



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 06:14 PM GMT

PDB ID : 3PG5
Title : Crystal structure of protein DIP2308 from Corynebacterium diphtheriae, Northeast Structural Genomics Consortium Target CdR78
Authors : Forouhar, F.; Lew, S.; Seetharaman, J.; Lee, D.; Ciccosanti, C.; Sahdev, S.; Nair, R.; Rost, B.; Acton, T.B.; Xiao, R.; Everett, J.K.; Montelione, G.T.; Hunt, J.F.; Tong, L.; Northeast Structural Genomics Consortium (NESG)
Deposited on : 2010-10-30
Resolution : 3.30 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

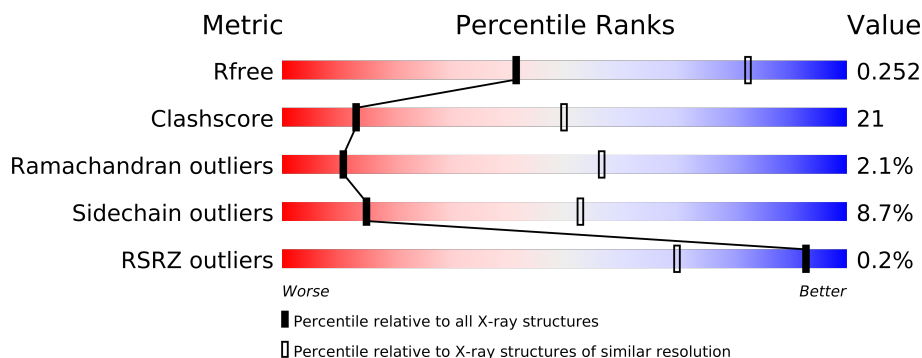
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.30 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}	66092	1341 (3.40-3.20)
Clashscore	79885	1696 (3.40-3.20)
Ramachandran outliers	78287	1664 (3.40-3.20)
Sidechain outliers	78261	1662 (3.40-3.20)
RSRZ outliers	66119	1342 (3.40-3.20)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	361	
1	B	361	
1	C	361	
1	D	361	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9613 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Uncharacterized protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	298	Total	C	N	O	S	Se	0	0	0
			2358	1495	412	442	3	6			
1	B	301	Total	C	N	O	S	Se	0	0	0
			2377	1506	416	446	3	6			
1	C	312	Total	C	N	O	S	Se	0	0	0
			2468	1566	430	463	3	6			
1	D	302	Total	C	N	O	S	Se	0	0	0
			2389	1516	418	446	3	6			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	354	LEU	-	EXPRESSION TAG	UNP Q6NEG6
A	355	GLU	-	EXPRESSION TAG	UNP Q6NEG6
A	356	HIS	-	EXPRESSION TAG	UNP Q6NEG6
A	357	HIS	-	EXPRESSION TAG	UNP Q6NEG6
A	358	HIS	-	EXPRESSION TAG	UNP Q6NEG6
A	359	HIS	-	EXPRESSION TAG	UNP Q6NEG6
A	360	HIS	-	EXPRESSION TAG	UNP Q6NEG6
A	361	HIS	-	EXPRESSION TAG	UNP Q6NEG6
B	354	LEU	-	EXPRESSION TAG	UNP Q6NEG6
B	355	GLU	-	EXPRESSION TAG	UNP Q6NEG6
B	356	HIS	-	EXPRESSION TAG	UNP Q6NEG6
B	357	HIS	-	EXPRESSION TAG	UNP Q6NEG6
B	358	HIS	-	EXPRESSION TAG	UNP Q6NEG6
B	359	HIS	-	EXPRESSION TAG	UNP Q6NEG6
B	360	HIS	-	EXPRESSION TAG	UNP Q6NEG6
B	361	HIS	-	EXPRESSION TAG	UNP Q6NEG6
C	354	LEU	-	EXPRESSION TAG	UNP Q6NEG6
C	355	GLU	-	EXPRESSION TAG	UNP Q6NEG6
C	356	HIS	-	EXPRESSION TAG	UNP Q6NEG6
C	357	HIS	-	EXPRESSION TAG	UNP Q6NEG6
C	358	HIS	-	EXPRESSION TAG	UNP Q6NEG6

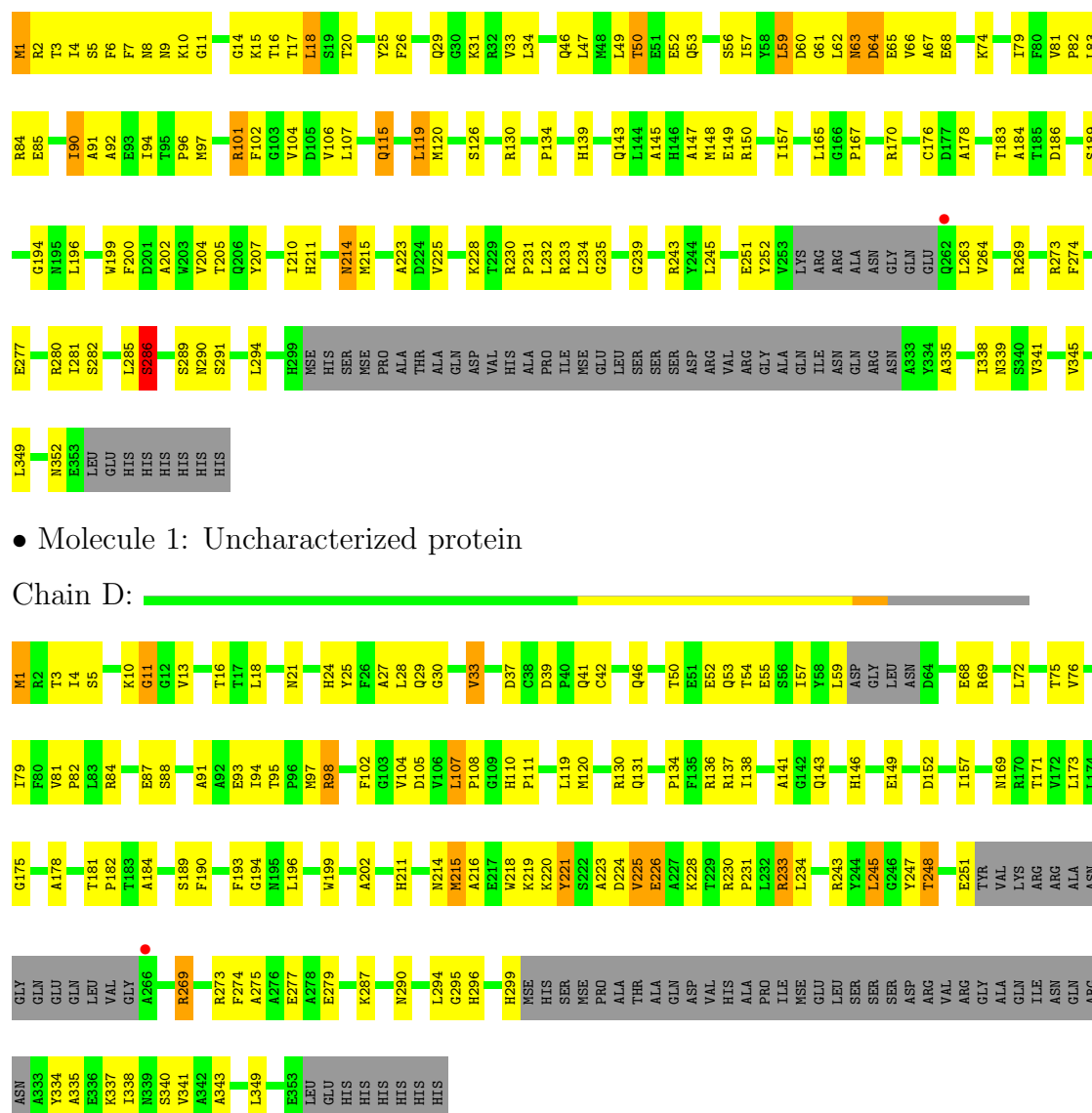
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Chain	Residue	Modelled	Actual	Comment	Reference
C	359	HIS	-	EXPRESSION TAG	UNP Q6NEG6
C	360	HIS	-	EXPRESSION TAG	UNP Q6NEG6
C	361	HIS	-	EXPRESSION TAG	UNP Q6NEG6
D	354	LEU	-	EXPRESSION TAG	UNP Q6NEG6
D	355	GLU	-	EXPRESSION TAG	UNP Q6NEG6
D	356	HIS	-	EXPRESSION TAG	UNP Q6NEG6
D	357	HIS	-	EXPRESSION TAG	UNP Q6NEG6
D	358	HIS	-	EXPRESSION TAG	UNP Q6NEG6
D	359	HIS	-	EXPRESSION TAG	UNP Q6NEG6
D	360	HIS	-	EXPRESSION TAG	UNP Q6NEG6
D	361	HIS	-	EXPRESSION TAG	UNP Q6NEG6

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	7	Total O 7 7	0	0
2	B	7	Total O 7 7	0	0
2	C	2	Total O 2 2	0	0
2	D	5	Total O 5 5	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α , β , γ	199.96Å 199.96Å 106.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.30 29.97 – 3.30	Depositor EDS
% Data completeness (in resolution range)	88.5 (20.00-3.30) 96.8 (29.97-3.30)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	0.19	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.71 (at 3.31Å)	Xtriage
Refinement program	CNS 1.2 & XtalView	Depositor
R, R_{free}	0.187 , 0.235 0.205 , 0.252	Depositor DCC
R_{free} test set	3152 reflections (9.89%)	DCC
Wilson B-factor (Å ²)	60.6	Xtriage
Anisotropy	0.231	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 13.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 62001 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	9613	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.77% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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	0.49	0/2408	0.59	1/3252 (0.0%)
1	B	0.46	0/2428	0.61	1/3281 (0.0%)
1	C	0.47	0/2522	0.60	1/3409 (0.0%)
1	D	0.46	0/2441	0.56	1/3297 (0.0%)
All	All	0.47	0/9799	0.59	4/13239 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	C	290	ASN	CB-CA-C	5.33	121.06	110.40
1	B	290	ASN	CB-CA-C	5.32	121.04	110.40
1	D	290	ASN	CB-CA-C	5.32	121.03	110.40
1	A	290	ASN	CB-CA-C	5.32	121.03	110.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	154	TYR	Sidechain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2358	0	2277	87	0
1	B	2377	0	2296	116	0
1	C	2468	0	2378	101	0
1	D	2389	0	2300	96	0
2	A	7	0	0	0	0
2	B	7	0	0	1	0
2	C	2	0	0	0	0
2	D	5	0	0	0	0
All	All	9613	0	9251	389	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 21.

All (389) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:1:MSE:HG3	1:D:149:GLU:HB2	1.43	1.00
1:B:33:VAL:HG13	1:B:104:VAL:HG23	1.52	0.92
1:A:219:LYS:HG3	1:A:225:VAL:HG11	1.51	0.91
1:B:178:ALA:HB1	1:B:245:LEU:HD13	1.57	0.85
1:B:8:ASN:HB3	1:B:15:LYS:HD3	1.55	0.85
1:B:201:ASP:O	1:B:205:THR:HG22	1.77	0.84
1:B:294:LEU:H	1:B:294:LEU:HD22	1.43	0.83
1:B:72:LEU:HD22	1:B:77:TYR:CD2	2.16	0.81
1:C:186:ASP:OD1	1:C:189:SER:HB2	1.83	0.79
1:D:84:ARG:HG2	1:D:119:LEU:HD13	1.65	0.79
1:C:119:LEU:HD12	1:C:120:MSE:HE2	1.65	0.78
1:C:3:THR:HG22	1:C:157:ILE:HB	1.64	0.78
1:B:293:LEU:HD23	1:B:295:GLY:H	1.50	0.77
1:A:198:ARG:HH11	1:A:198:ARG:HG2	1.50	0.76
1:A:224:ASP:HB3	1:A:228:LYS:HE3	1.67	0.76
1:C:79:ILE:HA	1:C:91:ALA:HB3	1.68	0.75
1:D:219:LYS:HG2	1:D:225:VAL:HG21	1.67	0.75
1:D:181:THR:HG21	1:D:193:PHE:HE2	1.51	0.75
1:C:90:ILE:HD12	1:C:143:GLN:HB3	1.70	0.74

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:186:ASP:OD1	1:A:189:SER:HB2	1.88	0.74
1:A:293:LEU:HD23	1:A:295:GLY:H	1.53	0.74
1:B:235:GLY:HA3	1:B:239:GLY:HA2	1.67	0.73
1:C:183:THR:HG22	1:C:184:ALA:H	1.55	0.72
1:D:294:LEU:HD22	1:D:294:LEU:H	1.54	0.72
1:B:4:ILE:HD12	1:B:178:ALA:O	1.91	0.70
1:B:130:ARG:HG3	1:B:130:ARG:HH11	1.55	0.70
1:A:178:ALA:HB1	1:A:245:LEU:HD13	1.73	0.69
1:C:49:LEU:HD21	1:C:106:VAL:CG1	2.23	0.69
1:B:33:VAL:HG13	1:B:104:VAL:CG2	2.20	0.69
1:A:10:LYS:HA	1:A:10:LYS:HE2	1.75	0.69
1:C:8:ASN:HB3	1:C:15:LYS:HD3	1.73	0.69
1:B:184:ALA:HB3	1:B:189:SER:OG	1.93	0.69
1:D:79:ILE:HA	1:D:91:ALA:HB3	1.75	0.69
1:C:184:ALA:HB3	1:C:189:SER:OG	1.93	0.68
1:C:210:ILE:O	1:C:214:ASN:HB2	1.94	0.68
1:A:8:ASN:HB3	1:A:15:LYS:HD3	1.76	0.68
1:B:233:ARG:HH11	1:B:233:ARG:HB3	1.58	0.67
1:B:229:THR:HG23	1:B:234:LEU:HD22	1.76	0.67
1:A:75:THR:HA	1:A:108:PRO:HG2	1.76	0.67
1:C:230:ARG:N	1:C:231:PRO:HD2	2.10	0.67
1:B:26:PHE:O	1:B:31:LYS:HB2	1.96	0.66
1:C:25:TYR:O	1:C:29:GLN:HG2	1.96	0.66
1:B:268:GLU:HG3	1:B:270:PHE:H	1.62	0.65
1:D:215:MSE:HA	1:D:215:MSE:HE3	1.79	0.65
1:C:94:ILE:HD12	1:C:96:PRO:HD3	1.78	0.65
1:A:53:GLN:O	1:A:56:SER:HB3	1.97	0.65
1:C:90:ILE:HD13	1:C:90:ILE:H	1.62	0.65
1:B:35:TYR:CD1	1:B:48:MSE:HE1	2.32	0.64
1:A:215:MSE:HE3	1:A:215:MSE:HA	1.79	0.64
1:D:75:THR:HA	1:D:108:PRO:HG2	1.78	0.64
1:D:33:VAL:O	1:D:104:VAL:HG23	1.99	0.63
1:A:230:ARG:N	1:A:231:PRO:HD2	2.13	0.63
1:A:1:MSE:HG3	1:A:149:GLU:HB2	1.79	0.63
1:C:63:ASN:HD21	1:C:66:VAL:HG23	1.64	0.63
1:C:183:THR:HG22	1:C:184:ALA:N	2.14	0.62
1:B:161:VAL:HB	1:B:169:ASN:ND2	2.14	0.62
1:D:219:LYS:NZ	1:D:219:LYS:HB3	2.14	0.62
1:C:84:ARG:NH2	1:C:115:GLN:HG2	2.14	0.62
1:B:33:VAL:O	1:B:104:VAL:HG23	2.00	0.62
1:A:294:LEU:H	1:A:294:LEU:HD22	1.65	0.62
1:D:4:ILE:HG12	1:D:5:SER:N	2.13	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:247:TYR:OH	1:B:275:ALA:HB2	2.01	0.60
1:C:26:PHE:O	1:C:31:LYS:HB2	2.01	0.60
1:B:94:ILE:HD11	1:B:107:LEU:HG	1.84	0.60
1:C:215:MSE:HE3	1:C:215:MSE:HA	1.83	0.60
1:C:63:ASN:ND2	1:C:66:VAL:HG23	2.16	0.60
1:C:8:ASN:HB3	1:C:15:LYS:CD	2.31	0.60
1:B:44:ALA:HB1	1:B:48:MSE:HE2	1.84	0.60
1:D:234:LEU:HD22	1:D:234:LEU:H	1.67	0.60
1:A:232:LEU:O	1:A:234:LEU:N	2.34	0.60
1:B:244:TYR:HB3	1:B:289:SER:HB3	1.84	0.59
1:D:181:THR:HG21	1:D:193:PHE:CE2	2.34	0.59
1:C:294:LEU:HD22	1:C:294:LEU:H	1.67	0.59
1:A:83:LEU:HD22	1:A:137:ARG:HG2	1.83	0.59
1:C:101:ARG:HD3	1:C:102:PHE:CE2	2.38	0.59
1:A:119:LEU:HG	1:A:120:MSE:HE2	1.85	0.59
1:A:185:THR:HA	1:A:274:PHE:CE2	2.38	0.58
1:A:184:ALA:HB3	1:A:189:SER:OG	2.03	0.58
1:B:187:LEU:HD13	1:D:54:THR:HG22	1.84	0.58
1:C:49:LEU:HD21	1:C:106:VAL:HG11	1.84	0.58
1:D:25:TYR:O	1:D:29:GLN:HG2	2.04	0.58
1:C:34:LEU:HD23	1:C:157:ILE:HD12	1.86	0.58
1:A:130:ARG:HG3	1:A:130:ARG:HH11	1.68	0.58
1:C:79:ILE:O	1:C:90:ILE:HB	2.05	0.57
1:D:28:LEU:HD12	1:D:29:GLN:N	2.20	0.57
1:C:286:SER:O	1:C:289:SER:HB2	2.04	0.57
1:C:335:ALA:HA	1:C:338:ILE:HG22	1.87	0.57
1:C:57:ILE:HD13	1:C:74:LYS:HE3	1.86	0.57
1:A:128:LEU:HD23	1:A:210:ILE:HD11	1.86	0.57
1:D:234:LEU:HD22	1:D:234:LEU:N	2.19	0.57
1:D:211:HIS:O	1:D:215:MSE:HB2	2.04	0.56
1:C:285:LEU:N	1:C:285:LEU:HD22	2.20	0.56
1:A:198:ARG:NH1	1:A:198:ARG:HG2	2.20	0.56
1:B:233:ARG:HH11	1:B:233:ARG:CB	2.18	0.56
1:D:28:LEU:C	1:D:30:GLY:H	2.09	0.56
1:C:56:SER:HA	1:C:60:ASP:HB2	1.86	0.56
1:A:337:LYS:HE3	1:A:337:LYS:HA	1.87	0.56
1:C:130:ARG:HG3	1:C:130:ARG:HH11	1.69	0.56
1:B:97:MSE:O	1:B:106:VAL:HG12	2.05	0.56
1:D:33:VAL:HG22	1:D:104:VAL:HG21	1.86	0.56
1:A:226:GLU:OE1	1:A:226:GLU:HA	2.06	0.55
1:B:45:THR:HG21	1:B:58:TYR:OH	2.05	0.55
1:B:182:PRO:HB3	1:B:248:THR:HG23	1.88	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:50:THR:OG1	1:D:53:GLN:HG3	2.05	0.55
1:A:3:THR:OG1	1:A:176:CYS:HA	2.06	0.55
1:B:126:SER:HB3	1:B:134:PRO:HG3	1.89	0.55
1:B:72:LEU:HD22	1:B:77:TYR:CE2	2.42	0.55
1:B:76:VAL:HG23	1:B:79:ILE:HD12	1.87	0.55
1:C:1:MSE:HE3	1:C:145:ALA:O	2.07	0.54
1:C:232:LEU:O	1:C:234:LEU:N	2.39	0.54
1:B:335:ALA:HB1	1:B:339:ASN:HD22	1.72	0.54
1:A:18:LEU:O	1:A:22:VAL:HG23	2.07	0.54
1:C:57:ILE:HD11	1:C:97:MSE:HE1	1.90	0.54
1:C:81:VAL:HA	1:D:221:TYR:OH	2.07	0.54
1:D:53:GLN:O	1:D:57:ILE:HG12	2.07	0.54
1:D:184:ALA:HB3	1:D:189:SER:CB	2.38	0.54
1:B:201:ASP:HA	1:B:284:SER:HB2	1.91	0.53
1:A:128:LEU:CD2	1:A:210:ILE:HD11	2.38	0.53
1:C:63:ASN:ND2	1:C:66:VAL:H	2.05	0.53
1:C:9:ASN:HB3	1:C:165:LEU:HD21	1.90	0.53
1:B:334:TYR:OH	1:B:338:ILE:HD12	2.08	0.53
1:C:194:GLY:HA2	1:C:277:GLU:HG2	1.89	0.53
1:D:97:MSE:HG3	1:D:98:ARG:H	1.74	0.53
1:B:41:GLN:O	1:B:42:CYS:HB2	2.08	0.53
1:D:94:ILE:HD11	1:D:107:LEU:HD11	1.89	0.53
1:D:84:ARG:HG2	1:D:119:LEU:CD1	2.37	0.53
1:A:135:PHE:O	1:A:138:ILE:HG12	2.07	0.53
1:A:125:GLN:O	1:A:128:LEU:HB2	2.09	0.53
1:B:182:PRO:HA	1:B:248:THR:O	2.09	0.53
1:C:90:ILE:CD1	1:C:143:GLN:HB3	2.39	0.53
1:D:76:VAL:O	1:D:79:ILE:HG12	2.09	0.52
1:B:135:PHE:O	1:B:138:ILE:HG12	2.09	0.52
1:B:184:ALA:O	1:B:185:THR:HB	2.09	0.52
1:B:150:ARG:HG3	1:B:151:ASP:OD2	2.09	0.52
1:A:10:LYS:HD2	1:A:189:SER:HA	1.91	0.52
1:D:224:ASP:HB2	1:D:228:LYS:HD2	1.91	0.52
1:C:235:GLY:HA3	1:C:239:GLY:HA2	1.92	0.52
1:A:161:VAL:HB	1:A:169:ASN:ND2	2.24	0.52
1:D:10:LYS:O	1:D:11:GLY:O	2.28	0.52
1:D:13:VAL:HA	1:D:16:THR:HG22	1.91	0.52
1:C:14:GLY:HA2	1:C:17:THR:HG22	1.90	0.51
1:C:14:GLY:O	1:C:17:THR:HG22	2.09	0.51
1:B:230:ARG:N	1:B:231:PRO:HD2	2.25	0.51
1:A:206:GLN:O	1:A:210:ILE:HG12	2.10	0.51
1:B:245:LEU:O	1:B:294:LEU:HD21	2.09	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:287:LYS:HG3	1:A:288:HIS:ND1	2.26	0.51
1:B:294:LEU:H	1:B:294:LEU:CD2	2.17	0.51
1:A:187:LEU:HD21	1:C:59:LEU:HD23	1.93	0.51
1:D:224:ASP:O	1:D:228:LYS:HB2	2.11	0.51
1:A:44:ALA:O	1:A:48:MSE:HG3	2.11	0.51
1:D:81:VAL:N	1:D:82:PRO:HD2	2.26	0.51
1:C:202:ALA:O	1:C:205:THR:HG22	2.11	0.51
1:B:70:ASN:O	1:B:74:LYS:HG3	2.11	0.51
1:B:335:ALA:C	1:B:337:LYS:H	2.13	0.51
1:C:178:ALA:HB1	1:C:245:LEU:HD13	1.92	0.51
1:C:81:VAL:N	1:C:82:PRO:HD2	2.26	0.51
1:B:143:GLN:HE21	1:B:232:LEU:CD2	2.24	0.50
1:B:50:THR:HG23	1:B:53:GLN:OE1	2.10	0.50
1:C:282:SER:HB2	1:C:291:SER:HB3	1.93	0.50
1:D:131:GLN:O	1:D:134:PRO:HD2	2.11	0.50
1:B:206:GLN:O	1:B:209:GLU:HB2	2.11	0.50
1:C:8:ASN:ND2	1:C:10:LYS:H	2.09	0.50
1:C:90:ILE:CD1	1:C:90:ILE:H	2.25	0.50
1:B:130:ARG:HG3	1:B:130:ARG:NH1	2.26	0.50
1:D:33:VAL:HG22	1:D:104:VAL:CG2	2.41	0.50
1:A:18:LEU:HD11	1:A:248:THR:HG21	1.93	0.50
1:C:251:GLU:CG	1:C:263:LEU:HD22	2.42	0.50
1:D:223:ALA:C	1:D:225:VAL:H	2.14	0.50
1:A:110:HIS:CE1	1:A:112:ALA:HB2	2.47	0.49
1:B:42:CYS:O	1:B:46:GLN:HG2	2.11	0.49
1:B:16:THR:HG21	1:B:43:ASN:HB2	1.94	0.49
1:C:50:THR:OG1	1:C:53:GLN:HG3	2.13	0.49
1:A:185:THR:O	1:A:185:THR:HG22	2.11	0.49
1:B:185:THR:HA	1:B:274:PHE:CE2	2.48	0.49
1:A:250:LEU:CD2	1:A:297:VAL:HB	2.42	0.49
1:A:188:PHE:CE1	1:C:46:GLN:HB3	2.47	0.49
1:A:245:LEU:HD21	1:A:349:LEU:HD23	1.95	0.49
1:C:167:PRO:HG3	1:C:170:ARG:NH2	2.27	0.49
1:A:165:LEU:N	1:A:165:LEU:HD23	2.27	0.49
1:B:294:LEU:N	1:B:294:LEU:HD22	2.22	0.49
1:B:293:LEU:HD23	1:B:295:GLY:N	2.24	0.49
1:A:185:THR:HA	1:A:274:PHE:HE2	1.77	0.49
1:C:101:ARG:HH11	1:C:101:ARG:HG2	1.77	0.49
1:D:296:HIS:H	1:D:337:LYS:HE3	1.76	0.49
1:D:178:ALA:HA	1:D:243:ARG:O	2.12	0.49
1:A:70:ASN:OD1	1:A:74:LYS:HE3	2.12	0.49
1:D:224:ASP:CB	1:D:228:LYS:HD2	2.43	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:18:LEU:O	1:B:22:VAL:HG23	2.12	0.49
1:B:232:LEU:O	1:B:234:LEU:N	2.42	0.48
1:B:161:VAL:HB	1:B:169:ASN:HD21	1.77	0.48
1:A:54:THR:HG22	1:A:55:GLU:N	2.28	0.48
1:D:295:GLY:HA3	1:D:341:VAL:HG22	1.94	0.48
1:C:126:SER:HB3	1:C:134:PRO:HG3	1.95	0.48
1:C:90:ILE:HD12	1:C:143:GLN:CB	2.41	0.48
1:D:143:GLN:HA	1:D:231:PRO:O	2.13	0.48
1:C:178:ALA:HA	1:C:243:ARG:O	2.13	0.48
1:C:119:LEU:HD22	1:D:131:GLN:HE22	1.78	0.48
1:C:184:ALA:HB3	1:C:189:SER:CB	2.43	0.48
1:A:184:ALA:O	1:A:185:THR:HB	2.13	0.48
1:D:88:SER:HB3	1:D:136:ARG:HE	1.77	0.48
1:A:132:THR:CG2	1:B:84:ARG:O	2.62	0.48
1:D:230:ARG:N	1:D:231:PRO:HD2	2.29	0.48
1:D:120:MSE:HG3	1:D:171:THR:HG21	1.96	0.48
1:C:263:LEU:HD12	1:C:263:LEU:O	2.14	0.47
1:A:54:THR:C	1:A:56:SER:H	2.18	0.47
1:D:146:HIS:HB2	1:D:233:ARG:HG3	1.96	0.47
1:B:2:ARG:O	1:B:156:VAL:HA	2.14	0.47
1:B:334:TYR:CZ	1:B:338:ILE:HB	2.50	0.47
1:B:120:MSE:HG3	1:B:171:THR:HG21	1.97	0.47
1:B:141:ALA:HB3	1:B:175:GLY:HA3	1.97	0.47
1:A:178:ALA:HA	1:A:243:ARG:O	2.14	0.47
1:B:293:LEU:C	1:B:293:LEU:HD23	2.36	0.47
1:C:6:PHE:CE2	1:C:18:LEU:HD13	2.50	0.47
1:A:104:VAL:HG23	1:A:104:VAL:O	2.14	0.47
1:A:184:ALA:HB3	1:A:189:SER:CB	2.45	0.46
1:D:224:ASP:C	1:D:226:GLU:H	2.18	0.46
1:A:132:THR:HG23	1:B:84:ARG:O	2.15	0.46
1:B:25:TYR:HA	1:B:28:LEU:HD12	1.97	0.46
1:D:182:PRO:HA	1:D:248:THR:HG23	1.97	0.46
1:A:190:PHE:HB2	1:A:274:PHE:CZ	2.51	0.46
1:B:178:ALA:HB1	1:B:245:LEU:CD1	2.37	0.46
1:B:4:ILE:HD12	1:B:178:ALA:C	2.35	0.46
1:B:143:GLN:HE21	1:B:232:LEU:HD21	1.81	0.46
1:C:335:ALA:O	1:C:339:ASN:HB2	2.16	0.46
1:B:110:HIS:ND1	1:B:111:PRO:HD2	2.30	0.46
1:B:83:LEU:HG	1:B:137:ARG:HD3	1.97	0.46
1:A:57:ILE:HG23	1:A:74:LYS:HB2	1.97	0.46
1:C:252:TYR:HD2	1:C:264:VAL:HB	1.81	0.46
1:D:340:SER:O	1:D:343:ALA:HB3	2.15	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:4:ILE:CG1	1:D:5:SER:N	2.77	0.46
1:A:180:VAL:HG12	1:A:181:THR:N	2.31	0.46
1:A:130:ARG:HG3	1:A:130:ARG:NH1	2.31	0.46
1:C:126:SER:CB	1:C:134:PRO:HG3	2.46	0.46
1:B:16:THR:HG22	1:B:16:THR:O	2.16	0.46
1:C:16:THR:O	1:C:20:THR:HG23	2.16	0.46
1:D:94:ILE:CD1	1:D:107:LEU:HD11	2.45	0.45
1:C:130:ARG:NH1	1:C:130:ARG:HG3	2.30	0.45
1:B:335:ALA:HB1	1:B:339:ASN:ND2	2.31	0.45
1:B:188:PHE:CE1	1:D:46:GLN:HB3	2.50	0.45
1:B:10:LYS:HB2	2:B:362:HOH:O	2.17	0.45
1:A:32:ARG:HG3	1:A:155:ASP:OD1	2.17	0.45
1:B:128:LEU:C	1:B:130:ARG:H	2.20	0.45
1:B:165:LEU:N	1:B:165:LEU:HD23	2.32	0.45
1:D:194:GLY:HA2	1:D:277:GLU:HG2	1.98	0.45
1:C:230:ARG:N	1:C:231:PRO:CD	2.79	0.45
1:B:178:ALA:HA	1:B:243:ARG:O	2.17	0.45
1:D:181:THR:HG22	1:D:181:THR:O	2.15	0.45
1:B:268:GLU:HG3	1:B:269:ARG:N	2.32	0.45
1:B:73:ALA:HA	1:B:78:ALA:HB2	1.97	0.45
1:B:78:ALA:HA	1:B:81:VAL:HG23	1.99	0.45
1:D:24:HIS:HB2	1:D:102:PHE:HD1	1.82	0.45
1:B:7:PHE:CD2	1:B:173:LEU:HD11	2.52	0.45
1:B:7:PHE:HE2	1:B:169:ASN:HB3	1.81	0.44
1:D:24:HIS:O	1:D:27:ALA:HB3	2.18	0.44
1:A:200:PHE:O	1:A:201:ASP:C	2.55	0.44
1:D:110:HIS:ND1	1:D:111:PRO:HD2	2.32	0.44
1:C:225:VAL:HA	1:C:228:LYS:HB3	1.98	0.44
1:C:5:SER:HB2	1:C:176:CYS:SG	2.58	0.44
1:D:88:SER:CB	1:D:136:ARG:HE	2.30	0.44
1:D:21:ASN:O	1:D:24:HIS:HB3	2.16	0.44
1:A:35:TYR:CE1	1:A:160:ASP:HB2	2.52	0.44
1:D:76:VAL:HA	1:D:107:LEU:HD22	1.99	0.44
1:B:49:LEU:HD21	1:B:106:VAL:CG1	2.47	0.44
1:A:7:PHE:HE2	1:A:169:ASN:HB3	1.83	0.44
1:C:223:ALA:HB2	1:D:69:ARG:NH1	2.33	0.44
1:D:216:ALA:O	1:D:220:LYS:HG2	2.18	0.44
1:D:294:LEU:H	1:D:294:LEU:CD2	2.26	0.44
1:D:226:GLU:O	1:D:230:ARG:HG2	2.17	0.44
1:C:4:ILE:HB	1:C:349:LEU:HD11	2.00	0.44
1:A:72:LEU:HD12	1:A:110:HIS:NE2	2.33	0.44
1:B:165:LEU:H	1:B:165:LEU:HD23	1.81	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:335:ALA:HA	1:D:338:ILE:HG22	1.98	0.44
1:A:336:GLU:HG2	1:A:337:LYS:N	2.33	0.44
1:B:100:GLU:C	1:B:102:PHE:H	2.21	0.44
1:C:352:ASN:N	1:C:352:ASN:HD22	2.13	0.44
1:C:83:LEU:C	1:C:85:GLU:H	2.21	0.44
1:A:250:LEU:HD22	1:A:297:VAL:HB	2.00	0.44
1:D:68:GLU:O	1:D:72:LEU:HD13	2.18	0.44
1:C:7:PHE:CD1	1:C:8:ASN:N	2.86	0.43
1:B:184:ALA:O	1:B:185:THR:CB	2.66	0.43
1:A:128:LEU:HD23	1:A:210:ILE:CD1	2.48	0.43
1:B:141:ALA:CB	1:B:175:GLY:HA3	2.48	0.43
1:C:150:ARG:O	1:C:150:ARG:HG2	2.17	0.43
1:B:194:GLY:HA2	1:B:277:GLU:HG2	2.00	0.43
1:B:200:PHE:O	1:B:204:VAL:HG23	2.18	0.43
1:A:293:LEU:HD23	1:A:295:GLY:N	2.27	0.43
1:D:234:LEU:CD2	1:D:234:LEU:H	2.32	0.43
1:C:1:MSE:HG3	1:C:149:GLU:HB2	2.00	0.43
1:C:269:ARG:O	1:C:273:ARG:NH1	2.52	0.43
1:C:33:VAL:HB	1:C:104:VAL:HG12	2.00	0.43
1:D:226:GLU:HA	1:D:226:GLU:OE1	2.18	0.43
1:D:215:MSE:HE1	1:D:218:TRP:HE3	1.83	0.43
1:A:235:GLY:HA3	1:A:239:GLY:HA2	2.01	0.43
1:A:34:LEU:HB2	1:A:154:TYR:CD2	2.53	0.43
1:D:190:PHE:CZ	1:D:273:ARG:HB3	2.54	0.43
1:D:294:LEU:HD22	1:D:294:LEU:N	2.28	0.43
1:D:33:VAL:HG13	1:D:104:VAL:CG2	2.49	0.43
1:B:58:TYR:O	1:B:59:LEU:HD23	2.18	0.43
1:D:98:ARG:HD2	1:D:98:ARG:HA	1.80	0.43
1:C:4:ILE:HG12	1:C:5:SER:N	2.34	0.43
1:C:341:VAL:O	1:C:345:VAL:HG23	2.19	0.43
1:A:81:VAL:N	1:A:82:PRO:HD2	2.34	0.43
1:C:139:HIS:HE1	1:C:207:TYR:OH	2.00	0.43
1:A:165:LEU:H	1:A:165:LEU:HD23	1.84	0.43
1:D:199:TRP:O	1:D:202:ALA:HB3	2.18	0.43
1:B:232:LEU:HB2	1:B:234:LEU:HD13	2.00	0.42
1:B:250:LEU:HD23	1:B:297:VAL:HG13	2.00	0.42
1:A:113:LEU:O	1:A:117:GLU:HG3	2.18	0.42
1:C:183:THR:HG21	1:C:274:PHE:CE1	2.54	0.42
1:B:177:ASP:OD2	1:B:233:ARG:NH2	2.51	0.42
1:A:294:LEU:N	1:A:294:LEU:HD22	2.31	0.42
1:C:294:LEU:HD22	1:C:294:LEU:N	2.32	0.42
1:B:187:LEU:HD11	1:D:55:GLU:HA	2.02	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:281:ILE:O	1:B:283:ASN:N	2.52	0.42
1:B:268:GLU:HB3	1:B:271:ARG:HB2	2.01	0.42
1:A:334:TYR:C	1:A:336:GLU:H	2.21	0.42
1:A:233:ARG:HH11	1:A:233:ARG:CB	2.32	0.42
1:D:87:GLU:O	1:D:137:ARG:HD3	2.19	0.42
1:D:214:ASN:O	1:D:218:TRP:HB2	2.19	0.42
1:C:294:LEU:CD2	1:C:294:LEU:H	2.29	0.42
1:B:49:LEU:HD21	1:B:106:VAL:HG11	2.02	0.42
1:D:184:ALA:HB3	1:D:189:SER:OG	2.20	0.42
1:C:199:TRP:O	1:C:202:ALA:HB3	2.19	0.42
1:B:1:MSE:HB2	1:B:155:ASP:O	2.20	0.42
1:A:184:ALA:O	1:A:185:THR:CB	2.67	0.42
1:B:229:THR:CG2	1:B:234:LEU:HD22	2.47	0.42
1:B:79:ILE:CG2	1:B:90:ILE:HB	2.50	0.42
1:D:130:ARG:HH11	1:D:130:ARG:HG3	1.84	0.42
1:A:191:HIS:HE1	1:C:68:GLU:OE2	2.03	0.42
1:D:215:MSE:HA	1:D:215:MSE:CE	2.48	0.42
1:C:200:PHE:O	1:C:204:VAL:HB	2.19	0.42
1:A:4:ILE:HG13	1:A:5:SER:N	2.35	0.42
1:A:39:ASP:OD2	1:A:40:PRO:N	2.53	0.42
1:D:39:ASP:OD2	1:D:41:GLN:HG2	2.20	0.42
1:D:141:ALA:HB1	1:D:175:GLY:HA3	2.02	0.42
1:B:57:ILE:HD11	1:B:97:MSE:SE	2.70	0.42
1:C:52:GLU:HG3	1:C:53:GLN:N	2.35	0.42
1:B:5:SER:O	1:B:179:PHE:HB2	2.20	0.42
1:D:219:LYS:HZ3	1:D:219:LYS:HB3	1.83	0.41
1:D:33:VAL:HG13	1:D:104:VAL:HG23	2.01	0.41
1:D:184:ALA:HB3	1:D:189:SER:HB2	2.01	0.41
1:C:4:ILE:HA	1:C:178:ALA:O	2.20	0.41
1:A:34:LEU:HB2	1:A:154:TYR:CG	2.55	0.41
1:B:61:GLY:HA3	1:B:66:VAL:HG13	2.01	0.41
1:B:82:PRO:O	1:B:87:GLU:HB2	2.19	0.41
1:D:3:THR:HG22	1:D:157:ILE:HB	2.01	0.41
1:B:173:LEU:O	1:B:176:CYS:HB2	2.20	0.41
1:B:10:LYS:HA	1:B:10:LYS:HD2	1.73	0.41
1:A:194:GLY:HA2	1:A:277:GLU:HG2	2.03	0.41
1:C:285:LEU:N	1:C:285:LEU:CD2	2.84	0.41
1:C:352:ASN:N	1:C:352:ASN:ND2	2.68	0.41
1:C:139:HIS:CE1	1:C:207:TYR:OH	2.73	0.41
1:D:334:TYR:CD1	1:D:334:TYR:C	2.94	0.41
1:B:165:LEU:HD12	1:B:199:TRP:CG	2.55	0.41
1:A:285:LEU:HB3	1:A:286:SER:H	1.50	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:207:TYR:O	1:A:208:ALA:C	2.59	0.41
1:D:245:LEU:HD12	1:D:245:LEU:HA	1.83	0.41
1:C:101:ARG:HG2	1:C:101:ARG:NH1	2.35	0.41
1:D:28:LEU:C	1:D:30:GLY:N	2.71	0.41
1:A:140:TRP:CZ2	1:A:172:VAL:HG22	2.56	0.41
1:D:215:MSE:HE2	1:D:225:VAL:CG2	2.51	0.41
1:C:20:THR:HG21	1:C:47:LEU:HD23	2.02	0.41
1:D:37:ASP:OD1	1:D:42:CYS:HA	2.21	0.41
1:D:225:VAL:O	1:D:225:VAL:HG13	2.21	0.41
1:B:128:LEU:HD21	1:B:206:GLN:OE1	2.21	0.41
1:B:94:ILE:HG13	1:B:107:LEU:HD11	2.03	0.41
1:A:5:SER:HB2	1:A:176:CYS:SG	2.60	0.41
1:B:70:ASN:HD22	1:B:70:ASN:HA	1.52	0.41
1:C:196:LEU:O	1:C:200:PHE:HD1	2.04	0.41
1:C:147:ALA:C	1:C:148:MSE:HE2	2.41	0.41
1:A:2:ARG:NH2	1:A:237:PHE:CD2	2.89	0.41
1:B:225:VAL:HG13	1:B:226:GLU:OE1	2.20	0.41
1:C:211:HIS:O	1:C:215:MSE:HB2	2.20	0.41
1:A:24:HIS:O	1:A:27:ALA:HB3	2.21	0.41
1:D:134:PRO:O	1:D:138:ILE:HG23	2.21	0.40
1:B:268:GLU:CG	1:B:269:ARG:N	2.83	0.40
1:B:344:ASN:HD22	1:B:344:ASN:N	2.19	0.40
1:C:61:GLY:HA3	1:C:67:ALA:HA	2.03	0.40
1:B:202:ALA:O	1:B:205:THR:CG2	2.69	0.40
1:B:131:GLN:O	1:B:134:PRO:HD2	2.21	0.40
1:A:183:THR:HG23	1:A:184:ALA:N	2.35	0.40
1:C:281:ILE:O	1:C:285:LEU:HD23	2.21	0.40
1:D:182:PRO:HA	1:D:248:THR:O	2.22	0.40
1:C:280:ARG:HG2	1:C:280:ARG:HH11	1.85	0.40
1:D:247:TYR:OH	1:D:275:ALA:HB2	2.21	0.40
1:D:193:PHE:O	1:D:196:LEU:HB3	2.22	0.40
1:B:131:GLN:HB3	1:B:134:PRO:HD2	2.03	0.40
1:B:277:GLU:HA	1:B:277:GLU:OE1	2.22	0.40
1:A:99:SER:O	1:A:103:GLY:N	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	290/361 (80%)	255 (88%)	31 (11%)	4 (1%)	16	67
1	B	295/361 (82%)	255 (86%)	32 (11%)	8 (3%)	8	49
1	C	306/361 (85%)	270 (88%)	30 (10%)	6 (2%)	11	58
1	D	294/361 (81%)	247 (84%)	40 (14%)	7 (2%)	9	53
All	All	1185/1444 (82%)	1027 (87%)	133 (11%)	25 (2%)	11	56

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	233	ARG
1	C	11	GLY
1	C	286	SER
1	B	11	GLY
1	B	294	LEU
1	C	92	ALA
1	D	11	GLY
1	D	93	GLU
1	D	221	TYR
1	D	225	VAL
1	A	93	GLU
1	B	282	SER
1	B	336	GLU
1	D	152	ASP
1	B	233	ARG
1	C	64	ASP
1	C	233	ARG
1	D	98	ARG
1	D	269	ARG
1	B	101	ARG
1	B	185	THR
1	B	334	TYR
1	C	62	LEU
1	A	11	GLY

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Mol	Chain	Res	Type
1	A	90	ILE

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	246/290 (85%)	219 (89%)	27 (11%)	9	38
1	B	248/290 (86%)	225 (91%)	23 (9%)	13	48
1	C	257/290 (89%)	242 (94%)	15 (6%)	28	73
1	D	248/290 (86%)	226 (91%)	22 (9%)	14	51
All	All	999/1160 (86%)	912 (91%)	87 (9%)	15	53

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MSE
1	A	2	ARG
1	A	9	ASN
1	A	10	LYS
1	A	21	ASN
1	A	52	GLU
1	A	65	GLU
1	A	84	ARG
1	A	100	GLU
1	A	106	VAL
1	A	107	LEU
1	A	118	ASP
1	A	132	THR
1	A	150	ARG
1	A	161	VAL
1	A	164	SER
1	A	198	ARG
1	A	219	LYS
1	A	220	LYS
1	A	232	LEU
1	A	233	ARG

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Mol	Chain	Res	Type
1	A	286	SER
1	A	288	HIS
1	A	291	SER
1	A	337	LYS
1	A	339	ASN
1	A	349	LEU
1	B	9	ASN
1	B	29	GLN
1	B	51	GLU
1	B	70	ASN
1	B	93	GLU
1	B	94	ILE
1	B	101	ARG
1	B	107	LEU
1	B	132	THR
1	B	143	GLN
1	B	150	ARG
1	B	187	LEU
1	B	205	THR
1	B	226	GLU
1	B	233	ARG
1	B	248	THR
1	B	269	ARG
1	B	277	GLU
1	B	290	ASN
1	B	291	SER
1	B	336	GLU
1	B	340	SER
1	B	344	ASN
1	C	1	MSE
1	C	2	ARG
1	C	18	LEU
1	C	50	THR
1	C	59	LEU
1	C	63	ASN
1	C	64	ASP
1	C	65	GLU
1	C	90	ILE
1	C	101	ARG
1	C	107	LEU
1	C	115	GLN
1	C	119	LEU

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Mol	Chain	Res	Type
1	C	214	ASN
1	C	286	SER
1	D	1	MSE
1	D	18	LEU
1	D	33	VAL
1	D	52	GLU
1	D	59	LEU
1	D	95	THR
1	D	105	ASP
1	D	107	LEU
1	D	169	ASN
1	D	173	LEU
1	D	215	MSE
1	D	226	GLU
1	D	233	ARG
1	D	245	LEU
1	D	248	THR
1	D	251	GLU
1	D	269	ARG
1	D	274	PHE
1	D	279	GLU
1	D	287	LYS
1	D	299	HIS
1	D	349	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	21	ASN
1	A	89	GLN
1	A	139	HIS
1	A	169	ASN
1	A	191	HIS
1	A	206	GLN
1	A	214	ASN
1	A	339	ASN
1	A	344	ASN
1	B	9	ASN
1	B	70	ASN
1	B	89	GLN
1	B	139	HIS

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Mol	Chain	Res	Type
1	B	169	ASN
1	B	214	ASN
1	B	290	ASN
1	B	339	ASN
1	B	344	ASN
1	C	8	ASN
1	C	63	ASN
1	C	89	GLN
1	C	139	HIS
1	C	169	ASN
1	C	206	GLN
1	C	339	ASN
1	C	344	ASN
1	C	352	ASN
1	D	8	ASN
1	D	53	GLN
1	D	70	ASN
1	D	131	GLN
1	D	139	HIS
1	D	169	ASN
1	D	214	ASN
1	D	283	ASN
1	D	339	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	298/361 (82%)	-0.26	0	100	100	19, 48, 80, 98	0
1	B	301/361 (83%)	-0.26	0	100	100	32, 54, 86, 121	0
1	C	312/361 (86%)	-0.21	1 (0%)	91	63	32, 54, 89, 106	0
1	D	302/361 (83%)	-0.14	1 (0%)	91	63	30, 55, 96, 107	0
All	All	1213/1444 (84%)	-0.22	2 (0%)	93	70	19, 54, 90, 121	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	262	GLN	2.8
1	D	266	ALA	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.