



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 02:56 AM UTC

PDB ID : 8GME / pdb_00008gme
Title : Crystal structure of the gp32-Dda-dT17 complex
Authors : He, X.; Yun, M.K.; White, S.W.
Deposited on : 2023-03-24
Resolution : 4.98 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

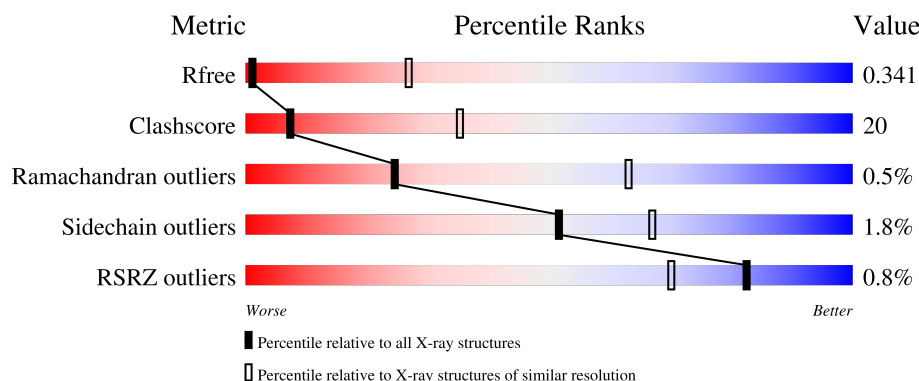
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.98 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}	180053	1047 (6.00-3.96)
Clashscore	190562	1007 (5.96-4.00)
Ramachandran outliers	187476	1014 (6.02-3.92)
Sidechain outliers	187428	1133 (6.06-3.90)
RSRZ outliers	180081	1042 (6.00-3.96)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	301	50% 31% 18%
1	B	301	% 40% 37% • 22%
2	C	459	54% 39% • •
2	D	459	% 47% 40% • 12%
3	P	17	29% 35% 35%

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Mol	Chain	Length	Quality of chain
3	Q	17	18% 35% 47%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10967 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 gp32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	246	Total	C	N	O	S	0	0	0
			1939	1228	317	384	10			
1	B	235	Total	C	N	O	S	0	0	0
			1870	1190	306	366	8			

- Molecule 2 is a protein called Dda helicase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	439	Total	C	N	O	S	0	0	0
			3506	2267	574	653	12			
2	D	406	Total	C	N	O	S	0	0	0
			3250	2099	539	601	11			

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-19	MET	-	initiating methionine	UNP A0A6B9WEE3
C	-18	GLY	-	expression tag	UNP A0A6B9WEE3
C	-17	SER	-	expression tag	UNP A0A6B9WEE3
C	-16	SER	-	expression tag	UNP A0A6B9WEE3
C	-15	HIS	-	expression tag	UNP A0A6B9WEE3
C	-14	HIS	-	expression tag	UNP A0A6B9WEE3
C	-13	HIS	-	expression tag	UNP A0A6B9WEE3
C	-12	HIS	-	expression tag	UNP A0A6B9WEE3
C	-11	HIS	-	expression tag	UNP A0A6B9WEE3
C	-10	HIS	-	expression tag	UNP A0A6B9WEE3
C	-9	SER	-	expression tag	UNP A0A6B9WEE3
C	-8	SER	-	expression tag	UNP A0A6B9WEE3
C	-7	GLY	-	expression tag	UNP A0A6B9WEE3
C	-6	LEU	-	expression tag	UNP A0A6B9WEE3
C	-5	VAL	-	expression tag	UNP A0A6B9WEE3
C	-4	PRO	-	expression tag	UNP A0A6B9WEE3

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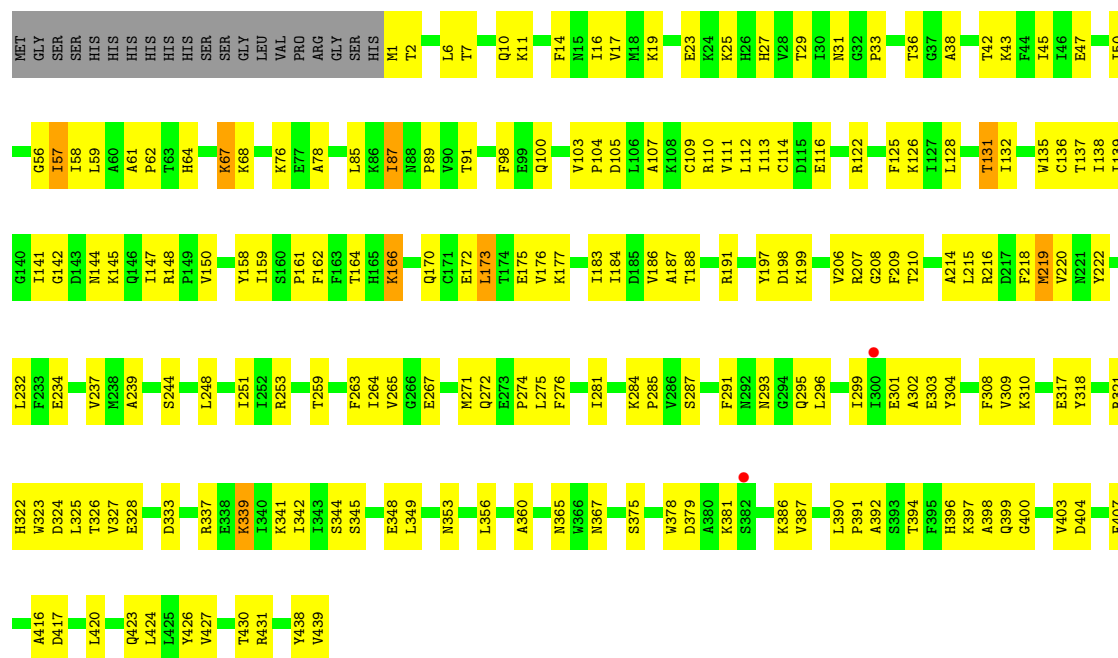
Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	ARG	-	expression tag	UNP A0A6B9WEE3
C	-2	GLY	-	expression tag	UNP A0A6B9WEE3
C	-1	SER	-	expression tag	UNP A0A6B9WEE3
C	0	HIS	-	expression tag	UNP A0A6B9WEE3
C	38	ALA	LYS	conflict	UNP A0A6B9WEE3
C	276	PHE	ILE	conflict	UNP A0A6B9WEE3
C	418	VAL	ALA	conflict	UNP A0A6B9WEE3
D	-19	MET	-	initiating methionine	UNP A0A6B9WEE3
D	-18	GLY	-	expression tag	UNP A0A6B9WEE3
D	-17	SER	-	expression tag	UNP A0A6B9WEE3
D	-16	SER	-	expression tag	UNP A0A6B9WEE3
D	-15	HIS	-	expression tag	UNP A0A6B9WEE3
D	-14	HIS	-	expression tag	UNP A0A6B9WEE3
D	-13	HIS	-	expression tag	UNP A0A6B9WEE3
D	-12	HIS	-	expression tag	UNP A0A6B9WEE3
D	-11	HIS	-	expression tag	UNP A0A6B9WEE3
D	-10	HIS	-	expression tag	UNP A0A6B9WEE3
D	-9	SER	-	expression tag	UNP A0A6B9WEE3
D	-8	SER	-	expression tag	UNP A0A6B9WEE3
D	-7	GLY	-	expression tag	UNP A0A6B9WEE3
D	-6	LEU	-	expression tag	UNP A0A6B9WEE3
D	-5	VAL	-	expression tag	UNP A0A6B9WEE3
D	-4	PRO	-	expression tag	UNP A0A6B9WEE3
D	-3	ARG	-	expression tag	UNP A0A6B9WEE3
D	-2	GLY	-	expression tag	UNP A0A6B9WEE3
D	-1	SER	-	expression tag	UNP A0A6B9WEE3
D	0	HIS	-	expression tag	UNP A0A6B9WEE3
D	38	ALA	LYS	conflict	UNP A0A6B9WEE3
D	276	PHE	ILE	conflict	UNP A0A6B9WEE3
D	418	VAL	ALA	conflict	UNP A0A6B9WEE3

- Molecule 3 is a DNA chain called dT17.

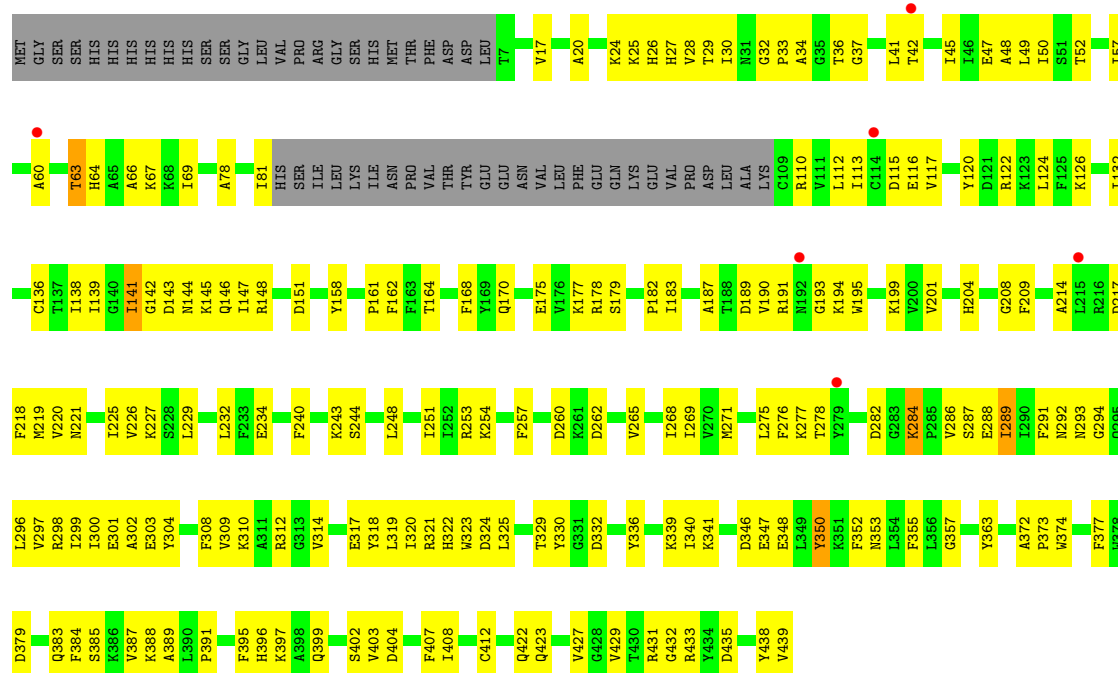
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	P	11	Total	C	N	O	P	0	0	0
			220	110	22	77	11			
3	Q	9	Total	C	N	O	P	0	0	0
			180	90	18	63	9			

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	Zn 1	0	0
4	B	1	Total 1	Zn 1	0	0



• Molecule 2: Dda helicase



• Molecule 3: dT17



● Molecule 3: dT17

Chain Q:  18% 35% 47%

T599	T600	T601	T602	T605	T606	T607	DT	DT	DT	DT	DT	DT	DT	DT
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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	109.86Å 114.35Å 147.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.56 – 4.98 29.56 – 4.98	Depositor EDS
% Data completeness (in resolution range)	96.9 (29.56-4.98) 96.3 (29.56-4.98)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.43 (at 5.05Å)	Xtriage
Refinement program	PHENIX 1.14 _3260	Depositor
R, R_{free}	0.286 , 0.313 0.321 , 0.341	Depositor DCC
R_{free} test set	7815 reflections (94.93%)	wwPDB-VP
Wilson B-factor (Å ²)	149.3	Xtriage
Anisotropy	0.428	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.22 , 162.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.23$, $\langle L^2 \rangle = 0.09$	Xtriage
Estimated twinning fraction	0.229 for k,h,-l	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	10967	wwPDB-VP
Average B, all atoms (Å ²)	200.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.19% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0.23	0/1980	0.50	0/2671
1	B	0.21	0/1910	0.49	0/2574
2	C	0.18	0/3586	0.48	0/4853
2	D	0.18	0/3323	0.48	0/4491
3	P	0.24	0/241	0.55	0/370
3	Q	0.25	0/197	0.55	0/302
All	All	0.20	0/11237	0.49	0/15261

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	1939	0	1871	70	0
1	B	1870	0	1805	94	0
2	C	3506	0	3516	150	0
2	D	3250	0	3269	139	0
3	P	220	0	133	9	0
3	Q	180	0	109	5	0
4	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	1	0	0	0	0
All	All	10967	0	10703	444	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 20.

All (444) 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)
2:C:399:GLN:HG2	2:C:427:VAL:HG11	1.50	0.94
2:D:276:PHE:HB3	2:D:287:SER:HB3	1.50	0.92
2:C:31:ASN:HB3	2:C:172:GLU:HG2	1.61	0.82
2:D:20:ALA:HB1	2:D:26:HIS:HB3	1.61	0.80
2:C:112:LEU:HB3	2:C:138:ILE:HA	1.64	0.79
1:B:140:GLY:H	1:B:143:ILE:HD12	1.49	0.78
2:D:34:ALA:HB1	2:D:177:LYS:HB2	1.64	0.77
1:A:134:VAL:HB	1:A:212:GLN:HB3	1.67	0.77
1:B:50:SER:HA	1:B:57:PRO:HA	1.68	0.76
2:D:145:LYS:HG3	2:D:191:ARG:HG3	1.65	0.75
1:A:61:LEU:HB3	1:A:114:SER:HB2	1.68	0.75
1:A:77:CYS:SG	1:A:79:SER:OG	2.43	0.75
2:C:6:LEU:H	2:C:11:LYS:HE3	1.49	0.75
1:B:39:GLY:HA3	1:B:179:GLN:HG2	1.70	0.74
2:D:234:GLU:HB3	2:D:404:ASP:HB2	1.71	0.72
2:C:198:ASP:HB2	2:C:207:ARG:HA	1.72	0.71
2:D:340:ILE:HD12	2:D:385:SER:HB2	1.72	0.71
2:C:62:PRO:HG3	2:C:116:GLU:HB2	1.71	0.71
2:C:234:GLU:HB3	2:C:404:ASP:HB2	1.71	0.71
2:C:367:ASN:ND2	1:B:193:ASN:OD1	2.25	0.70
2:C:29:THR:HG21	2:C:162:PHE:HB3	1.73	0.69
2:D:116:GLU:OE1	2:D:146:GLN:NE2	2.25	0.69
1:A:120:LEU:HD22	1:A:209:LEU:HD21	1.75	0.68
2:D:271:MET:HA	2:D:387:VAL:HG12	1.74	0.68
2:C:239:ALA:O	2:C:394:THR:HA	1.94	0.68
1:A:45:ILE:HG22	1:A:121:VAL:HA	1.77	0.67
2:D:17:VAL:HG22	2:D:28:VAL:HG11	1.76	0.67
2:C:112:LEU:N	2:C:137:THR:O	2.26	0.67
1:A:33:LEU:HD21	1:A:41:GLY:HA3	1.77	0.67
2:C:61:ALA:HB3	2:C:67:LYS:HB2	1.77	0.66
1:B:77:CYS:SG	1:B:111:ARG:NH2	2.69	0.66
2:C:150:VAL:HG11	3:P:603:DT:C4	2.31	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:85:ASP:OD1	1:B:91:GLN:NE2	2.29	0.66
2:C:148:ARG:NH2	2:C:417:ASP:OD2	2.29	0.65
2:C:27:HIS:HB3	2:C:138:ILE:HB	1.79	0.65
1:A:46:ARG:HD2	1:A:47:PHE:H	1.62	0.65
1:B:148:ASN:HA	1:B:151:ILE:HG12	1.78	0.65
2:C:323:TRP:HB3	2:C:325:LEU:HD13	1.79	0.64
1:B:265:PHE:HD1	2:D:251:ILE:HD11	1.61	0.64
2:D:299:ILE:HG21	2:D:302:ALA:HB2	1.78	0.64
1:B:58:PHE:HZ	1:B:165:THR:HG21	1.63	0.64
2:C:232:LEU:H	2:C:232:LEU:HD23	1.62	0.64
2:C:122:ARG:NH2	2:C:159:ILE:O	2.31	0.64
1:B:46:ARG:HD2	1:B:47:PHE:H	1.63	0.63
2:D:168:PHE:O	2:D:170:GLN:NE2	2.31	0.63
2:C:265:VAL:HG22	2:C:302:ALA:HB3	1.79	0.63
2:C:326:THR:HA	2:C:339:LYS:HA	1.81	0.63
2:C:275:LEU:HB3	2:C:291:PHE:H	1.63	0.63
1:B:87:CYS:HB3	1:B:90:CYS:HB2	1.81	0.63
2:D:64:HIS:HA	2:D:67:LYS:HB3	1.81	0.63
1:A:34:LYS:HB3	1:A:126:ALA:HB1	1.80	0.62
1:A:119:ILE:O	1:A:134:VAL:HA	1.98	0.62
2:C:103:VAL:HG13	2:C:131:THR:HA	1.81	0.62
1:B:34:LYS:HB3	1:B:126:ALA:HB1	1.81	0.62
2:C:397:LYS:HE2	3:P:603:DT:H5"	1.82	0.61
1:B:64:HIS:HA	1:B:111:ARG:HA	1.82	0.61
1:A:224:LYS:H	1:A:224:LYS:HD2	1.65	0.61
1:B:42:GLN:HE21	1:B:125:PRO:HG2	1.65	0.61
2:D:116:GLU:N	2:D:141:ILE:O	2.34	0.61
2:D:348:GLU:O	2:D:352:PHE:N	2.34	0.61
1:A:207:LYS:HA	1:A:210:PHE:HB3	1.82	0.61
2:D:151:ASP:HB2	2:D:158:TYR:HE2	1.65	0.60
2:D:63:THR:O	2:D:67:LYS:N	2.33	0.60
2:D:33:PRO:HB2	2:D:37:GLY:HA3	1.84	0.60
2:C:234:GLU:HA	2:C:403:VAL:HB	1.84	0.60
1:B:177:VAL:HG13	1:B:184:SER:HB3	1.84	0.60
1:A:46:ARG:O	1:A:120:LEU:N	2.30	0.59
2:C:31:ASN:OD1	2:C:144:ASN:N	2.24	0.59
2:C:328:GLU:OE1	2:C:337:ARG:NH2	2.36	0.59
1:B:44:VAL:HG22	1:B:174:VAL:HG22	1.84	0.59
1:A:116:TRP:HA	1:A:137:TYR:O	2.03	0.59
1:B:53:ASP:O	1:B:55:GLN:N	2.33	0.59
2:D:329:THR:OG1	2:D:336:TYR:N	2.28	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:SER:HB3	1:A:138:ARG:HG3	1.83	0.59
2:C:199:LYS:H	2:C:206:VAL:HB	1.67	0.59
1:B:249:ALA:O	1:B:253:LYS:HG3	2.03	0.59
2:D:66:ALA:HA	2:D:69:ILE:HG22	1.85	0.58
2:D:218:PHE:CG	2:D:439:VAL:HB	2.38	0.58
2:C:323:TRP:NE1	2:C:344:SER:HB2	2.19	0.58
1:A:157:MET:O	1:A:159:GLU:N	2.36	0.58
2:C:198:ASP:OD1	2:C:198:ASP:O	2.21	0.58
2:D:395:PHE:HZ	2:D:408:ILE:HG23	1.69	0.58
1:A:93:ILE:O	1:A:97:ASP:N	2.37	0.58
2:C:47:GLU:O	2:C:50:ILE:HG12	2.04	0.58
1:B:114:SER:HB3	1:B:138:ARG:HG3	1.85	0.58
3:Q:599:DT:H2''	3:Q:600:DT:H5''	1.84	0.58
2:C:16:ILE:HA	2:C:19:LYS:HD2	1.85	0.58
2:C:215:LEU:O	2:C:219:MET:N	2.36	0.58
2:D:30:ILE:HB	2:D:141:ILE:HA	1.85	0.57
2:D:304:TYR:CE2	2:D:321:ARG:HB3	2.39	0.57
2:D:310:LYS:HD3	2:D:317:GLU:HG2	1.86	0.57
1:A:177:VAL:HG22	1:A:186:TYR:HD1	1.68	0.57
1:A:116:TRP:CE2	1:A:138:ARG:HB2	2.39	0.57
2:C:367:ASN:ND2	1:B:193:ASN:H	2.01	0.57
2:D:243:LYS:NZ	3:Q:601:DT:OP2	2.36	0.57
2:C:416:ALA:HB1	2:C:420:LEU:HD23	1.87	0.57
2:D:399:GLN:HG2	2:D:427:VAL:HG11	1.86	0.57
2:D:217:ASP:HA	2:D:220:VAL:HG12	1.84	0.57
2:C:183:ILE:O	2:C:187:ALA:N	2.33	0.57
1:A:71:LYS:HE3	1:A:238:VAL:HA	1.87	0.57
2:C:396:HIS:HA	2:C:399:GLN:HE21	1.69	0.57
2:D:41:LEU:O	2:D:45:ILE:HG23	2.05	0.57
2:D:322:HIS:CE1	2:D:341:LYS:HD3	2.40	0.57
2:C:323:TRP:N	2:C:342:ILE:O	2.24	0.57
1:B:167:PRO:HA	1:B:197:ILE:HD12	1.87	0.56
3:P:602:DT:O2	3:P:603:DT:N3	2.39	0.56
1:B:229:GLU:HA	1:B:232:ASN:HB3	1.86	0.56
1:B:119:ILE:HD13	1:B:137:TYR:HB2	1.87	0.56
1:A:143:ILE:H	1:A:143:ILE:HD12	1.71	0.56
1:B:65:GLY:HA2	1:B:73:TYR:O	2.06	0.56
1:B:200:ILE:HG13	1:B:201:ASP:H	1.71	0.56
2:C:147:ILE:HD11	2:C:424:LEU:HA	1.88	0.56
1:B:224:LYS:H	1:B:224:LYS:HD2	1.71	0.56
2:C:378:TRP:HA	2:C:381:LYS:HB3	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:295:GLN:NE2	2:C:333:ASP:OD2	2.39	0.55
1:A:235:PHE:HA	1:A:238:VAL:HB	1.88	0.55
2:C:349:LEU:O	2:C:353:ASN:ND2	2.40	0.55
1:B:45:ILE:HG22	1:B:121:VAL:HA	1.88	0.55
2:D:339:LYS:HD2	2:D:339:LYS:O	2.07	0.55
2:D:64:HIS:CG	2:D:292:ASN:HB3	2.42	0.55
1:A:44:VAL:HG22	1:A:174:VAL:HG22	1.89	0.55
2:C:367:ASN:ND2	1:B:192:LEU:HB3	2.22	0.55
1:B:234:LYS:HD2	1:B:237:GLN:HE21	1.72	0.54
3:Q:605:DT:H2''	3:Q:606:DT:H5'	1.89	0.54
2:C:322:HIS:CE1	2:C:341:LYS:HD3	2.42	0.54
2:D:115:ASP:HA	2:D:141:ILE:HG23	1.89	0.54
2:C:398:ALA:O	2:C:431:ARG:HD2	2.07	0.54
1:A:206:GLN:O	1:A:210:PHE:N	2.41	0.54
2:C:57:ILE:HG22	2:C:113:ILE:HD13	1.90	0.54
1:B:40:ASN:HA	1:B:177:VAL:O	2.07	0.54
2:D:143:ASP:O	2:D:146:GLN:HB2	2.08	0.54
2:C:38:ALA:HB2	2:C:173:LEU:HD12	1.90	0.54
2:D:183:ILE:HG22	2:D:429:VAL:HG13	1.89	0.54
2:D:209:PHE:HB2	2:D:439:VAL:HG23	1.90	0.54
2:C:339:LYS:HD3	2:C:339:LYS:N	2.23	0.53
2:C:375:SER:O	2:C:379:ASP:HB2	2.09	0.53
1:B:43:ALA:HB3	1:B:175:LEU:HD12	1.91	0.53
2:D:187:ALA:HB2	2:D:429:VAL:HG11	1.91	0.53
2:D:271:MET:HB2	2:D:294:GLY:H	1.73	0.52
1:A:137:TYR:HE2	1:A:139:PHE:HB3	1.74	0.52
1:A:209:LEU:HD12	1:A:212:GLN:NE2	2.25	0.52
2:C:394:THR:O	2:C:398:ALA:N	2.41	0.52
1:B:46:ARG:NH2	1:B:166:CYS:O	2.26	0.52
2:C:232:LEU:HD21	2:C:390:LEU:HD23	1.90	0.52
2:D:143:ASP:HB3	2:D:146:GLN:HG3	1.92	0.52
1:A:268:ASP:OD2	2:C:216:ARG:NH1	2.32	0.52
2:C:244:SER:O	2:C:248:LEU:HG	2.09	0.52
1:B:63:ASN:HB2	1:B:75:GLU:O	2.10	0.52
1:A:70:GLY:HA3	3:P:600:DT:C6	2.45	0.52
1:A:163:ASP:O	1:A:170:GLY:HA2	2.10	0.52
2:C:107:ALA:HA	2:C:135:TRP:CZ2	2.45	0.52
2:C:308:PHE:HB3	2:C:317:GLU:HB2	1.92	0.52
1:B:46:ARG:HD3	1:B:172:ASN:OD1	2.10	0.52
2:D:276:PHE:CZ	2:D:289:ILE:HG23	2.45	0.52
2:C:209:PHE:HB2	2:C:439:VAL:HG23	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:78:SER:OG	1:B:83:ASP:O	2.23	0.52
1:B:73:TYR:HD2	1:B:238:VAL:HG21	1.75	0.51
2:D:64:HIS:HB2	2:D:293:ASN:O	2.10	0.51
2:C:29:THR:O	2:C:170:GLN:HB2	2.10	0.51
2:C:43:LYS:O	2:C:47:GLU:HG2	2.11	0.51
1:A:177:VAL:HG22	1:A:186:TYR:CD1	2.45	0.51
2:D:182:PRO:HG2	2:D:204:HIS:O	2.09	0.51
2:D:269:ILE:HG22	2:D:389:ALA:HA	1.92	0.51
2:D:300:ILE:HG22	2:D:301:GLU:HG3	1.93	0.51
1:B:42:GLN:HA	1:B:175:LEU:O	2.10	0.51
2:D:45:ILE:HA	2:D:48:ALA:HB3	1.93	0.51
2:C:184:ILE:O	2:C:188:THR:N	2.39	0.51
2:D:145:LYS:HG3	2:D:191:ARG:CG	2.36	0.51
1:A:71:LYS:HB2	1:A:238:VAL:HG13	1.93	0.51
1:B:97:ASP:HB3	1:B:100:ASN:OD1	2.10	0.51
1:A:137:TYR:CE2	1:A:139:PHE:HB3	2.46	0.51
2:D:24:LYS:HG2	2:D:25:LYS:H	1.74	0.50
2:D:265:VAL:HG22	2:D:302:ALA:HB3	1.94	0.50
1:A:99:TYR:HD1	1:A:106:TYR:CE2	2.29	0.50
2:C:59:LEU:HD11	2:C:76:LYS:HD3	1.93	0.50
2:D:253:ARG:NH1	2:D:262:ASP:O	2.35	0.50
2:C:19:LYS:O	2:C:23:GLU:N	2.30	0.50
2:C:274:PRO:HD3	2:C:293:ASN:HB2	1.92	0.50
2:D:148:ARG:HD2	2:D:158:TYR:HB3	1.92	0.50
2:C:303:GLU:O	2:C:324:ASP:N	2.41	0.50
2:C:367:ASN:HB3	1:B:192:LEU:HD22	1.93	0.50
1:B:93:ILE:HG23	1:B:98:LEU:HB2	1.93	0.50
2:D:120:TYR:CE2	2:D:124:LEU:HB3	2.45	0.50
1:B:266:ASN:HB3	2:D:254:LYS:HD2	1.93	0.50
2:D:277:LYS:O	2:D:288:GLU:HG3	2.11	0.50
2:D:312:ARG:O	2:D:363:TYR:OH	2.30	0.50
2:D:332:ASP:OD1	2:D:332:ASP:N	2.40	0.50
1:A:242:ALA:HA	1:A:249:ALA:HB2	1.94	0.50
2:D:120:TYR:CZ	2:D:124:LEU:HB3	2.47	0.50
2:C:293:ASN:HD22	3:P:605:DT:P	2.34	0.49
2:D:404:ASP:O	2:D:435:ASP:N	2.33	0.49
1:A:118:ASN:HD21	1:A:214:VAL:HG22	1.77	0.49
1:B:63:ASN:ND2	1:B:112:LYS:O	2.45	0.49
1:B:63:ASN:O	1:B:112:LYS:N	2.45	0.49
1:A:218:GLU:CD	1:B:85:ASP:HB2	2.37	0.49
1:B:221:SER:OG	1:B:222:LYS:N	2.34	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:175:GLU:OE1	2:D:178:ARG:N	2.44	0.49
2:C:309:VAL:O	2:C:318:TYR:N	2.44	0.49
2:D:309:VAL:O	2:D:318:TYR:N	2.41	0.49
2:C:218:PHE:O	2:C:222:TYR:N	2.42	0.49
1:B:65:GLY:HA2	1:B:74:ILE:HG12	1.94	0.49
1:B:166:CYS:HB3	1:B:170:GLY:N	2.28	0.49
2:C:304:TYR:HE1	2:C:321:ARG:HB3	1.78	0.49
2:D:27:HIS:O	2:D:168:PHE:HA	2.13	0.49
2:D:353:ASN:O	2:D:357:GLY:N	2.44	0.49
1:A:96:ASN:O	1:A:101:THR:OG1	2.21	0.49
2:D:117:VAL:HG22	2:D:142:GLY:HA3	1.95	0.49
1:B:33:LEU:HD23	1:B:35:LEU:HD23	1.94	0.49
1:B:88:PRO:HB2	1:B:235:PHE:CD2	2.47	0.49
1:B:173:PHE:HE2	1:B:175:LEU:HD23	1.78	0.49
2:C:175:GLU:O	2:C:177:LYS:N	2.46	0.48
2:D:32:GLY:H	2:D:143:ASP:HA	1.78	0.48
2:D:124:LEU:HG	3:Q:605:DT:H3	1.77	0.48
2:D:282:ASP:HB2	2:D:284:LYS:HE3	1.95	0.48
1:B:172:ASN:OD1	1:B:172:ASN:N	2.46	0.48
2:D:218:PHE:CZ	2:D:407:PHE:HD2	2.31	0.48
2:D:182:PRO:HB3	2:D:199:LYS:HG2	1.94	0.48
1:A:170:GLY:O	1:A:195:SER:N	2.46	0.48
2:D:48:ALA:O	2:D:52:THR:HG23	2.13	0.48
1:A:164:VAL:HA	1:A:171:ALA:H	1.78	0.48
2:D:396:HIS:O	2:D:399:GLN:HG3	2.14	0.48
1:B:122:VAL:HG21	1:B:172:ASN:HD22	1.79	0.48
2:D:304:TYR:HD1	2:D:323:TRP:CD1	2.31	0.48
2:D:187:ALA:HA	2:D:190:VAL:HB	1.94	0.48
2:C:210:THR:C	2:C:214:ALA:HB2	2.39	0.48
2:C:299:ILE:HA	2:C:327:VAL:HG23	1.95	0.48
1:B:90:CYS:SG	1:B:111:ARG:NH2	2.87	0.48
2:D:189:ASP:HB3	2:D:194:LYS:HD2	1.96	0.48
1:A:249:ALA:O	1:A:253:LYS:HG2	2.14	0.48
2:C:184:ILE:HA	2:C:187:ALA:HB3	1.95	0.48
2:C:7:THR:HG23	2:C:10:GLN:H	1.79	0.48
2:C:67:LYS:HG3	2:C:78:ALA:HB3	1.95	0.48
2:C:114:CYS:O	2:C:141:ILE:HG22	2.14	0.48
1:B:30:GLU:HB2	1:B:136:LYS:HE2	1.96	0.48
2:D:45:ILE:O	2:D:49:LEU:N	2.39	0.48
2:D:177:LYS:HE2	2:D:179:SER:HB3	1.96	0.48
1:A:30:GLU:HG3	1:A:137:TYR:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:128:LEU:HG	2:C:132:ILE:HD13	1.96	0.47
2:C:431:ARG:HA	2:C:431:ARG:HD3	1.72	0.47
1:B:142:LYS:HE3	1:B:142:LYS:HB3	1.75	0.47
2:D:113:ILE:HG13	2:D:139:ILE:HB	1.96	0.47
2:D:132:ILE:HG12	2:D:138:ILE:HD11	1.96	0.47
2:C:42:THR:O	2:C:45:ILE:HG12	2.14	0.47
1:A:218:GLU:HG3	1:B:85:ASP:OD1	2.15	0.47
1:A:237:GLN:HA	2:C:417:ASP:CB	2.45	0.47
2:C:208:GLY:HA2	2:C:438:TYR:O	2.15	0.47
2:C:232:LEU:HD12	2:C:391:PRO:HA	1.96	0.47
1:B:173:PHE:HB2	1:B:191:PHE:CZ	2.50	0.47
1:B:248:ALA:HB2	2:D:195:TRP:CD2	2.50	0.47
2:D:110:ARG:O	2:D:136:CYS:HA	2.15	0.47
2:D:193:GLY:O	2:D:422:GLN:NE2	2.48	0.47
2:D:240:PHE:HB3	2:D:412:CYS:SG	2.54	0.47
2:D:296:LEU:O	2:D:330:TYR:HB3	2.15	0.47
1:A:122:VAL:HG21	1:A:172:ASN:HD22	1.78	0.47
1:B:180:VAL:HB	1:B:185:ASN:HB2	1.95	0.47
2:D:232:LEU:HD23	2:D:232:LEU:H	1.80	0.47
1:A:66:PHE:CE1	1:A:109:VAL:HG13	2.49	0.47
2:C:122:ARG:NH1	2:C:161:PRO:HG3	2.29	0.47
2:D:234:GLU:HA	2:D:403:VAL:HB	1.97	0.47
1:A:66:PHE:CD1	1:A:109:VAL:HG13	2.50	0.47
1:B:202:ASP:HB3	1:B:205:PHE:HB3	1.97	0.47
2:C:272:GLN:HG2	2:C:387:VAL:HA	1.96	0.46
1:B:44:VAL:HB	1:B:123:LYS:HB2	1.97	0.46
1:B:58:PHE:HB3	1:B:116:TRP:O	2.15	0.46
2:D:209:PHE:CE1	2:D:218:PHE:HD1	2.33	0.46
2:D:234:GLU:HB3	2:D:404:ASP:CB	2.43	0.46
2:C:367:ASN:OD1	1:B:193:ASN:HB3	2.15	0.46
3:P:602:DT:H1'	3:P:603:DT:C4	2.49	0.46
2:C:323:TRP:HE1	2:C:344:SER:HB2	1.80	0.46
1:B:228:PHE:O	1:B:232:ASN:N	2.38	0.46
2:D:308:PHE:HA	2:D:319:LEU:HA	1.97	0.46
1:A:62:VAL:HB	1:A:80:THR:OG1	2.16	0.46
2:D:209:PHE:HB3	2:D:214:ALA:HB1	1.95	0.46
2:D:227:LYS:HD3	2:D:227:LYS:HA	1.78	0.46
2:D:268:ILE:HG13	2:D:298:ARG:HB2	1.97	0.46
2:C:271:MET:HA	2:C:387:VAL:HG12	1.96	0.46
1:B:30:GLU:HG2	1:B:136:LYS:O	2.15	0.46
1:B:47:PHE:HB2	1:B:165:THR:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:146:LYS:O	1:B:150:MET:HG2	2.15	0.46
1:A:116:TRP:CZ2	1:A:138:ARG:HB2	2.50	0.46
2:C:91:THR:HG23	2:C:378:TRP:HZ2	1.79	0.46
2:C:145:LYS:C	2:C:423:GLN:HG2	2.41	0.46
2:C:301:GLU:N	2:C:326:THR:OG1	2.49	0.46
1:B:58:PHE:CZ	1:B:165:THR:HG21	2.48	0.46
2:C:64:HIS:HB3	2:C:68:LYS:HE3	1.96	0.46
2:C:105:ASP:OD1	2:C:105:ASP:N	2.36	0.46
2:C:148:ARG:HH22	2:C:417:ASP:CG	2.24	0.46
2:C:125:PHE:CZ	2:C:161:PRO:HB2	2.51	0.46
2:D:260:ASP:OD1	2:D:260:ASP:N	2.49	0.46
2:C:110:ARG:C	2:C:136:CYS:HA	2.41	0.45
1:B:247:ALA:O	1:B:250:THR:OG1	2.26	0.45
2:C:259:THR:HG21	2:C:264:ILE:HD12	1.97	0.45
2:D:115:ASP:OD1	2:D:116:GLU:N	2.49	0.45
1:A:235:PHE:CZ	1:A:239:MET:HE2	2.52	0.45
1:A:35:LEU:HB3	1:A:39:GLY:HA2	1.97	0.45
2:C:85:LEU:O	2:C:100:GLN:HG3	2.15	0.45
2:C:400:GLY:H	2:C:431:ARG:CZ	2.30	0.45
2:D:278:THR:HA	2:D:286:VAL:O	2.16	0.45
1:A:69:ASN:C	1:A:71:LYS:H	2.24	0.45
2:D:291:PHE:CZ	2:D:336:TYR:HB2	2.52	0.45
2:C:56:GLY:HA3	2:C:110:ARG:H	1.81	0.45
1:B:31:TRP:HB3	1:B:119:ILE:HD11	1.97	0.45
1:A:71:LYS:HG3	1:A:238:VAL:O	2.16	0.45
1:B:210:PHE:HA	1:B:213:MET:HG3	1.98	0.45
2:D:144:ASN:OD1	2:D:145:LYS:N	2.49	0.45
1:A:230:GLU:O	1:A:233:THR:OG1	2.29	0.45
1:B:142:LYS:O	1:B:146:LYS:HG3	2.17	0.45
1:B:200:ILE:HG13	1:B:201:ASP:N	2.32	0.45
2:D:296:LEU:HD12	2:D:296:LEU:H	1.82	0.45
2:C:296:LEU:HD12	2:C:296:LEU:H	1.82	0.45
2:C:122:ARG:HH21	2:C:158:TYR:HA	1.81	0.44
2:C:323:TRP:CD1	2:C:344:SER:HB2	2.52	0.44
2:C:166:LYS:H	2:C:166:LYS:HG2	1.62	0.44
2:C:367:ASN:HD22	1:B:192:LEU:HB3	1.81	0.44
1:B:116:TRP:CZ2	1:B:138:ARG:HB2	2.52	0.44
2:D:42:THR:O	2:D:45:ILE:HG12	2.16	0.44
2:D:347:GLU:OE1	2:D:347:GLU:N	2.48	0.44
2:D:304:TYR:HA	2:D:323:TRP:HA	1.98	0.44
1:B:173:PHE:HB2	1:B:191:PHE:CE1	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:596:DT:H2''	3:P:597:DT:OP2	2.16	0.44
2:C:186:VAL:HG22	2:C:197:TYR:CE2	2.53	0.44
2:C:365:ASN:HB2	1:B:192:LEU:C	2.43	0.44
2:C:427:VAL:O	2:C:431:ARG:NE	2.51	0.44
2:D:57:ILE:H	2:D:57:ILE:HD12	1.83	0.44
2:D:244:SER:O	2:D:248:LEU:HG	2.18	0.44
2:C:89:PRO:HA	2:C:98:PHE:HA	1.99	0.44
2:D:187:ALA:O	2:D:191:ARG:N	2.37	0.44
2:D:431:ARG:HA	2:D:431:ARG:HD3	1.64	0.44
2:C:89:PRO:HD3	2:C:98:PHE:CE2	2.53	0.44
2:C:112:LEU:HD23	2:C:138:ILE:HG12	1.99	0.44
2:C:356:LEU:O	2:C:360:ALA:N	2.44	0.44
3:Q:601:DT:H2''	3:Q:602:DT:C6	2.53	0.44
2:C:147:ILE:HD13	2:C:424:LEU:HD23	1.99	0.43
2:C:237:VAL:O	2:C:392:ALA:HA	2.19	0.43
1:B:53:ASP:O	1:B:55:GLN:HG2	2.17	0.43
1:B:85:ASP:HA	1:B:91:GLN:HE21	1.83	0.43
1:A:114:SER:HB3	1:A:138:ARG:CG	2.47	0.43
2:C:1:MET:SD	2:C:2:THR:N	2.92	0.43
2:C:427:VAL:HG13	2:C:431:ARG:HH21	1.83	0.43
2:D:221:ASN:O	2:D:225:ILE:HG12	2.19	0.43
2:D:278:THR:HA	2:D:287:SER:HA	2.01	0.43
1:A:129:GLU:CD	1:A:129:GLU:H	2.26	0.43
2:C:199:LYS:O	2:C:206:VAL:N	2.51	0.43
2:C:345:SER:HB3	2:C:348:GLU:HB2	2.01	0.43
2:C:110:ARG:O	2:C:136:CYS:HA	2.18	0.43
1:B:146:LYS:O	1:B:150:MET:N	2.49	0.43
2:D:112:LEU:O	2:D:138:ILE:HA	2.19	0.43
1:A:235:PHE:HZ	1:A:239:MET:HE2	1.84	0.43
1:B:59:ALA:O	1:B:116:TRP:N	2.48	0.43
2:D:268:ILE:HA	2:D:297:VAL:O	2.19	0.43
1:A:150:MET:HG3	1:A:191:PHE:CD1	2.53	0.43
1:B:44:VAL:HG12	1:B:122:VAL:HB	2.01	0.43
2:D:64:HIS:HD2	2:D:293:ASN:HB3	1.83	0.43
2:D:388:LYS:NZ	2:D:397:LYS:HE3	2.33	0.43
1:A:98:LEU:HD22	1:A:102:ASP:HB3	2.01	0.43
1:A:73:TYR:CZ	1:A:75:GLU:HB2	2.54	0.42
2:C:218:PHE:CD1	2:C:439:VAL:HB	2.54	0.42
1:B:48:LEU:HB2	1:B:118:ASN:HB2	1.99	0.42
1:A:266:ASN:HA	2:C:251:ILE:HD11	2.02	0.42
2:C:29:THR:OG1	2:C:170:GLN:OE1	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:104:PRO:HD2	2:C:131:THR:HG23	2.01	0.42
2:C:263:PHE:HB2	2:C:323:TRP:CZ3	2.54	0.42
2:D:67:LYS:HG3	2:D:78:ALA:O	2.20	0.42
2:D:341:LYS:O	2:D:384:PHE:HA	2.19	0.42
1:A:49:PRO:HB2	1:A:50:SER:H	1.62	0.42
2:C:272:GLN:HB2	2:C:386:LYS:O	2.20	0.42
1:B:81:HIS:CD2	1:B:83:ASP:HB2	2.54	0.42
2:D:303:GLU:O	2:D:324:ASP:N	2.46	0.42
1:B:67:LYS:HB2	1:B:72:TRP:CE2	2.55	0.42
2:D:276:PHE:CB	2:D:287:SER:HB3	2.36	0.42
1:A:66:PHE:HB3	1:A:108:LEU:O	2.20	0.42
2:C:161:PRO:HA	2:C:164:THR:HG23	2.01	0.42
2:C:216:ARG:O	2:C:220:VAL:HG23	2.20	0.42
1:A:120:LEU:HD13	1:A:209:LEU:HD11	2.01	0.42
1:A:147:ILE:O	1:A:151:ILE:HG23	2.19	0.42
1:A:219:MET:O	1:A:224:LYS:NZ	2.45	0.42
2:C:112:LEU:O	2:C:139:ILE:N	2.47	0.42
2:D:117:VAL:HB	2:D:162:PHE:CD2	2.54	0.42
2:D:226:VAL:O	2:D:229:LEU:HB2	2.19	0.42
2:D:232:LEU:CD1	2:D:391:PRO:HA	2.50	0.42
2:C:107:ALA:HA	2:C:135:TRP:HZ2	1.83	0.42
2:C:218:PHE:CZ	2:C:407:PHE:HD2	2.37	0.42
1:B:124:ASP:CG	1:B:127:ALA:H	2.28	0.42
1:B:234:LYS:HA	1:B:237:GLN:NE2	2.34	0.42
2:D:402:SER:OG	2:D:433:ARG:HB3	2.20	0.42
2:C:87:ILE:HG22	2:C:98:PHE:C	2.44	0.42
2:C:89:PRO:O	2:C:284:LYS:HE3	2.19	0.42
2:C:126:LYS:H	2:C:126:LYS:HG2	1.51	0.42
2:C:394:THR:HG23	2:C:397:LYS:HD2	2.01	0.42
2:D:42:THR:HA	2:D:45:ILE:HG12	2.02	0.42
2:C:57:ILE:H	2:C:57:ILE:HG13	1.53	0.42
2:C:420:LEU:O	2:C:424:LEU:HG	2.20	0.42
2:D:60:ALA:HB1	2:D:81:ILE:HG23	2.00	0.42
2:D:275:LEU:HG	2:D:385:SER:OG	2.19	0.42
2:D:379:ASP:O	2:D:383:GLN:HB2	2.20	0.42
2:C:58:ILE:HD11	2:C:109:CYS:HB2	2.02	0.41
2:C:253:ARG:HH21	2:C:267:GLU:CD	2.28	0.41
2:D:122:ARG:O	2:D:126:LYS:HG2	2.20	0.41
2:D:314:VAL:HG11	2:D:355:PHE:HE1	1.85	0.41
2:D:403:VAL:O	2:D:432:GLY:HA2	2.20	0.41
2:C:276:PHE:HD2	2:C:287:SER:HB2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:304:TYR:CD1	2:D:323:TRP:CD1	3.08	0.41
2:C:145:LYS:HE3	2:C:191:ARG:HG3	2.02	0.41
2:C:304:TYR:CE1	2:C:321:ARG:HB3	2.54	0.41
2:D:29:THR:HG23	2:D:168:PHE:CG	2.55	0.41
2:D:126:LYS:HG2	2:D:126:LYS:H	1.61	0.41
1:A:50:SER:HA	1:A:57:PRO:HA	2.02	0.41
2:C:322:HIS:CE1	2:C:341:LYS:HB3	2.55	0.41
2:C:394:THR:HG21	3:P:603:DT:OP2	2.21	0.41
1:B:69:ASN:C	1:B:71:LYS:H	2.28	0.41
2:D:346:ASP:O	2:D:350:TYR:HB3	2.21	0.41
1:A:173:PHE:HZ	1:A:189:SER:HB3	1.85	0.41
2:D:69:ILE:HD12	2:D:69:ILE:HA	1.92	0.41
2:C:31:ASN:HA	2:C:142:GLY:O	2.20	0.41
1:B:65:GLY:HA3	1:B:112:LYS:HD2	2.01	0.41
1:A:243:VAL:O	1:A:247:ALA:N	2.51	0.41
2:C:14:PHE:HA	2:C:17:VAL:HB	2.02	0.41
2:C:57:ILE:HG23	2:C:111:VAL:HB	2.02	0.41
2:C:426:TYR:O	2:C:430:THR:HG23	2.21	0.41
1:B:216:LEU:O	1:B:220:THR:HG23	2.20	0.41
2:D:36:THR:H	2:D:177:LYS:HD3	1.86	0.41
2:D:372:ALA:HA	2:D:373:PRO:HD3	1.87	0.41
2:C:33:PRO:HD2	2:C:36:THR:HG21	2.03	0.41
2:D:161:PRO:HA	2:D:164:THR:HG1	1.85	0.41
2:C:145:LYS:HG3	2:C:191:ARG:HG3	2.02	0.41
1:A:51:LYS:HG2	1:A:215:ASP:HB2	2.03	0.40
2:C:310:LYS:HB3	2:C:317:GLU:HB3	2.03	0.40
1:B:51:LYS:HE3	1:B:210:PHE:HE1	1.85	0.40
1:B:102:ASP:CG	1:B:105:GLU:H	2.28	0.40
2:D:63:THR:HG1	2:D:66:ALA:H	1.64	0.40
2:D:147:ILE:HG12	2:D:423:GLN:HB3	2.02	0.40
2:D:253:ARG:HG2	2:D:257:PHE:CE2	2.56	0.40
2:D:25:LYS:HZ2	2:D:27:HIS:CE1	2.39	0.40
2:C:284:LYS:HD3	2:C:285:PRO:HD2	2.03	0.40
2:C:430:THR:OG1	2:C:431:ARG:NH2	2.54	0.40
1:A:207:LYS:HA	1:A:207:LYS:HD3	1.68	0.40
2:C:150:VAL:HG11	3:P:603:DT:C5	2.56	0.40
1:B:115:TYR:OH	1:B:141:LYS:HB3	2.21	0.40
2:D:47:GLU:O	2:D:50:ILE:HG13	2.21	0.40
2:D:208:GLY:HA2	2:D:438:TYR:O	2.22	0.40
1:A:145:ASP:O	1:A:149:ALA:N	2.46	0.40
1:B:34:LYS:HB3	1:B:126:ALA:CB	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:182:PRO:HG3	2:D:201:VAL:HB	2.04	0.40
2:D:374:TRP:HE3	2:D:377:PHE:HB2	1.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	244/301 (81%)	229 (94%)	12 (5%)	3 (1%)	10	42
1	B	229/301 (76%)	212 (93%)	15 (7%)	2 (1%)	14	50
2	C	437/459 (95%)	412 (94%)	24 (6%)	1 (0%)	43	77
2	D	402/459 (88%)	384 (96%)	18 (4%)	0	100	100
All	All	1312/1520 (86%)	1237 (94%)	69 (5%)	6 (0%)	24	63

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	176	VAL
1	A	49	PRO
1	A	221	SER
1	B	49	PRO
1	A	158	GLY
1	B	221	SER

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	211/258 (82%)	209 (99%)	2 (1%)	70	77
1	B	204/258 (79%)	203 (100%)	1 (0%)	81	82
2	C	382/402 (95%)	372 (97%)	10 (3%)	40	61
2	D	353/402 (88%)	345 (98%)	8 (2%)	44	63
All	All	1150/1320 (87%)	1129 (98%)	21 (2%)	51	67

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	175	LEU
1	A	223	ASP
2	C	25	LYS
2	C	57	ILE
2	C	67	LYS
2	C	87	ILE
2	C	131	THR
2	C	166	LYS
2	C	173	LEU
2	C	219	MET
2	C	281	ILE
2	C	339	LYS
1	B	172	ASN
2	D	63	THR
2	D	141	ILE
2	D	219	MET
2	D	284	LYS
2	D	289	ILE
2	D	320	ILE
2	D	325	LEU
2	D	350	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	ASN
1	A	185	ASN
1	A	194	GLN
1	A	212	GLN

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Mol	Chain	Res	Type
1	A	266	ASN
2	C	12	ASN
2	C	100	GLN
2	C	146	GLN
2	C	204	HIS
2	C	295	GLN
2	C	322	HIS
2	C	367	ASN
2	C	383	GLN
2	C	396	HIS
2	C	399	GLN
1	B	42	GLN
1	B	81	HIS
1	B	91	GLN
1	B	193	ASN
1	B	199	ASN
1	B	237	GLN
2	D	64	HIS
2	D	170	GLN
2	D	295	GLN
2	D	399	GLN
2	D	422	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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	246/301 (81%)	-0.26	1 (0%) 88 78	115, 155, 216, 315	0
1	B	235/301 (78%)	-0.28	2 (0%) 81 68	113, 186, 261, 301	0
2	C	439/459 (95%)	-0.21	2 (0%) 87 76	124, 204, 301, 353	0
2	D	406/459 (88%)	-0.11	6 (1%) 72 58	136, 209, 337, 366	0
3	P	11/17 (64%)	-0.01	0 100 100	202, 222, 239, 239	0
3	Q	9/17 (52%)	0.03	0 100 100	176, 194, 231, 234	0
All	All	1346/1554 (86%)	-0.20	11 (0%) 82 70	113, 192, 303, 366	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	114	CYS	4.2
2	D	60	ALA	3.8
1	B	261	ASP	3.7
2	C	382	SER	3.4
2	D	192	ASN	2.7
1	A	161	PRO	2.5
2	D	42	THR	2.4
2	C	300	ILE	2.3
2	D	215	LEU	2.3
1	B	113	THR	2.0
2	D	279	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	ZN	B	500	1/1	0.98	0.06	174,174,174,174	0
4	ZN	A	500	1/1	0.99	0.07	156,156,156,156	0

6.5 Other polymers [i](#)

There are no such residues in this entry.