Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:48 PM GMT

PDB ID	:	4DI3
Title	:	Crystal structure of a 2:1 complex of Treponema pallidum TatP(T) (Tp0957) bound to TatT (Tp0956)
Authors	:	Brautigam, C.A.; Deka, R.K.; Norgard, M.V.
Deposited on	:	2012-01-30
Resolution	:	3.05 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 ①) were used in the production of this report:

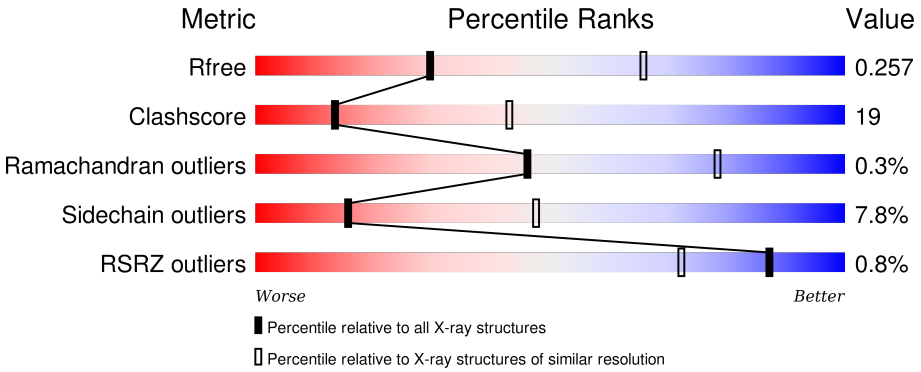
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.05 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	1191 (3.10-3.02)
Clashscore	102246	1303 (3.10-3.02)
Ramachandran outliers	100387	1254 (3.10-3.02)
Sidechain outliers	100360	1254 (3.10-3.02)
RSRZ outliers	91569	1197 (3.10-3.02)

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 <=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	D	324	51% 39% 6%
1	E	324	56% 35% 6%
2	A	301	63% 26% 9%
2	B	301	65% 24% 9%
2	C	301	62% 27% 9%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11376 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 Tp33 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	303	Total	C	N	O	S	0	0	0
			2385	1527	416	431	11			
1	E	317	Total	C	N	O	S	0	0	0
			2493	1594	435	453	11			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	5	GLY	-	EXPRESSION TAG	UNP O83923
D	6	ARG	-	EXPRESSION TAG	UNP O83923
D	185	VAL	ALA	ENGINEERED MUTATION	UNP O83923
E	5	GLY	-	EXPRESSION TAG	UNP O83923
E	6	ARG	-	EXPRESSION TAG	UNP O83923
E	185	VAL	ALA	ENGINEERED MUTATION	UNP O83923

- Molecule 2 is a protein called Uncharacterized protein TP_0956.

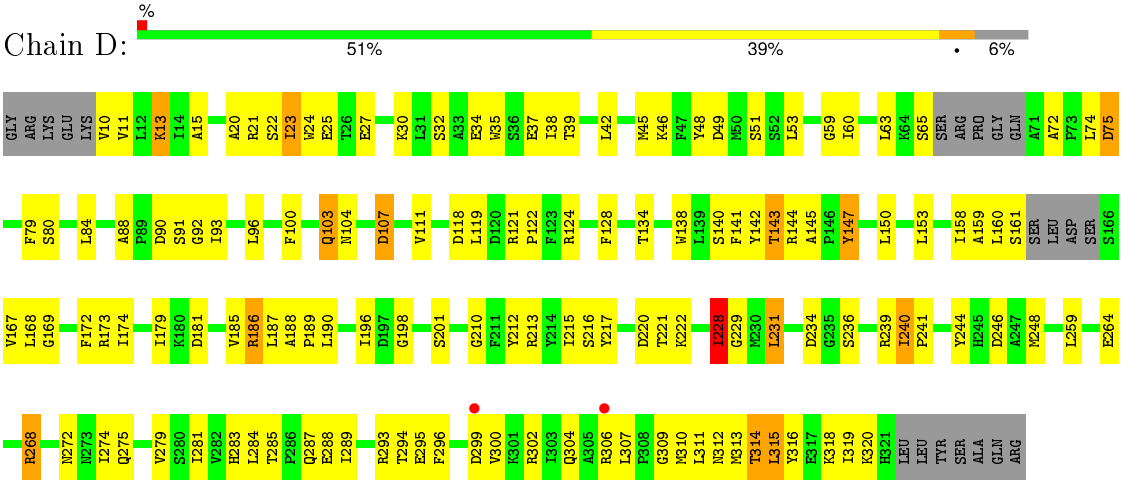
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	273	Total	C	N	O	S	0	0	0
			2166	1386	374	398	8			
2	B	273	Total	C	N	O	S	0	0	0
			2166	1386	374	398	8			
2	C	273	Total	C	N	O	S	0	0	0
			2166	1386	374	398	8			

3 Residue-property plots (i)

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.

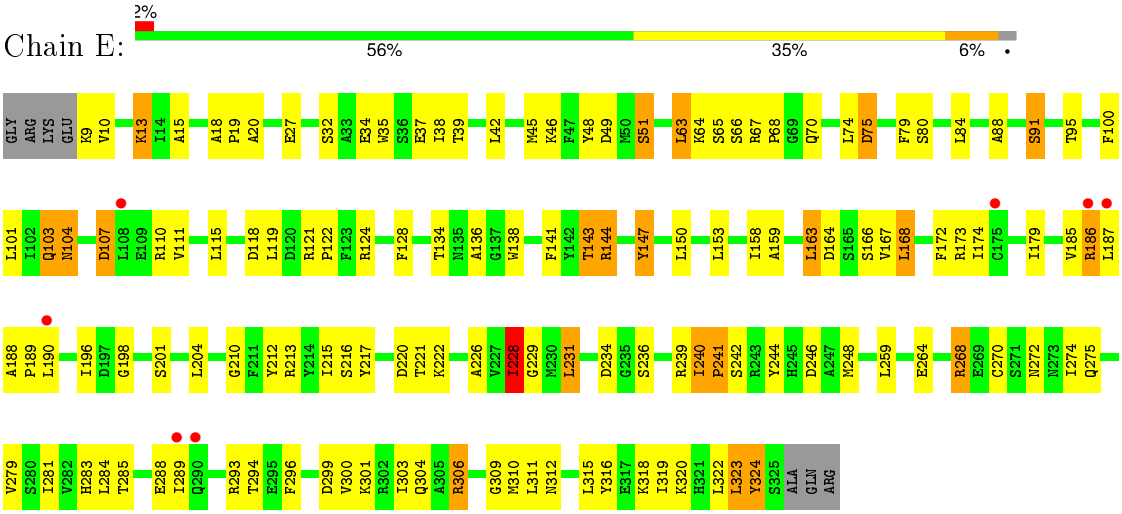
- Molecule 1: Tp33 protein

Chain D:



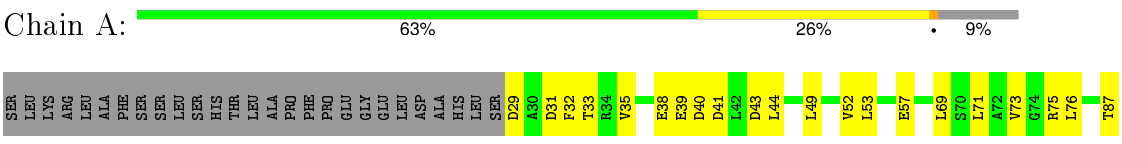
- Molecule 1: Tp33 protein

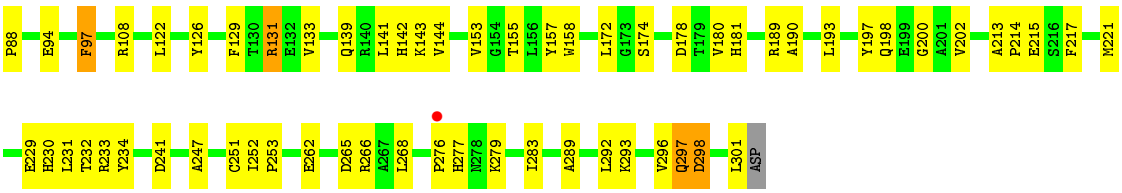
Chain E:



- Molecule 2: Uncharacterized protein TP_0956

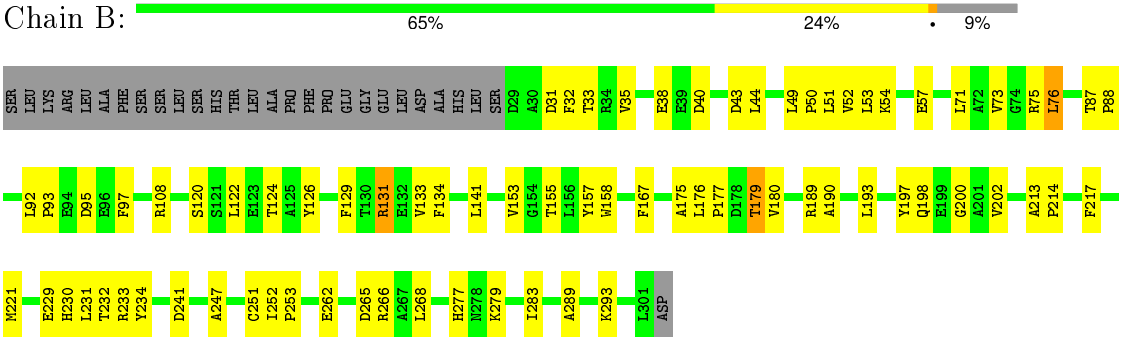
Chain A:





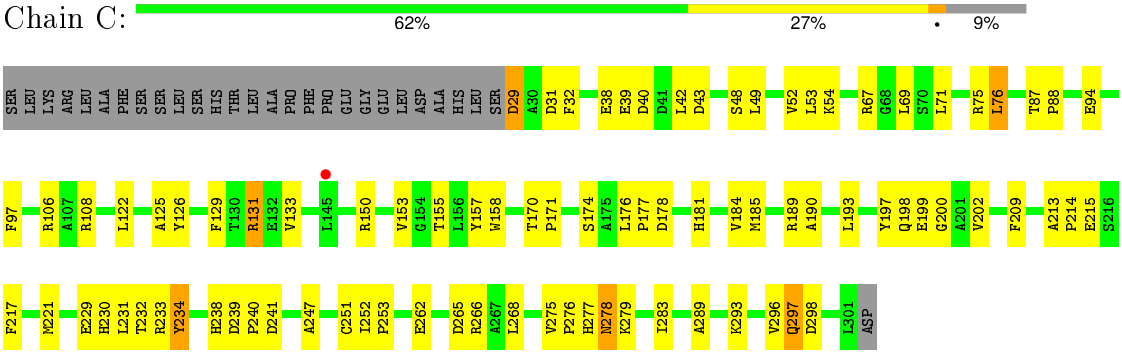
• Molecule 2: Uncharacterized protein TP_0956

Chain B:



• Molecule 2: Uncharacterized protein TP_0956

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 2 2	Depositor
Cell constants a, b, c, α, β, γ	148.93Å 148.93Å 212.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.65 – 3.05 49.64 – 3.05	Depositor EDS
% Data completeness (in resolution range)	98.9 (49.65-3.05) 99.0 (49.64-3.05)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.96 (at 3.07Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.7.1_743)	Depositor
R, R_{free}	0.203 , 0.263 0.196 , 0.257	Depositor DCC
R_{free} test set	2322 reflections (5.08%)	DCC
Wilson B-factor (Å^2)	97.6	Xtriage
Anisotropy	0.302	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 82.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Outliers	0 of 45737 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	11376	wwPDB-VP
Average B, all atoms (Å^2)	117.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.99% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 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	D	0.41	0/2434	0.67	0/3292
1	E	0.42	0/2546	0.64	0/3446
2	A	0.45	0/2224	0.61	0/3029
2	B	0.45	0/2224	0.59	0/3029
2	C	0.47	0/2224	0.60	0/3029
All	All	0.44	0/11652	0.62	0/15825

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	D	0	1
1	E	0	2
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	228	ILE	Peptide
1	E	228	ILE	Peptide
1	E	241	PRO	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	D	2385	0	2423	118	0
1	E	2493	0	2535	130	0
2	A	2166	0	2100	58	0
2	B	2166	0	2100	64	0
2	C	2166	0	2100	68	1
All	All	11376	0	11258	424	1

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 19.

All (424) 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:104:ASN:HB3	1:D:107:ASP:HB2	1.23	1.14
1:E:65:SER:HA	1:E:66:SER:HB2	1.23	1.13
1:E:104:ASN:HB3	1:E:107:ASP:HB2	1.28	1.13
1:D:213:ARG:NH2	2:A:178:ASP:OD1	1.80	1.13
2:B:176:LEU:HD12	2:B:177:PRO:HD2	1.36	1.07
1:D:285:THR:HG22	1:D:288:GLU:HG3	1.51	0.92
1:E:186:ARG:HH11	1:E:190:LEU:HD21	1.36	0.90
1:E:110:ARG:NH2	1:E:322:LEU:HB3	1.87	0.89
1:E:196:ILE:HG22	1:E:198:GLY:H	1.37	0.89
1:D:186:ARG:HH11	1:D:190:LEU:HD21	1.35	0.89
1:E:144:ARG:HH11	1:E:144:ARG:HG3	1.37	0.88
1:E:65:SER:CA	1:E:66:SER:HB2	2.03	0.88
1:E:67:ARG:H	1:E:70:GLN:HB3	1.39	0.87
1:E:67:ARG:HB3	1:E:68:PRO:HD2	1.57	0.85
1:D:75:ASP:HB3	1:D:236:SER:OG	1.78	0.83
1:D:196:ILE:HG22	1:D:198:GLY:H	1.44	0.83
1:D:22:SER:O	1:D:23:ILE:HG23	1.80	0.82
2:B:176:LEU:HB2	2:B:217:PHE:CD1	2.15	0.82
2:B:176:LEU:HA	2:B:217:PHE:HE1	1.46	0.81
1:D:240:ILE:HG21	1:D:248:MET:CE	2.11	0.81
1:E:75:ASP:HB3	1:E:236:SER:OG	1.81	0.81
1:E:324:TYR:N	1:E:324:TYR:HD2	1.79	0.80
1:E:64:LYS:HG3	1:E:65:SER:H	1.45	0.80
2:B:176:LEU:HD13	2:B:217:PHE:CD1	2.16	0.80
1:E:210:GLY:HA2	1:E:212:TYR:CE2	2.17	0.79
1:E:66:SER:N	1:E:67:ARG:HA	1.97	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:143:THR:HG21	1:E:147:TYR:HE2	1.47	0.78
1:E:285:THR:OG1	1:E:288:GLU:HG3	1.83	0.78
1:D:35:TRP:NE1	1:D:248:MET:HB2	1.99	0.78
1:D:143:THR:HG21	1:D:147:TYR:HE2	1.46	0.78
1:E:163:LEU:HD11	1:E:173:ARG:HH22	1.48	0.77
2:B:129:PHE:O	2:B:133:VAL:HG12	1.85	0.77
2:C:38:GLU:OE2	2:C:277:HIS:HA	1.86	0.76
1:E:324:TYR:N	1:E:324:TYR:CD2	2.53	0.76
1:E:240:ILE:HG21	1:E:248:MET:CE	2.16	0.75
2:B:175:ALA:O	2:B:217:PHE:CZ	2.41	0.74
1:E:35:TRP:NE1	1:E:248:MET:HB2	2.02	0.73
1:D:240:ILE:HG21	1:D:248:MET:HE1	1.70	0.73
1:E:240:ILE:HG21	1:E:248:MET:HE1	1.69	0.73
1:D:210:GLY:HA2	1:D:212:TYR:CE2	2.24	0.72
1:D:315:LEU:O	1:D:319:ILE:HG13	1.88	0.72
2:B:131:ARG:HB2	2:B:131:ARG:HH11	1.53	0.72
2:C:131:ARG:HH11	2:C:131:ARG:HB2	1.55	0.72
2:A:139:GLN:O	2:A:143:LYS:HB2	1.91	0.71
1:E:210:GLY:HA2	1:E:212:TYR:HE2	1.54	0.70
1:D:32:SER:OG	2:A:94:GLU:OE1	2.09	0.70
2:B:54:LYS:NZ	2:C:39:GLU:OE1	2.21	0.70
1:D:296:PHE:O	1:D:300:VAL:HG23	1.93	0.69
2:A:214:PRO:HD2	2:A:217:PHE:CD2	2.28	0.69
2:A:229:GLU:O	2:A:232:THR:OG1	2.10	0.69
1:D:143:THR:HG21	1:D:147:TYR:CE2	2.27	0.68
2:A:141:LEU:O	2:A:144:VAL:HG12	1.93	0.68
2:B:214:PRO:HD2	2:B:217:PHE:CD2	2.28	0.68
2:C:38:GLU:OE1	2:C:276:PRO:O	2.12	0.68
1:D:22:SER:HB2	1:D:24:TRP:HE3	1.59	0.68
1:E:143:THR:HG21	1:E:147:TYR:CE2	2.27	0.68
2:B:176:LEU:HA	2:B:217:PHE:CE1	2.27	0.67
2:B:176:LEU:HD12	2:B:177:PRO:CD	2.20	0.67
2:C:214:PRO:HD2	2:C:217:PHE:CD2	2.30	0.67
2:A:131:ARG:HH11	2:A:131:ARG:HB2	1.59	0.67
2:B:40:ASP:HB3	2:B:279:LYS:HD3	1.77	0.66
2:C:38:GLU:OE1	2:C:276:PRO:C	2.34	0.65
1:D:299:ASP:OD2	1:D:302:ARG:NH1	2.29	0.65
1:D:34:GLU:O	1:D:38:ILE:HG13	1.97	0.65
2:B:229:GLU:O	2:B:232:THR:OG1	2.13	0.65
1:D:210:GLY:HA2	1:D:212:TYR:HE2	1.62	0.64
1:D:299:ASP:HA	1:D:302:ARG:NH1	2.13	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:214:PRO:HD2	2:A:217:PHE:HD2	1.63	0.63
2:B:176:LEU:HD13	2:B:217:PHE:CE1	2.33	0.63
2:B:134:PHE:CE1	2:B:179:THR:HG22	2.34	0.63
1:D:15:ALA:HB2	1:D:74:LEU:HD21	1.79	0.63
2:A:32:PHE:O	2:A:35:VAL:HG22	1.99	0.63
1:D:35:TRP:CD1	1:D:248:MET:HB2	2.35	0.62
1:E:103:GLN:O	1:E:103:GLN:NE2	2.32	0.62
2:A:40:ASP:HB3	2:A:279:LYS:HD3	1.82	0.62
1:D:100:PHE:HB3	1:D:293:ARG:HD3	1.81	0.62
1:E:144:ARG:CG	1:E:144:ARG:HH11	2.12	0.62
1:E:215:ILE:O	1:E:215:ILE:HD12	2.00	0.62
2:C:53:LEU:HD12	2:C:76:LEU:HG	1.81	0.62
2:C:238:HIS:HB3	2:C:275:VAL:HG11	1.81	0.62
2:C:40:ASP:HB3	2:C:279:LYS:HD3	1.82	0.62
1:D:231:LEU:HD12	1:D:231:LEU:N	2.15	0.62
2:B:87:THR:HB	2:B:88:PRO:HD3	1.82	0.62
1:D:119:LEU:O	1:D:122:PRO:HD2	1.98	0.61
1:D:32:SER:HB2	1:D:45:MET:HB2	1.81	0.61
1:D:241:PRO:HG2	1:D:244:TYR:CD2	2.35	0.61
1:E:159:ALA:HB2	1:E:196:ILE:HD13	1.83	0.61
1:D:240:ILE:HG21	1:D:248:MET:HE3	1.81	0.61
1:D:215:ILE:O	1:D:215:ILE:HD12	2.00	0.61
1:D:118:ASP:OD1	1:D:318:LYS:NZ	2.28	0.61
1:E:213:ARG:NH2	2:C:178:ASP:OD1	2.33	0.61
1:E:35:TRP:CD1	1:E:248:MET:HB2	2.36	0.61
2:C:176:LEU:HD12	2:C:177:PRO:HD2	1.81	0.61
1:E:32:SER:HB2	1:E:45:MET:HB2	1.81	0.61
2:C:214:PRO:HD2	2:C:217:PHE:HD2	1.65	0.60
1:D:306:ARG:O	1:D:307:LEU:HD12	2.02	0.60
2:C:252:ILE:HB	2:C:253:PRO:HD3	1.83	0.60
1:E:318:LYS:O	1:E:322:LEU:HG	2.02	0.59
1:D:190:LEU:HD12	1:D:196:ILE:HD11	1.84	0.59
1:E:80:SER:HA	1:E:228:ILE:HG22	1.83	0.59
1:E:67:ARG:HB3	1:E:68:PRO:CD	2.30	0.59
1:E:67:ARG:H	1:E:70:GLN:CB	2.13	0.59
1:E:100:PHE:CE2	1:E:289:ILE:HG23	2.38	0.59
2:A:262:GLU:O	2:A:266:ARG:HG3	2.02	0.59
1:E:241:PRO:HG2	1:E:244:TYR:CD2	2.38	0.59
1:E:34:GLU:O	1:E:38:ILE:HG13	2.02	0.59
2:C:262:GLU:O	2:C:266:ARG:HG3	2.03	0.59
1:D:160:LEU:O	1:D:161:SER:HB3	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:122:LEU:HD13	2:C:129:PHE:CZ	2.38	0.58
2:A:252:ILE:HB	2:A:253:PRO:HD3	1.85	0.58
2:C:38:GLU:O	2:C:279:LYS:HD2	2.03	0.58
1:D:313:MET:HA	1:D:316:TYR:HB3	1.86	0.58
1:D:80:SER:HA	1:D:228:ILE:HG22	1.85	0.58
1:D:39:THR:HB	1:D:42:LEU:HB3	1.84	0.58
1:E:119:LEU:O	1:E:122:PRO:HD2	2.03	0.58
2:C:38:GLU:CD	2:C:277:HIS:HA	2.24	0.58
1:E:163:LEU:O	1:E:166:SER:N	2.36	0.57
1:D:168:LEU:HG	1:D:168:LEU:O	2.03	0.57
1:D:159:ALA:HB2	1:D:196:ILE:HD13	1.84	0.57
2:B:262:GLU:O	2:B:266:ARG:HG3	2.03	0.57
2:B:252:ILE:HB	2:B:253:PRO:HD3	1.85	0.57
2:C:153:VAL:HG13	2:C:190:ALA:HB1	1.85	0.57
1:E:67:ARG:N	1:E:70:GLN:HB3	2.14	0.57
1:E:190:LEU:HD12	1:E:196:ILE:HD11	1.87	0.57
1:E:49:ASP:OD1	1:E:51:SER:OG	2.22	0.57
2:C:229:GLU:O	2:C:232:THR:OG1	2.19	0.57
1:E:304:GLN:HE22	1:E:311:LEU:HD12	1.70	0.57
1:E:103:GLN:O	1:E:104:ASN:HB2	2.04	0.56
1:D:79:PHE:O	1:D:229:GLY:HA3	2.05	0.56
1:D:173:ARG:NH1	1:D:179:ILE:O	2.37	0.56
1:E:63:LEU:HD12	1:E:74:LEU:HB3	1.87	0.56
2:A:298:ASP:OD1	2:A:298:ASP:N	2.36	0.56
1:E:220:ASP:OD1	1:E:268:ARG:NH2	2.38	0.56
1:E:65:SER:HA	1:E:66:SER:CB	2.15	0.56
2:C:157:TYR:HD1	2:C:202:VAL:HG22	1.70	0.56
2:B:214:PRO:HD2	2:B:217:PHE:HD2	1.69	0.56
2:C:29:ASP:O	2:C:32:PHE:HB3	2.05	0.56
1:E:144:ARG:NH1	1:E:144:ARG:HG3	2.16	0.56
2:A:276:PRO:HB2	2:A:277:HIS:ND1	2.21	0.56
2:B:176:LEU:CA	2:B:217:PHE:CE1	2.89	0.56
2:B:176:LEU:HB2	2:B:217:PHE:HD1	1.70	0.55
1:E:304:GLN:NE2	1:E:311:LEU:HD12	2.22	0.55
2:B:32:PHE:O	2:B:35:VAL:HG22	2.06	0.55
1:E:15:ALA:HB2	1:E:74:LEU:HD21	1.87	0.55
2:A:122:LEU:HD13	2:A:129:PHE:CZ	2.41	0.55
2:B:53:LEU:HD12	2:B:76:LEU:HG	1.89	0.55
1:D:10:VAL:HG13	1:D:10:VAL:O	2.07	0.55
1:D:107:ASP:O	1:D:111:VAL:HG23	2.06	0.55
1:E:79:PHE:O	1:E:229:GLY:HA3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:46:LYS:HE3	2:C:94:GLU:OE2	2.07	0.54
2:C:53:LEU:CD1	2:C:76:LEU:HG	2.36	0.54
1:E:100:PHE:CD2	1:E:289:ILE:HG23	2.42	0.54
1:E:10:VAL:HG13	1:E:10:VAL:O	2.06	0.54
1:E:272:ASN:O	1:E:275:GLN:HB3	2.06	0.54
1:E:110:ARG:HH21	1:E:322:LEU:HB3	1.66	0.54
2:B:189:ARG:NH2	2:B:193:LEU:HD21	2.22	0.54
1:E:300:VAL:HG13	1:E:301:LYS:N	2.22	0.54
2:A:126:TYR:O	2:A:129:PHE:HB2	2.08	0.54
1:E:231:LEU:N	1:E:231:LEU:HD12	2.22	0.54
2:B:268:LEU:HD21	2:B:289:ALA:HB3	1.90	0.54
2:B:53:LEU:CD1	2:B:76:LEU:HG	2.38	0.54
2:A:189:ARG:NH2	2:A:193:LEU:HD21	2.23	0.53
2:A:153:VAL:HG13	2:A:190:ALA:HB1	1.90	0.53
1:E:274:ILE:HG22	1:E:279:VAL:HB	1.91	0.53
1:E:240:ILE:HG21	1:E:248:MET:HE3	1.91	0.53
1:E:107:ASP:O	1:E:111:VAL:HG23	2.09	0.53
1:E:173:ARG:NH1	1:E:179:ILE:O	2.42	0.53
1:E:39:THR:HB	1:E:42:LEU:HB3	1.90	0.53
1:D:91:SER:C	1:D:93:ILE:H	2.11	0.53
1:E:323:LEU:C	1:E:324:TYR:HD2	2.11	0.52
1:D:39:THR:HG22	1:D:244:TYR:CG	2.44	0.52
1:E:10:VAL:HG12	1:E:42:LEU:HG	1.89	0.52
1:D:59:GLY:O	1:D:63:LEU:HD12	2.09	0.52
1:E:100:PHE:HB3	1:E:293:ARG:HD3	1.92	0.52
1:E:84:LEU:HD11	1:E:229:GLY:HA2	1.91	0.52
2:B:126:TYR:O	2:B:129:PHE:HB2	2.08	0.52
2:C:71:LEU:HD13	2:C:155:THR:HA	1.91	0.52
1:D:158:ILE:HA	1:D:198:GLY:O	2.10	0.52
2:B:122:LEU:HD13	2:B:129:PHE:CZ	2.45	0.52
2:C:71:LEU:CD1	2:C:155:THR:HA	2.39	0.52
1:E:299:ASP:O	1:E:303:ILE:HD13	2.10	0.52
1:D:49:ASP:OD1	1:D:51:SER:OG	2.25	0.52
2:B:157:TYR:HD1	2:B:202:VAL:HG22	1.75	0.52
1:D:96:LEU:HD23	1:D:319:ILE:HD13	1.91	0.52
1:D:272:ASN:O	1:D:275:GLN:HB3	2.10	0.52
1:E:13:LYS:HB3	1:E:48:TYR:CE2	2.45	0.51
2:C:157:TYR:CD1	2:C:202:VAL:HG22	2.45	0.51
1:D:161:SER:HA	1:D:181:ASP:OD2	2.10	0.51
1:E:64:LYS:HG3	1:E:65:SER:N	2.20	0.51
1:E:46:LYS:NZ	2:C:298:ASP:OD2	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:315:LEU:HD11	1:E:319:ILE:HD11	1.91	0.51
2:C:131:ARG:HH11	2:C:131:ARG:CB	2.21	0.51
2:B:131:ARG:CB	2:B:131:ARG:HH11	2.20	0.51
2:C:181:HIS:O	2:C:185:MET:HG2	2.11	0.51
1:E:210:GLY:HA2	1:E:212:TYR:CD2	2.45	0.50
1:E:163:LEU:HD12	1:E:164:ASP:N	2.26	0.50
1:D:274:ILE:HG22	1:D:279:VAL:HB	1.93	0.50
2:A:53:LEU:CD1	2:A:76:LEU:HG	2.42	0.50
2:A:53:LEU:HD12	2:A:76:LEU:HG	1.94	0.50
2:C:87:THR:HB	2:C:88:PRO:HD3	1.93	0.50
1:E:158:ILE:HA	1:E:198:GLY:O	2.11	0.50
1:D:84:LEU:HD11	1:D:229:GLY:HA2	1.94	0.50
2:C:265:ASP:OD1	2:C:293:LYS:HE3	2.12	0.50
2:C:126:TYR:O	2:C:129:PHE:HB2	2.11	0.50
1:E:101:LEU:HD13	1:E:316:TYR:HE1	1.77	0.50
1:E:168:LEU:C	1:E:168:LEU:HD22	2.31	0.50
2:B:176:LEU:HB2	2:B:217:PHE:CE1	2.46	0.50
1:E:322:LEU:HD23	1:E:322:LEU:N	2.27	0.50
1:D:100:PHE:CE2	1:D:289:ILE:HG23	2.46	0.50
2:B:265:ASP:OD1	2:B:293:LYS:HE3	2.12	0.50
1:E:323:LEU:HB3	1:E:324:TYR:CE2	2.47	0.49
1:D:134:THR:N	1:D:228:ILE:O	2.39	0.49
2:B:153:VAL:HG13	2:B:190:ALA:HB1	1.94	0.49
2:A:38:GLU:O	2:A:279:LYS:HD2	2.13	0.49
2:B:175:ALA:O	2:B:217:PHE:CE1	2.65	0.49
2:C:277:HIS:O	2:C:278:ASN:CB	2.59	0.49
2:A:268:LEU:HD21	2:A:289:ALA:HB3	1.94	0.49
2:C:176:LEU:HD12	2:C:177:PRO:CD	2.43	0.49
2:A:87:THR:HB	2:A:88:PRO:HD3	1.93	0.49
2:A:38:GLU:OE2	2:A:277:HIS:HA	2.12	0.49
1:D:220:ASP:OD1	1:D:268:ARG:NH2	2.45	0.49
1:E:221:THR:HG21	1:E:284:LEU:HB2	1.95	0.49
1:E:39:THR:HG22	1:E:244:TYR:CG	2.48	0.49
2:A:252:ILE:CB	2:A:253:PRO:HD3	2.42	0.49
1:E:88:ALA:O	1:E:91:SER:HB3	2.12	0.49
2:A:131:ARG:CB	2:A:131:ARG:HH11	2.24	0.49
2:A:75:ARG:HG3	2:A:158:TRP:CZ2	2.47	0.49
1:E:164:ASP:OD1	1:E:164:ASP:N	2.46	0.48
1:D:167:VAL:O	1:D:167:VAL:CG1	2.61	0.48
2:C:296:VAL:HG13	2:C:297:GLN:N	2.28	0.48
2:A:71:LEU:CD1	2:A:155:THR:HA	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:71:LEU:HD13	2:B:155:THR:HA	1.94	0.48
2:B:176:LEU:CD1	2:B:217:PHE:CE1	2.96	0.48
1:D:100:PHE:CD2	1:D:289:ILE:HG23	2.49	0.48
2:B:176:LEU:CA	2:B:217:PHE:HE1	2.19	0.48
1:E:296:PHE:O	1:E:299:ASP:N	2.41	0.48
2:A:265:ASP:OD1	2:A:293:LYS:HE3	2.13	0.48
2:B:176:LEU:CB	2:B:217:PHE:CD1	2.94	0.48
1:D:60:ILE:HA	1:D:63:LEU:CD1	2.43	0.48
1:D:268:ARG:NE	1:D:268:ARG:HA	2.28	0.48
1:D:264:GLU:HA	1:D:264:GLU:OE2	2.12	0.48
2:C:252:ILE:CB	2:C:253:PRO:HD3	2.43	0.48
2:C:279:LYS:O	2:C:283:ILE:HG12	2.13	0.48
2:A:157:TYR:HD1	2:A:202:VAL:HG22	1.78	0.48
2:A:157:TYR:CD1	2:A:202:VAL:HG22	2.48	0.48
1:D:241:PRO:HG2	1:D:244:TYR:CE2	2.49	0.48
1:E:309:GLY:C	1:E:311:LEU:H	2.17	0.48
2:B:38:GLU:O	2:B:279:LYS:HD2	2.14	0.47
1:D:316:TYR:CE2	1:D:320:LYS:NZ	2.74	0.47
2:A:71:LEU:HD13	2:A:155:THR:HA	1.95	0.47
1:E:144:ARG:NH1	1:E:144:ARG:CG	2.75	0.47
1:E:143:THR:HG23	1:E:217:TYR:HB2	1.96	0.47
1:E:163:LEU:CD1	1:E:164:ASP:N	2.77	0.47
2:C:276:PRO:O	2:C:279:LYS:HB2	2.14	0.47
2:B:252:ILE:CB	2:B:253:PRO:HD3	2.44	0.47
2:B:71:LEU:CD1	2:B:155:THR:HA	2.44	0.47
1:E:118:ASP:OD1	1:E:318:LYS:HD2	2.15	0.47
1:D:316:TYR:HE2	1:D:320:LYS:HZ3	1.54	0.47
1:E:323:LEU:C	1:E:324:TYR:CD2	2.88	0.47
1:D:241:PRO:HG2	1:D:244:TYR:HD2	1.77	0.47
1:D:312:ASN:O	1:D:313:MET:HB2	2.15	0.47
1:E:185:VAL:HG21	2:C:215:GLU:OE1	2.13	0.47
1:D:309:GLY:O	1:D:311:LEU:N	2.47	0.47
2:C:268:LEU:HD21	2:C:289:ALA:HB3	1.95	0.47
2:B:176:LEU:CB	2:B:217:PHE:CE1	2.98	0.47
1:E:241:PRO:HG2	1:E:244:TYR:HD2	1.79	0.47
1:D:138:TRP:CD1	1:D:222:LYS:HE3	2.50	0.47
2:C:75:ARG:HG3	2:C:158:TRP:CZ2	2.49	0.47
1:E:300:VAL:HG13	1:E:301:LYS:H	1.79	0.47
1:E:186:ARG:HD2	1:E:190:LEU:HG	1.97	0.47
2:B:157:TYR:CD1	2:B:202:VAL:HG22	2.50	0.47
2:A:197:TYR:CE2	2:A:198:GLN:HG2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:96:LEU:CD2	1:D:319:ILE:HD13	2.45	0.46
2:C:170:THR:HG23	2:C:171:PRO:HD2	1.95	0.46
2:A:279:LYS:O	2:A:283:ILE:HG12	2.14	0.46
2:B:167:PHE:CD1	2:B:180:VAL:HG21	2.51	0.46
1:D:304:GLN:CG	1:D:311:LEU:HD23	2.45	0.46
1:D:60:ILE:HA	1:D:63:LEU:HD13	1.97	0.46
1:E:138:TRP:CD1	1:E:222:LYS:HE3	2.50	0.46
1:E:204:LEU:HD12	1:E:270:CYS:SG	2.56	0.46
2:C:200:GLY:O	2:C:231:LEU:HD13	2.15	0.46
1:D:285:THR:HG23	1:D:287:GLN:HB2	1.96	0.46
2:A:230:HIS:CD2	2:A:233:ARG:HE	2.34	0.46
1:D:124:ARG:HA	1:D:128:PHE:O	2.15	0.46
1:D:285:THR:CG2	1:D:288:GLU:HG3	2.35	0.46
2:A:189:ARG:CZ	2:A:193:LEU:HD21	2.45	0.46
1:E:124:ARG:HA	1:E:128:PHE:O	2.16	0.46
2:B:197:TYR:CE2	2:B:198:GLN:HG2	2.51	0.46
1:D:210:GLY:HA2	1:D:212:TYR:CD2	2.52	0.45
1:D:160:LEU:HB3	1:D:161:SER:H	1.62	0.45
1:D:91:SER:HA	1:D:92:GLY:HA3	1.67	0.45
2:C:171:PRO:O	2:C:174:SER:N	2.47	0.45
2:B:51:LEU:HD13	2:C:48:SER:HB2	1.97	0.45
1:D:221:THR:HG21	1:D:284:LEU:HB2	1.98	0.45
2:A:252:ILE:HG22	2:A:253:PRO:N	2.30	0.45
1:D:143:THR:HG23	1:D:217:TYR:HB2	1.97	0.45
1:E:187:LEU:HA	1:E:187:LEU:HD23	1.78	0.45
1:D:10:VAL:HG12	1:D:42:LEU:HG	1.98	0.45
2:C:230:HIS:CD2	2:C:233:ARG:HE	2.35	0.45
2:A:133:VAL:HG23	2:A:141:LEU:CD1	2.46	0.45
1:D:84:LEU:HA	1:D:84:LEU:HD23	1.75	0.45
1:D:188:ALA:HB3	1:D:189:PRO:HD3	1.99	0.45
2:C:184:VAL:HG21	2:C:209:PHE:CZ	2.52	0.45
1:D:216:SER:HB2	1:D:217:TYR:CD2	2.52	0.45
2:A:141:LEU:HG	2:A:142:HIS:N	2.32	0.45
1:D:75:ASP:CB	1:D:236:SER:OG	2.59	0.45
2:B:122:LEU:HD23	2:B:122:LEU:HA	1.70	0.45
2:B:44:LEU:HD23	2:B:44:LEU:HA	1.73	0.45
1:E:306:ARG:O	1:E:306:ARG:HD2	2.17	0.45
2:B:230:HIS:CD2	2:B:233:ARG:HE	2.35	0.45
2:C:275:VAL:O	2:C:275:VAL:HG23	2.17	0.45
2:C:76:LEU:HA	2:C:76:LEU:HD12	1.81	0.45
1:E:18:ALA:HA	1:E:19:PRO:HD3	1.83	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:160:LEU:O	1:D:161:SER:CB	2.64	0.45
1:D:150:LEU:O	1:D:153:LEU:N	2.50	0.44
2:B:95:ASP:N	2:B:95:ASP:OD1	2.50	0.44
1:D:65:SER:HB3	1:D:72:ALA:HA	1.98	0.44
1:E:281:ILE:HG22	1:E:283:HIS:CD2	2.52	0.44
1:D:281:ILE:HG22	1:D:283:HIS:CD2	2.53	0.44
2:C:239:ASP:HA	2:C:240:PRO:HD3	1.88	0.44
1:E:95:THR:OG1	1:E:311:LEU:HA	2.17	0.44
2:C:252:ILE:HG22	2:C:253:PRO:N	2.32	0.44
1:E:39:THR:HA	1:E:244:TYR:CE1	2.52	0.44
2:B:57:GLU:HA	2:B:73:VAL:HG21	1.99	0.44
2:B:120:SER:O	2:B:124:THR:OG1	2.27	0.44
1:E:163:LEU:HD11	1:E:173:ARG:NH2	2.24	0.44
1:D:284:LEU:HA	1:D:284:LEU:HD23	1.83	0.44
2:A:292:LEU:HA	2:A:292:LEU:HD23	1.79	0.44
2:A:200:GLY:O	2:A:231:LEU:HD13	2.18	0.44
1:E:268:ARG:NE	1:E:268:ARG:HA	2.32	0.44
2:A:44:LEU:HD23	2:A:44:LEU:HA	1.86	0.44
1:E:241:PRO:HG2	1:E:244:TYR:CE2	2.53	0.44
1:D:63:LEU:N	1:D:63:LEU:HD12	2.33	0.44
1:D:174:ILE:O	1:D:174:ILE:CG2	2.66	0.44
2:B:176:LEU:HD13	2:B:217:PHE:HD1	1.76	0.43
1:D:259:LEU:HD23	1:D:259:LEU:HA	1.82	0.43
2:A:41:ASP:CG	2:C:106:ARG:HE	2.22	0.43
2:B:75:ARG:HG3	2:B:158:TRP:CZ2	2.52	0.43
1:D:103:GLN:O	1:D:104:ASN:HB2	2.19	0.43
1:E:79:PHE:N	1:E:229:GLY:O	2.40	0.43
2:B:265:ASP:OD1	2:B:293:LYS:CE	2.66	0.43
1:E:284:LEU:HD23	1:E:284:LEU:HA	1.78	0.43
2:C:234:TYR:CD2	2:C:234:TYR:N	2.85	0.43
1:E:216:SER:HB2	1:E:217:TYR:CD2	2.53	0.43
1:E:100:PHE:HE2	1:E:289:ILE:HG23	1.84	0.43
2:A:122:LEU:HA	2:A:122:LEU:HD23	1.72	0.43
2:C:197:TYR:CE2	2:C:198:GLN:HG2	2.54	0.43
1:E:84:LEU:HA	1:E:84:LEU:HD23	1.73	0.43
2:A:69:LEU:HA	2:A:69:LEU:HD23	1.64	0.43
1:E:236:SER:HA	1:E:239:ARG:HD3	2.01	0.43
1:D:236:SER:HA	1:D:239:ARG:HD3	2.01	0.42
2:C:38:GLU:OE1	2:C:277:HIS:HA	2.19	0.42
2:C:213:ALA:HB1	2:C:217:PHE:HB3	2.00	0.42
1:E:115:LEU:CD2	1:E:319:ILE:HG13	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:306:ARG:CD	1:E:306:ARG:O	2.67	0.42
2:A:39:GLU:OE1	2:C:54:LYS:NZ	2.34	0.42
1:E:84:LEU:HD21	1:E:231:LEU:HD11	2.02	0.42
1:D:88:ALA:C	1:D:90:ASP:H	2.23	0.42
1:D:296:PHE:C	1:D:300:VAL:HG23	2.40	0.42
2:A:49:LEU:O	2:A:52:VAL:N	2.50	0.42
2:A:57:GLU:HA	2:A:73:VAL:HG21	2.01	0.42
1:D:187:LEU:HA	1:D:187:LEU:HD23	1.69	0.42
1:D:240:ILE:HG12	1:D:240:ILE:H	1.64	0.42
2:C:54:LYS:HA	2:C:54:LYS:HD3	1.54	0.42
1:D:141:PHE:CD1	1:D:158:ILE:HD13	2.55	0.42
2:C:275:VAL:O	2:C:276:PRO:C	2.58	0.42
2:B:189:ARG:CZ	2:B:193:LEU:HD21	2.49	0.42
1:D:150:LEU:HD23	1:D:295:GLU:OE2	2.19	0.42
1:D:140:SER:HB2	1:D:142:TYR:CZ	2.54	0.42
1:D:13:LYS:HB3	1:D:48:TYR:CE2	2.55	0.42
2:A:178:ASP:O	2:A:181:HIS:HB3	2.19	0.42
1:D:186:ARG:NH1	1:D:190:LEU:HD21	2.17	0.42
1:D:22:SER:O	1:D:23:ILE:CG2	2.60	0.42
1:E:174:ILE:O	1:E:174:ILE:CG2	2.68	0.42
2:C:189:ARG:NH2	2:C:193:LEU:HD21	2.34	0.42
2:B:247:ALA:HA	2:B:251:CYS:HB2	2.02	0.42
2:B:279:LYS:O	2:B:283:ILE:HG12	2.20	0.42
2:C:69:LEU:HD23	2:C:69:LEU:HA	1.70	0.42
2:B:200:GLY:O	2:B:231:LEU:HD13	2.20	0.42
1:E:186:ARG:NH1	1:E:190:LEU:HD21	2.18	0.42
2:C:213:ALA:HA	2:C:214:PRO:HD3	1.92	0.42
1:D:314:THR:O	1:D:318:LYS:HB2	2.20	0.42
1:D:167:VAL:C	1:D:169:GLY:H	2.23	0.42
1:E:174:ILE:HD11	1:E:306:ARG:HG3	2.02	0.41
1:E:27:GLU:OE2	1:E:27:GLU:HA	2.20	0.41
1:E:188:ALA:HB3	1:E:189:PRO:HD3	2.02	0.41
1:D:46:LYS:NZ	2:A:298:ASP:OD2	2.49	0.41
2:A:296:VAL:HG13	2:A:297:GLN:N	2.34	0.41
1:E:323:LEU:N	1:E:323:LEU:HD13	2.35	0.41
1:E:259:LEU:HD23	1:E:259:LEU:HA	1.85	0.41
1:E:264:GLU:HA	1:E:264:GLU:OE2	2.20	0.41
2:C:67:ARG:CZ	2:C:125:ALA:HB2	2.51	0.41
2:B:92:LEU:HA	2:B:93:PRO:HD3	1.90	0.41
1:D:185:VAL:CG2	2:A:215:GLU:HB2	2.50	0.41
1:E:118:ASP:HA	1:E:121:ARG:NH1	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:277:HIS:O	2:C:278:ASN:HB2	2.20	0.41
2:C:265:ASP:OD1	2:C:293:LYS:CE	2.69	0.41
1:E:150:LEU:O	1:E:153:LEU:N	2.52	0.41
1:D:186:ARG:HD2	1:D:190:LEU:HG	2.01	0.41
2:B:49:LEU:N	2:B:50:PRO:CD	2.83	0.41
1:E:309:GLY:O	1:E:310:MET:HB3	2.20	0.41
2:C:49:LEU:O	2:C:52:VAL:N	2.52	0.41
1:D:20:ALA:O	1:D:25:GLU:CD	2.59	0.41
1:D:59:GLY:O	1:D:63:LEU:CD1	2.69	0.41
2:B:49:LEU:O	2:B:52:VAL:N	2.54	0.41
2:A:213:ALA:HB1	2:A:217:PHE:HB3	2.02	0.41
1:E:134:THR:N	1:E:228:ILE:O	2.37	0.41
1:D:304:GLN:HG3	1:D:311:LEU:HD23	2.02	0.41
2:C:247:ALA:HA	2:C:251:CYS:HB2	2.02	0.41
1:D:30:LYS:HA	2:A:97:PHE:CE2	2.56	0.41
2:A:213:ALA:HA	2:A:214:PRO:HD3	1.88	0.41
2:B:213:ALA:HB1	2:B:217:PHE:HB3	2.02	0.40
2:B:38:GLU:OE2	2:B:277:HIS:HA	2.21	0.40
1:D:27:GLU:OE2	1:D:27:GLU:HA	2.21	0.40
1:E:141:PHE:CD1	1:E:158:ILE:HD13	2.56	0.40
1:E:323:LEU:CB	1:E:324:TYR:CD2	3.04	0.40
2:A:247:ALA:HA	2:A:251:CYS:HB2	2.03	0.40
1:D:143:THR:OG1	1:D:145:ALA:O	2.30	0.40
1:D:39:THR:HA	1:D:244:TYR:CE1	2.57	0.40
2:C:42:LEU:HD23	2:C:42:LEU:HA	1.93	0.40
2:A:277:HIS:N	2:A:277:HIS:ND1	2.68	0.40
1:D:121:ARG:HB3	1:D:122:PRO:HD3	2.03	0.40
1:E:136:ALA:HB3	1:E:226:ALA:HB3	2.03	0.40
1:D:53:LEU:HD21	2:A:301:LEU:HD12	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:150:ARG:NH2	2:C:199:GLU:OE2[7_464]	2.12	0.08

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	D	297/324 (92%)	272 (92%)	24 (8%)	1 (0%)	46 78
1	E	315/324 (97%)	293 (93%)	19 (6%)	3 (1%)	19 56
2	A	271/301 (90%)	263 (97%)	8 (3%)	0	100 100
2	B	271/301 (90%)	258 (95%)	13 (5%)	0	100 100
2	C	271/301 (90%)	260 (96%)	11 (4%)	0	100 100
All	All	1425/1551 (92%)	1346 (94%)	75 (5%)	4 (0%)	46 78

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	23	ILE
1	E	242	SER
1	E	20	ALA
1	E	104	ASN

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	254/272 (93%)	231 (91%)	23 (9%)	12 38
1	E	267/272 (98%)	237 (89%)	30 (11%)	7 28
2	A	223/247 (90%)	208 (93%)	15 (7%)	20 53
2	B	223/247 (90%)	211 (95%)	12 (5%)	27 62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	C	223/247 (90%)	210 (94%)	13 (6%)	25 59
All	All	1190/1285 (93%)	1097 (92%)	93 (8%)	16 47

All (93) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	11	VAL
1	D	13	LYS
1	D	21	ARG
1	D	37	GLU
1	D	75	ASP
1	D	103	GLN
1	D	107	ASP
1	D	143	THR
1	D	144	ARG
1	D	147	TYR
1	D	172	PHE
1	D	186	ARG
1	D	201	SER
1	D	228	ILE
1	D	231	LEU
1	D	234	ASP
1	D	240	ILE
1	D	246	ASP
1	D	268	ARG
1	D	294	THR
1	D	310	MET
1	D	314	THR
1	D	315	LEU
1	E	9	LYS
1	E	13	LYS
1	E	37	GLU
1	E	51	SER
1	E	63	LEU
1	E	75	ASP
1	E	91	SER
1	E	103	GLN
1	E	107	ASP
1	E	143	THR
1	E	144	ARG
1	E	147	TYR
1	E	163	LEU

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Mol	Chain	Res	Type
1	E	167	VAL
1	E	168	LEU
1	E	172	PHE
1	E	186	ARG
1	E	201	SER
1	E	228	ILE
1	E	231	LEU
1	E	234	ASP
1	E	240	ILE
1	E	246	ASP
1	E	268	ARG
1	E	294	THR
1	E	306	ARG
1	E	312	ASN
1	E	320	LYS
1	E	323	LEU
1	E	324	TYR
2	A	29	ASP
2	A	31	ASP
2	A	33	THR
2	A	43	ASP
2	A	97	PHE
2	A	108	ARG
2	A	131	ARG
2	A	172	LEU
2	A	174	SER
2	A	180	VAL
2	A	221	MET
2	A	234	TYR
2	A	241	ASP
2	A	297	GLN
2	A	298	ASP
2	B	31	ASP
2	B	33	THR
2	B	43	ASP
2	B	76	LEU
2	B	97	PHE
2	B	108	ARG
2	B	131	ARG
2	B	141	LEU
2	B	179	THR
2	B	221	MET

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Mol	Chain	Res	Type
2	B	234	TYR
2	B	241	ASP
2	C	29	ASP
2	C	31	ASP
2	C	43	ASP
2	C	76	LEU
2	C	97	PHE
2	C	108	ARG
2	C	131	ARG
2	C	133	VAL
2	C	221	MET
2	C	234	TYR
2	C	241	ASP
2	C	278	ASN
2	C	297	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	283	HIS
1	E	283	HIS
1	E	304	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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	D	303/324 (93%)	-0.08	2 (0%) 89 75	90, 129, 173, 200	0
1	E	317/324 (97%)	0.05	7 (2%) 65 40	80, 128, 169, 210	0
2	A	273/301 (90%)	-0.28	1 (0%) 93 84	71, 103, 144, 177	0
2	B	273/301 (90%)	-0.25	0 100 100	66, 101, 146, 176	0
2	C	273/301 (90%)	-0.22	1 (0%) 93 84	73, 106, 147, 177	0
All	All	1439/1551 (92%)	-0.15	11 (0%) 87 72	66, 114, 163, 210	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	186	ARG	4.0
1	D	306	ARG	3.0
1	E	289	ILE	2.5
1	E	108	LEU	2.4
1	E	290	GLN	2.3
1	D	299	ASP	2.3
2	A	276	PRO	2.2
1	E	187	LEU	2.2
2	C	145	LEU	2.1
1	E	190	LEU	2.1
1	E	175	CYS	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.