UNP Q9I6J1
A	22	PRO	-	EXPRESSION TAG	UNP Q9I6J1
A	23	LEU	-	EXPRESSION TAG	UNP Q9I6J1
A	24	GLY	-	EXPRESSION TAG	UNP Q9I6J1
A	25	SER	-	EXPRESSION TAG	UNP Q9I6J1
B	21	GLY	-	EXPRESSION TAG	UNP Q9I6J1
B	22	PRO	-	EXPRESSION TAG	UNP Q9I6J1
B	23	LEU	-	EXPRESSION TAG	UNP Q9I6J1
B	24	GLY	-	EXPRESSION TAG	UNP Q9I6J1
B	25	SER	-	EXPRESSION TAG	UNP Q9I6J1
C	21	GLY	-	EXPRESSION TAG	UNP Q9I6J1
C	22	PRO	-	EXPRESSION TAG	UNP Q9I6J1
C	23	LEU	-	EXPRESSION TAG	UNP Q9I6J1
C	24	GLY	-	EXPRESSION TAG	UNP Q9I6J1
C	25	SER	-	EXPRESSION TAG	UNP Q9I6J1

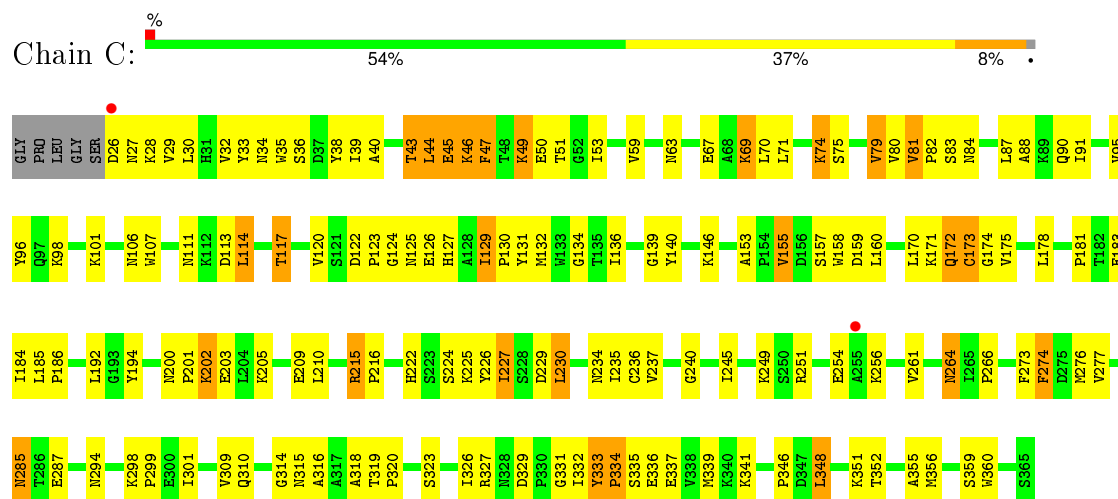
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	49	Total	O	0	0
			49	49		
2	B	50	Total	O	0	0
			50	50		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	33	Total	O	0	0
			33	33		



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	47.77Å 108.98Å 228.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.97 40.86 – 2.50	Depositor EDS
% Data completeness (in resolution range)	85.3 (20.00-2.97) 86.3 (40.86-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.56 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.4.0077	Depositor
R, R_{free}	0.215 , 0.288 0.212 , 0.285	Depositor DCC
R_{free} test set	1086 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	52.6	Xtriage
Anisotropy	0.405	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 38.3	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 36560 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8157	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.64% 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	0.36	0/2742	0.57	2/3724 (0.1%)
1	B	0.39	0/2742	0.59	2/3724 (0.1%)
1	C	0.37	0/2742	0.57	2/3724 (0.1%)
All	All	0.37	0/8226	0.57	6/11172 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	333	TYR	C-N-CD	-7.78	103.48	120.60
1	A	333	TYR	C-N-CD	-7.31	104.52	120.60
1	B	173	CYS	CA-CB-SG	6.67	126.01	114.00
1	C	333	TYR	C-N-CA	5.57	145.41	122.00
1	B	333	TYR	C-N-CD	-5.48	108.55	120.60
1	A	333	TYR	C-N-CA	5.25	144.04	122.00

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	2675	0	2658	191	0
1	B	2675	0	2658	151	0
1	C	2675	0	2658	152	0
2	A	49	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	50	0	0	3	0
2	C	33	0	0	1	0
All	All	8157	0	7974	494	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 31.

All (494) 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:34:ASN:ND2	1:A:35:TRP:H	1.34	1.24
1:B:336:GLU:HA	1:B:339:MET:CG	1.77	1.15
1:A:336:GLU:HA	1:A:339:MET:CG	1.76	1.14
1:C:34:ASN:ND2	1:C:35:TRP:H	1.47	1.13
1:C:87:LEU:O	1:C:91:ILE:HG12	1.48	1.12
1:C:336:GLU:HA	1:C:339:MET:CG	1.81	1.11
1:C:336:GLU:HA	1:C:339:MET:HG3	1.23	1.10
1:B:336:GLU:HA	1:B:339:MET:HG2	1.29	1.08
1:A:28:LYS:HD2	1:A:28:LYS:N	1.65	1.07
1:B:34:ASN:ND2	1:B:35:TRP:H	1.57	1.02
1:A:336:GLU:HA	1:A:339:MET:HG2	1.38	1.02
1:A:34:ASN:ND2	1:A:35:TRP:N	2.10	0.99
1:A:87:LEU:O	1:A:91:ILE:HG12	1.64	0.96
1:C:172:GLN:HG2	1:C:173:CYS:H	1.30	0.96
1:B:222:HIS:CD2	1:B:225:LYS:H	1.82	0.95
1:B:34:ASN:HD22	1:B:35:TRP:H	1.18	0.91
1:C:84:ASN:HD22	1:C:274:PHE:H	1.15	0.91
1:A:40:ALA:HB1	1:A:41:PRO:HD2	1.52	0.91
1:A:34:ASN:HD22	1:A:35:TRP:H	1.10	0.90
1:B:28:LYS:N	1:B:28:LYS:HD2	1.84	0.90
1:A:222:HIS:CD2	1:A:225:LYS:H	1.88	0.90
1:A:30:LEU:HD22	1:A:32:VAL:HG23	1.51	0.90
1:A:28:LYS:HD2	1:A:28:LYS:H	1.36	0.90
1:A:67:GLU:HG3	1:A:90:GLN:HE21	1.35	0.90
1:A:120:VAL:O	1:A:120:VAL:HG12	1.71	0.89
1:C:336:GLU:CA	1:C:339:MET:HG3	2.03	0.88
1:C:34:ASN:ND2	1:C:35:TRP:N	2.23	0.87
1:C:222:HIS:CD2	1:C:225:LYS:H	1.92	0.86
1:B:84:ASN:HD22	1:B:274:PHE:H	1.18	0.86
1:B:34:ASN:ND2	1:B:35:TRP:N	2.22	0.86
1:B:113:ASP:O	1:B:117:THR:HG22	1.75	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:84:ASN:ND2	1:C:274:PHE:H	1.74	0.85
1:C:28:LYS:HD2	1:C:28:LYS:N	1.92	0.84
1:A:63:ASN:HD21	1:A:83:SER:HB2	1.41	0.82
1:C:348:LEU:H	1:C:348:LEU:HD12	1.43	0.81
1:A:84:ASN:HD22	1:A:274:PHE:H	1.24	0.81
1:C:34:ASN:HD22	1:C:35:TRP:H	1.24	0.81
1:A:51:THR:HG22	1:A:53:ILE:HG13	1.62	0.81
1:C:32:VAL:HG22	1:C:79:VAL:HG13	1.62	0.81
1:B:222:HIS:HD2	1:B:224:SER:H	1.28	0.80
1:B:84:ASN:ND2	1:B:274:PHE:H	1.79	0.79
1:A:34:ASN:ND2	1:A:81:VAL:HG11	1.96	0.79
1:B:332:ILE:C	1:B:334:PRO:HD2	2.03	0.79
1:B:113:ASP:O	1:B:117:THR:CG2	2.30	0.79
1:A:81:VAL:O	1:A:81:VAL:HG22	1.82	0.78
1:B:34:ASN:ND2	1:B:81:VAL:HG11	1.99	0.78
1:B:106:ASN:H	1:B:294:ASN:HD21	1.30	0.78
1:B:332:ILE:O	1:B:334:PRO:HD2	1.83	0.77
1:C:172:GLN:HG2	1:C:173:CYS:N	2.00	0.77
1:A:34:ASN:HD22	1:A:35:TRP:N	1.79	0.77
1:C:332:ILE:C	1:C:334:PRO:HD2	2.04	0.77
1:B:120:VAL:O	1:B:120:VAL:HG12	1.82	0.76
1:A:32:VAL:HG22	1:A:79:VAL:HG13	1.68	0.76
1:B:87:LEU:O	1:B:91:ILE:HG12	1.86	0.76
1:B:81:VAL:O	1:B:81:VAL:HG22	1.86	0.75
1:A:336:GLU:HA	1:A:339:MET:HG3	1.69	0.75
1:C:222:HIS:HD2	1:C:225:LYS:H	1.32	0.75
1:C:44:LEU:HD12	1:C:44:LEU:H	1.51	0.75
1:A:333:TYR:N	1:A:334:PRO:CD	2.48	0.74
1:A:224:SER:O	1:A:227:ILE:HG13	1.87	0.74
1:B:329:ASP:HB3	1:B:332:ILE:HD12	1.70	0.74
1:A:222:HIS:HD2	1:A:225:LYS:H	1.33	0.73
1:C:185:LEU:HB2	1:C:186:PRO:HD3	1.68	0.73
1:A:332:ILE:C	1:A:334:PRO:HD2	2.07	0.73
1:C:332:ILE:C	1:C:334:PRO:CD	2.57	0.73
1:C:332:ILE:O	1:C:334:PRO:HD2	1.89	0.73
1:C:333:TYR:N	1:C:334:PRO:CD	2.49	0.73
1:C:81:VAL:HG22	1:C:81:VAL:O	1.88	0.73
1:B:44:LEU:H	1:B:44:LEU:HD12	1.54	0.73
1:A:185:LEU:HB2	1:A:186:PRO:HD3	1.71	0.72
1:A:336:GLU:CA	1:A:339:MET:HG2	2.18	0.72
1:B:336:GLU:CA	1:B:339:MET:HG2	2.13	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:ASN:ND2	1:A:81:VAL:CG1	2.53	0.71
1:A:113:ASP:O	1:A:117:THR:HG22	1.90	0.71
1:C:205:LYS:O	1:C:209:GLU:HG3	1.91	0.71
1:C:34:ASN:ND2	1:C:81:VAL:HG11	2.05	0.70
1:B:30:LEU:HD11	1:B:292:PHE:HB2	1.74	0.70
1:A:44:LEU:HD12	1:A:44:LEU:H	1.55	0.69
1:C:175:VAL:HA	1:C:237:VAL:O	1.92	0.69
1:B:34:ASN:ND2	1:B:81:VAL:CG1	2.55	0.69
1:C:224:SER:O	1:C:227:ILE:HG13	1.93	0.69
1:A:274:PHE:CD2	1:A:274:PHE:N	2.58	0.69
1:C:140:TYR:CE2	1:C:155:VAL:HG21	2.27	0.69
1:A:81:VAL:HA	1:A:276:MET:O	1.93	0.68
1:A:249:LYS:HA	1:A:261:VAL:HB	1.74	0.68
1:A:84:ASN:ND2	1:A:274:PHE:H	1.90	0.68
1:B:126:GLU:HB2	1:B:127:HIS:CD2	2.28	0.68
1:B:336:GLU:HA	1:B:339:MET:HG3	1.75	0.68
1:B:222:HIS:HD2	1:B:225:LYS:H	1.38	0.68
1:B:30:LEU:HD22	1:B:32:VAL:HG23	1.76	0.68
1:B:333:TYR:N	1:B:334:PRO:CD	2.57	0.68
1:B:74:LYS:HB2	1:B:74:LYS:HZ3	1.59	0.67
1:A:157:SER:HB2	1:A:267:LYS:HE2	1.74	0.67
1:C:222:HIS:HD2	1:C:224:SER:H	1.43	0.67
1:C:172:GLN:CG	1:C:173:CYS:H	2.00	0.66
1:C:172:GLN:O	1:C:174:GLY:N	2.29	0.66
1:A:51:THR:CG2	1:A:53:ILE:HG13	2.26	0.66
1:B:172:GLN:HG3	1:B:172:GLN:O	1.95	0.66
1:A:222:HIS:HD2	1:A:224:SER:H	1.43	0.66
1:A:126:GLU:HB2	1:A:127:HIS:HD2	1.61	0.66
1:C:335:SER:C	1:C:337:GLU:H	2.00	0.66
1:A:336:GLU:O	1:A:336:GLU:CG	2.44	0.65
1:A:63:ASN:ND2	1:A:83:SER:HB2	2.11	0.65
1:C:172:GLN:CG	1:C:173:CYS:N	2.58	0.65
1:A:89:LYS:HG2	1:A:347:ASP:OD2	1.95	0.65
1:B:348:LEU:HD12	1:B:348:LEU:H	1.62	0.65
1:A:106:ASN:H	1:A:294:ASN:HD21	1.44	0.65
1:B:319:THR:HB	1:B:320:PRO:HD3	1.79	0.64
1:C:158:TRP:CE2	1:C:266:PRO:HG2	2.33	0.64
1:C:129:ILE:CD1	1:C:277:VAL:HB	2.28	0.64
1:B:32:VAL:HG22	1:B:79:VAL:HG13	1.80	0.64
1:B:34:ASN:HD22	1:B:35:TRP:N	1.91	0.63
1:C:126:GLU:HB2	1:C:127:HIS:CD2	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:LYS:CD	1:A:28:LYS:N	2.50	0.63
1:B:332:ILE:C	1:B:334:PRO:CD	2.67	0.63
1:A:63:ASN:HD21	1:A:83:SER:CB	2.10	0.63
1:A:114:LEU:HA	1:A:117:THR:HG23	1.80	0.62
1:A:126:GLU:HB2	1:A:127:HIS:CD2	2.34	0.62
1:A:82:PRO:HD2	1:A:276:MET:O	1.98	0.62
1:A:333:TYR:N	1:A:334:PRO:HD2	1.97	0.62
1:C:51:THR:CG2	1:C:53:ILE:HG13	2.29	0.62
1:C:336:GLU:HA	1:C:339:MET:CB	2.28	0.62
1:C:126:GLU:HB2	1:C:127:HIS:HD2	1.64	0.62
1:A:222:HIS:CD2	1:A:224:SER:H	2.18	0.62
1:A:336:GLU:HA	1:A:339:MET:CB	2.31	0.61
1:B:222:HIS:CD2	1:B:224:SER:H	2.16	0.61
1:A:232:ASN:HB2	1:A:234:ASN:ND2	2.16	0.61
1:C:34:ASN:ND2	1:C:81:VAL:CG1	2.63	0.61
1:B:123:PRO:O	1:B:126:GLU:HG3	1.99	0.61
1:C:51:THR:HG22	1:C:53:ILE:HG13	1.81	0.61
1:B:335:SER:C	1:B:337:GLU:H	2.02	0.61
1:C:34:ASN:HD22	1:C:35:TRP:N	1.93	0.61
1:B:153:ALA:O	1:B:155:VAL:N	2.34	0.61
1:C:82:PRO:HD2	1:C:276:MET:O	2.01	0.61
1:B:106:ASN:H	1:B:294:ASN:ND2	1.98	0.61
1:B:335:SER:O	1:B:337:GLU:N	2.34	0.61
1:B:335:SER:HB2	1:B:338:VAL:HG23	1.82	0.61
1:A:130:PRO:HG2	1:A:314:GLY:HA3	1.82	0.61
1:C:30:LEU:HD22	1:C:32:VAL:HG23	1.83	0.61
1:A:332:ILE:O	1:A:334:PRO:HD2	2.00	0.61
1:B:140:TYR:CE2	1:B:155:VAL:HG21	2.36	0.60
1:B:333:TYR:N	1:B:334:PRO:HD2	2.04	0.60
1:C:320:PRO:HA	1:C:327:ARG:HD3	1.83	0.60
1:A:332:ILE:C	1:A:334:PRO:CD	2.70	0.60
1:B:28:LYS:CD	1:B:28:LYS:N	2.59	0.60
1:A:336:GLU:HG2	1:A:336:GLU:O	2.01	0.60
1:A:229:ASP:HA	1:A:234:ASN:HD22	1.66	0.60
1:C:106:ASN:H	1:C:294:ASN:HD21	1.48	0.60
1:A:123:PRO:O	1:A:126:GLU:HG3	2.02	0.60
1:A:91:ILE:HD12	1:A:127:HIS:ND1	2.17	0.60
1:B:181:PRO:HB3	1:B:360:TRP:HB2	1.84	0.59
1:B:51:THR:HG22	1:B:53:ILE:HG13	1.82	0.59
1:A:175:VAL:HA	1:A:237:VAL:O	2.02	0.59
1:C:178:LEU:HG	1:C:240:GLY:HA2	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:200:ASN:HB3	1:C:203:GLU:HG3	1.85	0.59
1:A:120:VAL:CG1	1:A:120:VAL:O	2.44	0.58
1:C:33:TYR:HB3	1:C:80:VAL:HG12	1.85	0.58
1:C:215:ARG:N	1:C:216:PRO:HD2	2.18	0.58
1:C:120:VAL:HG12	1:C:120:VAL:O	2.03	0.58
1:B:232:ASN:HD22	1:B:232:ASN:N	1.99	0.58
1:A:158:TRP:CE2	1:A:266:PRO:HG2	2.38	0.58
1:B:336:GLU:O	1:B:336:GLU:CD	2.42	0.58
1:C:113:ASP:O	1:C:117:THR:HG22	2.02	0.58
1:C:329:ASP:C	1:C:331:GLY:H	2.07	0.58
1:A:67:GLU:HG3	1:A:90:GLN:NE2	2.13	0.58
1:C:274:PHE:N	1:C:274:PHE:CD2	2.71	0.58
1:A:30:LEU:HD22	1:A:32:VAL:CG2	2.30	0.58
1:B:27:ASN:C	1:B:28:LYS:HD2	2.23	0.57
1:A:335:SER:C	1:A:337:GLU:H	2.07	0.57
1:A:140:TYR:CE2	1:A:155:VAL:HG21	2.39	0.57
1:B:81:VAL:HA	1:B:276:MET:O	2.04	0.57
1:B:215:ARG:N	1:B:216:PRO:HD2	2.20	0.57
1:A:192:LEU:HD21	1:A:210:LEU:HD22	1.87	0.57
1:B:249:LYS:HA	1:B:261:VAL:HB	1.87	0.57
1:A:40:ALA:HB1	1:A:41:PRO:CD	2.29	0.56
1:B:39:ILE:HG12	1:B:43:THR:OG1	2.04	0.56
1:C:29:VAL:O	1:C:29:VAL:HG23	2.04	0.56
1:C:91:ILE:HD12	1:C:127:HIS:ND1	2.20	0.56
1:C:155:VAL:HA	1:C:160:LEU:HD22	1.86	0.56
1:C:332:ILE:C	1:C:334:PRO:HD3	2.24	0.56
1:B:120:VAL:CG1	1:B:120:VAL:O	2.54	0.56
1:A:178:LEU:HG	1:A:240:GLY:HA2	1.87	0.56
1:C:90:GLN:HB3	1:C:96:TYR:HE2	1.70	0.56
1:A:200:ASN:O	1:A:204:LEU:HG	2.05	0.56
1:A:47:PHE:O	1:A:50:GLU:N	2.23	0.56
1:A:67:GLU:O	1:A:71:LEU:HD13	2.06	0.56
1:A:298:LYS:O	1:A:299:PRO:C	2.44	0.56
1:C:215:ARG:HD3	1:C:215:ARG:C	2.26	0.55
1:B:129:ILE:CD1	1:B:277:VAL:HB	2.36	0.55
1:C:43:THR:HG22	1:C:301:ILE:HG23	1.89	0.55
1:A:29:VAL:HG23	1:A:29:VAL:O	2.06	0.55
1:A:336:GLU:CA	1:A:339:MET:CG	2.68	0.55
1:A:104:LEU:N	1:A:105:PRO:HD3	2.20	0.55
1:B:26:ASP:O	1:B:29:VAL:HG22	2.07	0.55
1:C:44:LEU:O	1:C:47:PHE:HB3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:ALA:HB1	1:B:41:PRO:HD2	1.89	0.55
1:B:126:GLU:HB2	1:B:127:HIS:HD2	1.70	0.55
1:A:214:ILE:C	1:A:216:PRO:HD2	2.27	0.55
1:C:336:GLU:CG	1:C:336:GLU:O	2.54	0.55
1:C:39:ILE:HG12	1:C:43:THR:OG1	2.06	0.55
1:A:134:GLY:HA3	1:A:273:PHE:CE2	2.40	0.54
1:A:199:ASP:OD1	1:A:352:THR:OG1	2.25	0.54
1:C:81:VAL:HA	1:C:276:MET:O	2.08	0.54
1:A:30:LEU:HD12	1:A:47:PHE:CE2	2.42	0.54
1:A:306:THR:O	1:A:310:GLN:HA	2.08	0.54
1:A:200:ASN:C	1:A:200:ASN:OD1	2.46	0.54
1:B:133:TRP:HB2	1:B:273:PHE:O	2.08	0.54
1:A:49:LYS:O	1:A:49:LYS:HG3	2.06	0.54
1:A:40:ALA:HB3	1:A:43:THR:OG1	2.08	0.54
1:A:215:ARG:C	1:A:215:ARG:HD3	2.29	0.53
1:A:188:ALA:HB2	1:A:211:PHE:CE2	2.43	0.53
1:A:336:GLU:O	1:A:336:GLU:CD	2.47	0.53
1:C:285:ASN:C	1:C:285:ASN:HD22	2.10	0.53
1:C:298:LYS:O	1:C:299:PRO:C	2.47	0.53
1:B:71:LEU:C	1:B:73:GLY:H	2.12	0.53
1:B:87:LEU:HD22	1:B:276:MET:HG3	1.89	0.53
1:C:329:ASP:C	1:C:331:GLY:N	2.62	0.53
1:A:215:ARG:N	1:A:216:PRO:HD2	2.23	0.53
1:B:350:ALA:HB1	1:B:354:ARG:HE	1.73	0.53
1:A:30:LEU:HD11	1:A:292:PHE:HB2	1.91	0.53
1:A:285:ASN:C	1:A:285:ASN:HD22	2.11	0.53
1:B:251:ARG:O	1:B:254:GLU:HB3	2.09	0.53
1:A:222:HIS:HD2	1:A:225:LYS:N	2.06	0.53
1:C:226:TYR:O	1:C:230:LEU:HB2	2.09	0.53
1:A:39:ILE:HG12	1:A:43:THR:OG1	2.08	0.52
1:B:139:GLY:CA	1:B:245:ILE:HD13	2.39	0.52
1:B:139:GLY:HA3	1:B:245:ILE:HD13	1.90	0.52
1:B:82:PRO:HD2	1:B:276:MET:O	2.09	0.52
1:C:319:THR:HB	1:C:320:PRO:HD3	1.91	0.52
1:C:114:LEU:HA	1:C:117:THR:HG23	1.90	0.52
1:C:67:GLU:HG3	1:C:90:GLN:HE21	1.74	0.52
1:C:335:SER:C	1:C:337:GLU:N	2.63	0.52
1:C:153:ALA:O	1:C:155:VAL:N	2.43	0.52
1:A:171:LYS:HG3	1:A:171:LYS:O	2.10	0.52
1:A:30:LEU:HD12	1:A:47:PHE:HE2	1.74	0.52
1:B:274:PHE:N	1:B:274:PHE:CD2	2.77	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:254:GLU:C	1:B:256:LYS:H	2.13	0.52
1:B:124:GLY:O	1:B:125:ASN:C	2.47	0.52
1:A:114:LEU:HG	1:A:274:PHE:HE1	1.74	0.52
1:B:175:VAL:HA	1:B:237:VAL:O	2.10	0.52
1:A:28:LYS:CD	1:A:28:LYS:H	2.16	0.52
1:A:47:PHE:O	1:A:48:THR:C	2.47	0.52
1:A:106:ASN:H	1:A:294:ASN:ND2	2.07	0.52
1:B:34:ASN:O	1:B:59:VAL:HA	2.10	0.52
1:A:267:LYS:NZ	2:A:384:HOH:O	2.42	0.51
1:C:335:SER:O	1:C:336:GLU:HB3	2.11	0.51
1:B:67:GLU:HG3	1:B:90:GLN:HE21	1.76	0.51
1:B:104:LEU:N	1:B:105:PRO:HD3	2.26	0.51
1:A:134:GLY:CA	1:A:273:PHE:CE2	2.94	0.51
1:B:67:GLU:O	1:B:71:LEU:HD13	2.10	0.51
1:A:33:TYR:HB3	1:A:80:VAL:HG12	1.93	0.51
1:A:122:ASP:OD1	1:A:127:HIS:CD2	2.63	0.51
1:C:336:GLU:CD	1:C:336:GLU:O	2.48	0.51
1:C:178:LEU:HB2	1:C:184:ILE:HD11	1.92	0.51
1:A:31:HIS:HB3	1:A:77:TYR:HA	1.93	0.51
1:B:222:HIS:HD2	1:B:224:SER:N	2.04	0.50
1:A:162:PHE:HB3	1:A:191:TYR:CE2	2.47	0.50
1:B:40:ALA:HB3	1:B:43:THR:HG23	1.93	0.50
1:A:215:ARG:HG3	1:A:363:ILE:O	2.12	0.50
1:A:50:GLU:O	1:A:50:GLU:HG2	2.12	0.50
1:B:81:VAL:O	1:B:81:VAL:CG2	2.59	0.50
1:B:47:PHE:CE1	1:B:292:PHE:HA	2.47	0.50
1:A:329:ASP:O	1:A:331:GLY:N	2.45	0.50
1:C:113:ASP:O	1:C:117:THR:CG2	2.60	0.50
1:C:332:ILE:O	1:C:334:PRO:CD	2.57	0.50
1:C:254:GLU:O	1:C:256:LYS:HD2	2.11	0.50
1:C:45:GLU:O	1:C:46:LYS:C	2.50	0.50
1:B:158:TRP:CE2	1:B:266:PRO:HG2	2.47	0.50
1:C:106:ASN:H	1:C:294:ASN:ND2	2.09	0.49
1:A:30:LEU:HB3	1:A:55:VAL:HG13	1.93	0.49
1:A:352:THR:O	1:A:355:ALA:N	2.45	0.49
1:A:348:LEU:H	1:A:348:LEU:HD12	1.76	0.49
1:B:34:ASN:HD22	1:B:81:VAL:CG1	2.25	0.49
1:A:113:ASP:O	1:A:117:THR:CG2	2.60	0.49
1:A:274:PHE:HD2	1:A:274:PHE:N	2.07	0.49
1:B:336:GLU:HA	1:B:339:MET:CB	2.40	0.49
1:C:34:ASN:O	1:C:59:VAL:HA	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:LEU:O	1:A:47:PHE:HB3	2.12	0.49
1:B:86:PHE:O	1:B:87:LEU:C	2.50	0.49
1:C:91:ILE:HD12	1:C:127:HIS:CG	2.47	0.49
1:A:352:THR:O	1:A:355:ALA:HB3	2.13	0.49
1:C:170:LEU:C	1:C:172:GLN:N	2.65	0.49
1:C:134:GLY:HA3	1:C:273:PHE:CE2	2.48	0.49
1:A:232:ASN:HB2	1:A:234:ASN:HD21	1.76	0.48
1:C:40:ALA:HB3	1:C:43:THR:OG1	2.13	0.48
1:A:106:ASN:OD1	1:A:294:ASN:O	2.30	0.48
1:C:249:LYS:HA	1:C:261:VAL:HB	1.94	0.48
1:A:334:PRO:HG2	1:A:339:MET:CE	2.43	0.48
1:B:69:LYS:HD2	1:B:69:LYS:HA	1.61	0.48
1:A:335:SER:C	1:A:337:GLU:N	2.65	0.48
1:A:97:GLN:NE2	1:A:280:PRO:O	2.42	0.48
1:A:74:LYS:HA	1:A:74:LYS:HZ2	1.79	0.48
1:B:335:SER:C	1:B:337:GLU:N	2.66	0.48
1:A:47:PHE:CE1	1:A:292:PHE:HA	2.48	0.48
1:A:250:SER:O	1:A:252:ALA:N	2.46	0.48
1:C:171:LYS:O	1:C:172:GLN:O	2.32	0.48
1:C:173:CYS:O	1:C:235:ILE:HA	2.14	0.48
1:C:123:PRO:O	1:C:126:GLU:HG3	2.14	0.47
1:A:188:ALA:HB2	1:A:211:PHE:HE2	1.79	0.47
1:B:51:THR:HG21	1:B:53:ILE:HD12	1.97	0.47
1:C:50:GLU:O	1:C:50:GLU:HG2	2.14	0.47
1:C:329:ASP:O	1:C:331:GLY:N	2.47	0.47
1:B:185:LEU:HB2	1:B:186:PRO:HD3	1.96	0.47
1:A:153:ALA:O	1:A:155:VAL:N	2.48	0.47
1:A:78:ASP:HB3	1:A:289:ALA:HB2	1.95	0.47
1:B:29:VAL:HG23	1:B:29:VAL:O	2.14	0.47
1:C:69:LYS:HD2	1:C:75:SER:HA	1.97	0.47
1:C:63:ASN:HD21	1:C:83:SER:HB2	1.79	0.47
1:C:30:LEU:HD22	1:C:32:VAL:CG2	2.45	0.47
1:A:156:ASP:O	1:A:266:PRO:HA	2.14	0.47
1:B:146:LYS:HE2	1:B:146:LYS:HB3	1.69	0.47
1:B:200:ASN:OD1	1:B:200:ASN:C	2.51	0.47
1:B:336:GLU:CG	1:B:336:GLU:O	2.63	0.47
1:C:251:ARG:O	1:C:254:GLU:HB3	2.15	0.47
1:A:34:ASN:CG	1:A:35:TRP:N	2.67	0.47
1:B:129:ILE:HD13	1:B:129:ILE:H	1.79	0.47
1:B:189:LEU:HD21	1:B:204:LEU:HD23	1.97	0.47
1:C:139:GLY:CA	1:C:245:ILE:HD13	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:39:ILE:HG12	1:C:43:THR:HG1	1.80	0.46
1:A:133:TRP:HB2	1:A:273:PHE:O	2.15	0.46
1:B:119:GLU:C	1:B:121:SER:H	2.18	0.46
1:A:329:ASP:C	1:A:331:GLY:N	2.69	0.46
1:A:250:SER:C	1:A:252:ALA:N	2.67	0.46
1:C:63:ASN:HD21	1:C:83:SER:CB	2.29	0.46
1:C:222:HIS:CD2	1:C:224:SER:H	2.27	0.46
1:B:329:ASP:CB	1:B:332:ILE:HD12	2.44	0.46
1:C:323:SER:HB3	1:C:326:ILE:HD12	1.98	0.46
1:A:136:ILE:O	1:A:136:ILE:HG22	2.16	0.46
1:C:122:ASP:OD1	1:C:127:HIS:CD2	2.68	0.46
1:A:309:VAL:O	1:A:310:GLN:HB2	2.14	0.46
1:C:336:GLU:CA	1:C:339:MET:CG	2.72	0.46
1:A:346:PRO:HG2	1:A:348:LEU:HG	1.98	0.46
1:A:146:LYS:HG2	1:A:146:LYS:O	2.16	0.46
1:C:74:LYS:HZ2	1:C:74:LYS:HA	1.80	0.46
1:C:264:ASN:HA	1:C:264:ASN:HD22	1.59	0.46
1:A:173:CYS:O	1:A:235:ILE:HA	2.16	0.46
1:C:84:ASN:HD22	1:C:274:PHE:N	1.98	0.46
1:C:129:ILE:HD13	1:C:277:VAL:HB	1.97	0.46
1:C:200:ASN:OD1	1:C:202:LYS:N	2.48	0.45
1:C:101:LYS:HE3	1:C:107:TRP:CZ2	2.51	0.45
1:C:131:TYR:CE2	1:C:132:MET:HE2	2.51	0.45
1:A:336:GLU:OE1	1:A:336:GLU:O	2.34	0.45
1:B:337:GLU:O	1:B:341:LYS:HG3	2.15	0.45
1:C:136:ILE:CD1	1:C:183:GLU:HB3	2.46	0.45
1:B:110:LEU:HD13	1:B:115:MET:HE2	1.98	0.45
1:C:124:GLY:O	1:C:125:ASN:C	2.55	0.45
1:B:200:ASN:HA	1:B:201:PRO:HD2	1.70	0.45
1:B:132:MET:HG2	1:B:312:PRO:O	2.16	0.45
1:B:337:GLU:HB2	2:B:19:HOH:O	2.16	0.45
1:C:111:ASN:HA	1:C:316:ALA:HB2	1.99	0.45
1:B:36:SER:OG	1:B:61:ASP:OD2	2.22	0.45
1:B:130:PRO:HG2	1:B:314:GLY:HA3	1.99	0.45
1:A:124:GLY:O	1:A:125:ASN:C	2.55	0.45
1:A:40:ALA:HB3	1:A:43:THR:HG23	1.98	0.45
1:C:129:ILE:HB	1:C:130:PRO:HD2	1.99	0.45
1:C:74:LYS:HZ3	1:C:74:LYS:HB2	1.80	0.45
1:A:40:ALA:CB	1:A:43:THR:HG23	2.47	0.45
1:A:32:VAL:HG22	1:A:79:VAL:CG1	2.41	0.45
1:C:346:PRO:HA	2:C:382:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:178:LEU:HG	1:B:240:GLY:HA2	1.99	0.45
1:B:114:LEU:HA	1:B:117:THR:HG23	1.99	0.45
1:B:329:ASP:O	1:B:331:GLY:N	2.50	0.45
1:A:146:LYS:HE2	1:A:146:LYS:HB3	1.78	0.45
1:B:140:TYR:CZ	1:B:155:VAL:HG21	2.52	0.45
1:C:90:GLN:HB3	1:C:96:TYR:CE2	2.51	0.45
1:A:87:LEU:HD22	1:A:276:MET:CB	2.47	0.44
1:C:352:THR:O	1:C:355:ALA:HB3	2.16	0.44
1:A:95:VAL:O	1:A:95:VAL:CG1	2.65	0.44
1:A:245:ILE:HD13	1:A:263:TYR:HD1	1.83	0.44
1:A:224:SER:O	1:A:225:LYS:C	2.55	0.44
1:C:67:GLU:O	1:C:71:LEU:HD13	2.17	0.44
1:B:189:LEU:HD23	1:B:207:ALA:HB2	1.99	0.44
1:C:336:GLU:CD	1:C:336:GLU:C	2.75	0.44
1:B:128:ALA:HB1	1:B:276:MET:HB3	2.00	0.44
1:C:134:GLY:CA	1:C:273:PHE:CE2	3.00	0.44
1:A:45:GLU:O	1:A:46:LYS:C	2.55	0.44
1:C:40:ALA:HB3	1:C:43:THR:HG23	2.00	0.44
1:A:329:ASP:C	1:A:331:GLY:H	2.21	0.44
1:B:183:GLU:HA	1:B:345:PHE:CE1	2.52	0.44
1:C:336:GLU:HG2	1:C:336:GLU:O	2.17	0.44
1:B:122:ASP:OD1	1:B:127:HIS:CD2	2.71	0.44
1:A:189:LEU:HD13	1:A:198:THR:HG22	1.98	0.44
1:A:63:ASN:CB	1:A:86:PHE:CE1	3.00	0.44
1:C:45:GLU:O	1:C:47:PHE:N	2.50	0.44
1:C:356:MET:O	1:C:359:SER:HB2	2.18	0.44
1:B:63:ASN:HD21	1:B:83:SER:CB	2.30	0.44
1:B:163:LYS:O	1:B:164:PRO:C	2.52	0.44
1:B:28:LYS:O	1:B:54:LYS:N	2.50	0.44
1:B:232:ASN:ND2	1:B:232:ASN:N	2.66	0.44
1:A:100:ASP:OD1	1:A:103:LYS:HD2	2.18	0.44
1:B:205:LYS:O	1:B:208:GLU:HB3	2.18	0.43
1:B:43:THR:HG22	1:B:301:ILE:HG23	2.00	0.43
1:B:63:ASN:HD21	1:B:83:SER:HB2	1.83	0.43
1:C:336:GLU:HA	1:C:339:MET:HB2	1.99	0.43
1:B:51:THR:CG2	1:B:53:ILE:HG13	2.46	0.43
1:C:111:ASN:OD1	1:C:113:ASP:HB2	2.17	0.43
1:C:273:PHE:C	1:C:274:PHE:CD2	2.92	0.43
1:C:49:LYS:O	1:C:49:LYS:HG2	2.19	0.43
1:C:192:LEU:HD21	1:C:210:LEU:HD22	2.01	0.43
1:B:32:VAL:HG22	1:B:79:VAL:CG1	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:VAL:HG11	1:A:239:ILE:CD1	2.49	0.43
1:A:34:ASN:O	1:A:59:VAL:HA	2.17	0.43
1:C:95:VAL:CG1	1:C:95:VAL:O	2.65	0.43
1:B:352:THR:O	1:B:355:ALA:HB3	2.19	0.43
1:A:104:LEU:HD23	1:A:294:ASN:HB2	2.00	0.43
1:B:255:ALA:O	1:B:256:LYS:C	2.56	0.43
1:B:195:LYS:HG3	2:B:399:HOH:O	2.18	0.43
1:B:85:SER:HB3	2:B:403:HOH:O	2.19	0.42
1:B:157:SER:HB2	1:B:267:LYS:HE2	2.00	0.42
1:B:33:TYR:HB3	1:B:80:VAL:HG12	2.00	0.42
1:A:132:MET:HB2	1:A:132:MET:HE3	1.93	0.42
1:A:32:VAL:CG1	1:A:33:TYR:N	2.83	0.42
1:C:28:LYS:CD	1:C:28:LYS:N	2.69	0.42
1:B:309:VAL:O	1:B:310:GLN:HB2	2.18	0.42
1:C:70:LEU:HD11	1:C:80:VAL:HG21	2.00	0.42
1:A:254:GLU:C	1:A:256:LYS:H	2.22	0.42
1:A:289:ALA:O	1:A:292:PHE:HB3	2.19	0.42
1:A:352:THR:O	1:A:353:GLN:C	2.58	0.42
1:C:132:MET:HE3	1:C:132:MET:HB2	1.83	0.42
1:A:336:GLU:CA	1:A:339:MET:HG3	2.44	0.42
1:A:250:SER:C	1:A:252:ALA:H	2.23	0.42
1:B:48:THR:HG22	1:B:49:LYS:N	2.33	0.42
1:B:140:TYR:HA	1:B:236:CYS:O	2.20	0.42
1:A:129:ILE:HD13	1:A:129:ILE:H	1.84	0.42
1:A:250:SER:O	1:A:251:ARG:C	2.58	0.42
1:B:100:ASP:OD1	1:B:103:LYS:HD2	2.20	0.42
1:C:348:LEU:H	1:C:348:LEU:CD1	2.21	0.42
1:B:104:LEU:HD23	1:B:294:ASN:HB2	2.02	0.42
1:A:175:VAL:HG13	1:A:237:VAL:HB	2.01	0.42
1:C:200:ASN:C	1:C:200:ASN:OD1	2.58	0.42
1:A:31:HIS:CB	1:A:77:TYR:HA	2.49	0.42
1:C:254:GLU:C	1:C:256:LYS:H	2.23	0.42
1:B:185:LEU:HD23	1:B:185:LEU:HA	1.74	0.42
1:B:285:ASN:C	1:B:285:ASN:HD22	2.23	0.42
1:A:34:ASN:HD22	1:A:81:VAL:CG1	2.27	0.42
1:B:104:LEU:HA	1:B:294:ASN:HD22	1.84	0.42
1:A:350:ALA:O	1:A:353:GLN:HB3	2.20	0.42
1:B:134:GLY:HA3	1:B:273:PHE:CE2	2.55	0.42
1:A:95:VAL:O	1:A:95:VAL:HG12	2.20	0.42
1:C:157:SER:C	1:C:159:ASP:N	2.74	0.42
1:A:333:TYR:HA	1:A:334:PRO:HD2	1.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:214:ILE:C	1:B:216:PRO:HD2	2.40	0.41
1:A:215:ARG:HD3	1:A:215:ARG:O	2.20	0.41
1:C:140:TYR:HA	1:C:236:CYS:O	2.19	0.41
1:B:195:LYS:HA	1:B:196:PRO:HD3	1.85	0.41
1:A:98:LYS:H	1:A:98:LYS:HD2	1.84	0.41
1:C:229:ASP:HA	1:C:234:ASN:HD22	1.85	0.41
1:A:27:ASN:ND2	1:A:285:ASN:OD1	2.54	0.41
1:A:27:ASN:C	1:A:28:LYS:HD2	2.36	0.41
1:C:139:GLY:HA3	1:C:245:ILE:HD13	2.02	0.41
1:B:95:VAL:O	1:B:95:VAL:HG12	2.19	0.41
1:C:309:VAL:O	1:C:310:GLN:HB2	2.20	0.41
1:B:30:LEU:HD12	1:B:47:PHE:CE2	2.55	0.41
1:C:194:TYR:CD1	1:C:203:GLU:CD	2.93	0.41
1:C:34:ASN:CG	1:C:81:VAL:HG11	2.41	0.41
1:C:140:TYR:CZ	1:C:155:VAL:HG21	2.54	0.41
1:B:189:LEU:HD13	1:B:198:THR:HG22	2.02	0.41
1:C:130:PRO:HG2	1:C:314:GLY:HA3	2.02	0.41
1:A:230:LEU:HD23	1:A:230:LEU:HA	1.77	0.41
1:A:129:ILE:CD1	1:A:277:VAL:HB	2.51	0.41
1:A:87:LEU:HD22	1:A:276:MET:HB2	2.01	0.41
1:A:312:PRO:HD3	1:A:332:ILE:HG23	2.02	0.41
1:A:33:TYR:O	1:A:80:VAL:HA	2.21	0.41
1:A:78:ASP:O	1:A:279:ILE:HG23	2.20	0.41
1:A:131:TYR:CE2	1:A:132:MET:HE2	2.55	0.41
1:A:69:LYS:HD2	1:A:69:LYS:HA	1.56	0.41
1:A:91:ILE:HD12	1:A:127:HIS:CG	2.55	0.41
1:C:200:ASN:HA	1:C:201:PRO:HD2	1.66	0.41
1:B:254:GLU:C	1:B:256:LYS:N	2.73	0.41
1:B:33:TYR:HB2	1:B:77:TYR:CD1	2.55	0.41
1:C:315:ASN:HB3	1:C:318:ALA:HB3	2.03	0.41
1:A:59:VAL:O	1:A:59:VAL:HG23	2.21	0.41
1:C:84:ASN:ND2	1:C:274:PHE:N	2.57	0.41
1:A:157:SER:C	1:A:159:ASP:N	2.74	0.41
1:B:197:ASP:O	1:B:198:THR:C	2.59	0.41
1:A:181:PRO:HD2	1:A:182:THR:H	1.86	0.41
1:A:292:PHE:O	1:A:295:PHE:HB3	2.21	0.40
1:A:45:GLU:O	1:A:47:PHE:N	2.54	0.40
1:B:329:ASP:C	1:B:331:GLY:H	2.24	0.40
1:B:140:TYR:CE1	1:B:262:LYS:HB3	2.55	0.40
1:A:97:GLN:HG2	1:A:97:GLN:H	1.65	0.40
1:B:34:ASN:HD22	1:B:81:VAL:HG13	1.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:329:ASP:C	1:B:331:GLY:N	2.75	0.40
1:C:215:ARG:O	1:C:215:ARG:HD3	2.21	0.40
1:C:181:PRO:HG3	1:C:360:TRP:CG	2.57	0.40
1:A:136:ILE:CD1	1:A:183:GLU:HB3	2.51	0.40
1:B:352:THR:O	1:B:353:GLN:C	2.58	0.40
1:A:129:ILE:HB	1:A:130:PRO:HD2	2.02	0.40
1:B:215:ARG:N	1:B:216:PRO:CD	2.83	0.40
1:B:100:ASP:OD1	1:B:103:LYS:HG3	2.21	0.40
1:A:195:LYS:HG3	1:A:195:LYS:H	1.65	0.40
1:A:87:LEU:HD21	1:A:128:ALA:HB3	2.03	0.40
1:B:47:PHE:O	1:B:48:THR:C	2.59	0.40
1:A:139:GLY:CA	1:A:245:ILE:HD13	2.51	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	338/345 (98%)	287 (85%)	40 (12%)	11 (3%)	5	24
1	B	338/345 (98%)	292 (86%)	40 (12%)	6 (2%)	11	43
1	C	338/345 (98%)	288 (85%)	42 (12%)	8 (2%)	7	34
All	All	1014/1035 (98%)	867 (86%)	122 (12%)	25 (2%)	7	33

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	47	PHE
1	C	172	GLN
1	C	173	CYS
1	A	45	GLU
1	A	251	ARG

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Mol	Chain	Res	Type
1	C	45	GLU
1	C	47	PHE
1	A	46	LYS
1	A	48	THR
1	A	353	GLN
1	B	45	GLU
1	B	47	PHE
1	B	224	SER
1	B	324	GLU
1	B	334	PRO
1	C	46	LYS
1	A	324	GLU
1	A	364	LYS
1	B	255	ALA
1	C	49	LYS
1	C	88	ALA
1	A	334	PRO
1	C	334	PRO
1	A	120	VAL
1	A	299	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	291/294 (99%)	265 (91%)	26 (9%)	12	40
1	B	291/294 (99%)	268 (92%)	23 (8%)	15	46
1	C	291/294 (99%)	264 (91%)	27 (9%)	11	38
All	All	873/882 (99%)	797 (91%)	76 (9%)	13	41

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	ASP
1	A	27	ASN

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Mol	Chain	Res	Type
1	A	28	LYS
1	A	33	TYR
1	A	36	SER
1	A	38	TYR
1	A	43	THR
1	A	44	LEU
1	A	74	LYS
1	A	79	VAL
1	A	98	LYS
1	A	117	THR
1	A	122	ASP
1	A	129	ILE
1	A	155	VAL
1	A	171	LYS
1	A	195	LYS
1	A	215	ARG
1	A	219	THR
1	A	227	ILE
1	A	230	LEU
1	A	251	ARG
1	A	274	PHE
1	A	285	ASN
1	A	287	GLU
1	A	309	VAL
1	B	27	ASN
1	B	28	LYS
1	B	38	TYR
1	B	43	THR
1	B	69	LYS
1	B	74	LYS
1	B	79	VAL
1	B	114	LEU
1	B	117	THR
1	B	129	ILE
1	B	151	ASP
1	B	168	GLN
1	B	195	LYS
1	B	209	GLU
1	B	215	ARG
1	B	230	LEU
1	B	247	GLN
1	B	262	LYS

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Mol	Chain	Res	Type
1	B	284	GLU
1	B	285	ASN
1	B	287	GLU
1	B	309	VAL
1	B	359	SER
1	C	26	ASP
1	C	27	ASN
1	C	36	SER
1	C	38	TYR
1	C	43	THR
1	C	44	LEU
1	C	69	LYS
1	C	74	LYS
1	C	79	VAL
1	C	81	VAL
1	C	98	LYS
1	C	114	LEU
1	C	117	THR
1	C	129	ILE
1	C	146	LYS
1	C	155	VAL
1	C	202	LYS
1	C	215	ARG
1	C	227	ILE
1	C	230	LEU
1	C	264	ASN
1	C	274	PHE
1	C	285	ASN
1	C	287	GLU
1	C	341	LYS
1	C	348	LEU
1	C	351	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	ASN
1	A	34	ASN
1	A	63	ASN
1	A	84	ASN
1	A	106	ASN
1	A	127	HIS

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Mol	Chain	Res	Type
1	A	222	HIS
1	A	232	ASN
1	A	234	ASN
1	A	264	ASN
1	A	285	ASN
1	A	294	ASN
1	B	27	ASN
1	B	34	ASN
1	B	84	ASN
1	B	106	ASN
1	B	127	HIS
1	B	168	GLN
1	B	172	GLN
1	B	222	HIS
1	B	232	ASN
1	B	234	ASN
1	B	285	ASN
1	B	294	ASN
1	C	34	ASN
1	C	84	ASN
1	C	106	ASN
1	C	127	HIS
1	C	222	HIS
1	C	232	ASN
1	C	234	ASN
1	C	247	GLN
1	C	264	ASN
1	C	285	ASN
1	C	294	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 carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	340/345 (98%)	-0.62	1 (0%) 94 86	19, 37, 53, 68	0
1	B	340/345 (98%)	-0.65	0 100 100	19, 33, 47, 57	0
1	C	340/345 (98%)	-0.34	2 (0%) 90 77	29, 48, 62, 71	0
All	All	1020/1035 (98%)	-0.54	3 (0%) 94 86	19, 40, 56, 71	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	26	ASP	2.9
1	C	26	ASP	2.8
1	C	255	ALA	2.2

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.