Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 08:23 PM GMT

PDB ID	:	1K28
Title	:	The Structure of the Bacteriophage T4 Cell-Puncturing Device
Authors	:	Kanamaru, S.; Leiman, P.G.; Kostyuchenko, V.A.; Chipman, P.R.; Mesyanzhinov, V.V.; Arisaka, F.; Rossmann, M.G.
Deposited on	:	2001-09-26
Resolution	:	2.90 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

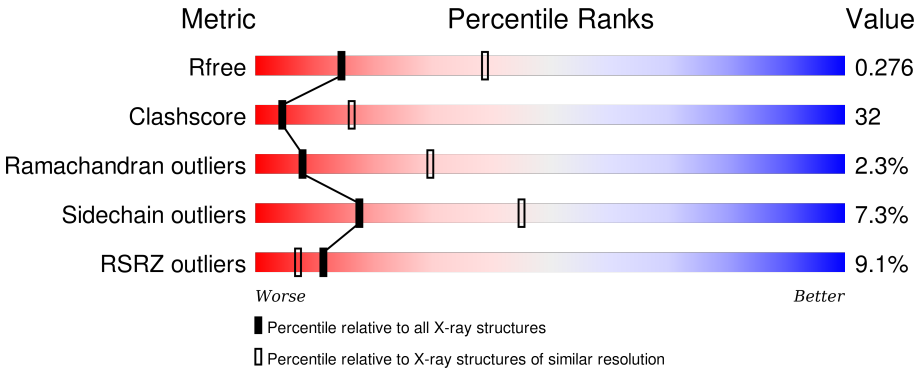
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.90 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	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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	A	584	% 57% 33% 6% 5%
2	D	391	19% 38% 49% 6% 7%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7614 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 TAIL-ASSOCIATED LYSOZYME.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	557	Total	C	N	O	S	0	0	0
			4309	2672	763	853	21			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	576	SER	-	EXPRESSION TAG	UNP P16009
A	577	VAL	-	EXPRESSION TAG	UNP P16009
A	578	ASP	-	EXPRESSION TAG	UNP P16009
A	579	HIS	-	EXPRESSION TAG	UNP P16009
A	580	HIS	-	EXPRESSION TAG	UNP P16009
A	581	HIS	-	EXPRESSION TAG	UNP P16009
A	582	HIS	-	EXPRESSION TAG	UNP P16009
A	583	HIS	-	EXPRESSION TAG	UNP P16009
A	584	HIS	-	EXPRESSION TAG	UNP P16009

- Molecule 2 is a protein called BASEPLATE STRUCTURAL PROTEIN GP27.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	D	364	Total	C	N	O	S	Se	0	0	0
			2912	1858	478	559	2	15			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1	MSE	MET	MODIFIED RESIDUE	UNP P17172
D	3	MSE	MET	MODIFIED RESIDUE	UNP P17172
D	40	MSE	MET	MODIFIED RESIDUE	UNP P17172
D	51	MSE	MET	MODIFIED RESIDUE	UNP P17172
D	64	MSE	MET	MODIFIED RESIDUE	UNP P17172
D	135	MSE	MET	MODIFIED RESIDUE	UNP P17172
D	168	ASN	THR	SEE REMARK 999	UNP P17172

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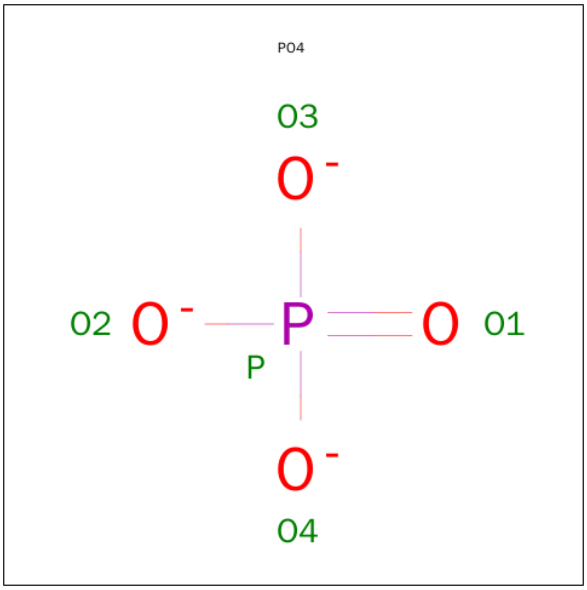
Chain	Residue	Modelled	Actual	Comment	Reference
D	193	MSE	MET	MODIFIED RESIDUE	UNP P17172
D	197	MSE	MET	MODIFIED RESIDUE	UNP P17172
D	198	MSE	MET	MODIFIED RESIDUE	UNP P17172
D	202	MSE	MET	MODIFIED RESIDUE	UNP P17172
D	203	MSE	MET	MODIFIED RESIDUE	UNP P17172
D	211	MSE	MET	MODIFIED RESIDUE	UNP P17172
D	248	MSE	MET	MODIFIED RESIDUE	UNP P17172
D	262	SER	GLU	SEE REMARK 999	UNP P17172
D	265	MSE	MET	MODIFIED RESIDUE	UNP P17172
D	286	MSE	MET	MODIFIED RESIDUE	UNP P17172
D	301	MSE	MET	MODIFIED RESIDUE	UNP P17172
D	308	ALA	LEU	SEE REMARK 999	UNP P17172
D	357	MSE	MET	MODIFIED RESIDUE	UNP P17172

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total K 1 1	0	0

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O P 3 2 1	0	0

- Molecule 5 is water.

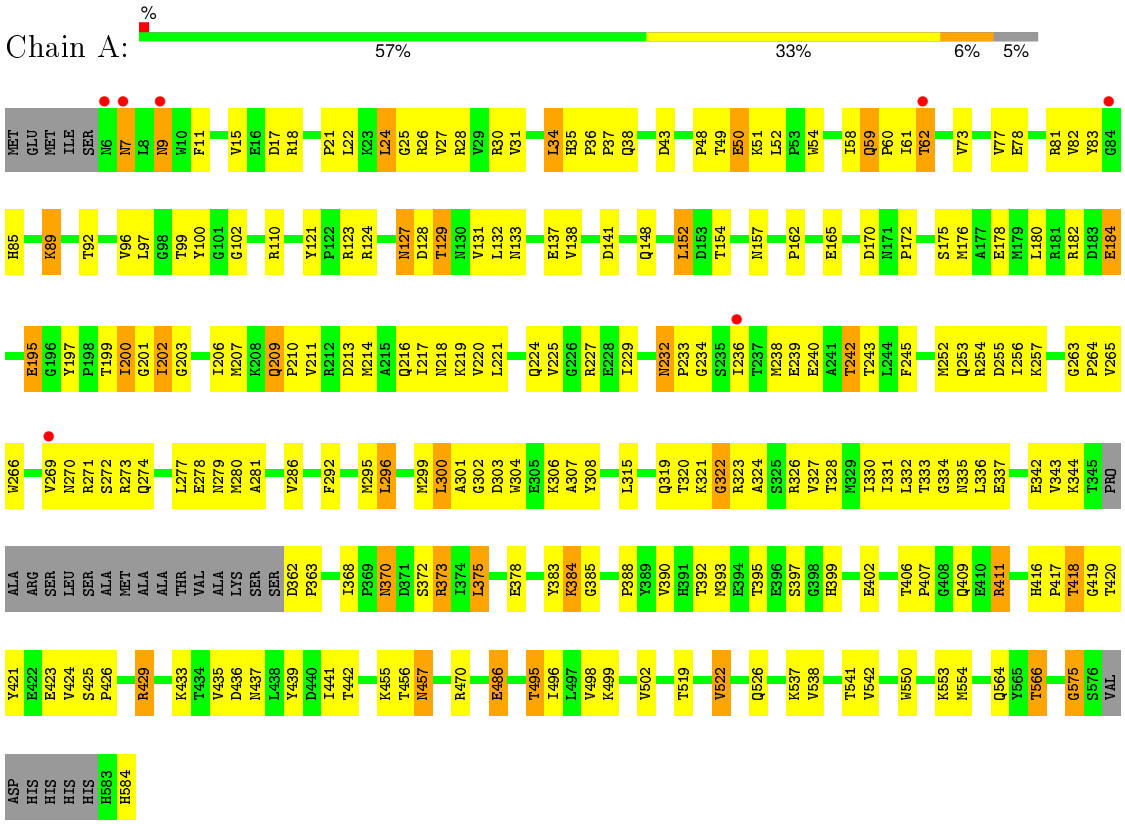
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	307	Total O 307 307	0	0
5	D	82	Total O 82 82	0	0

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.

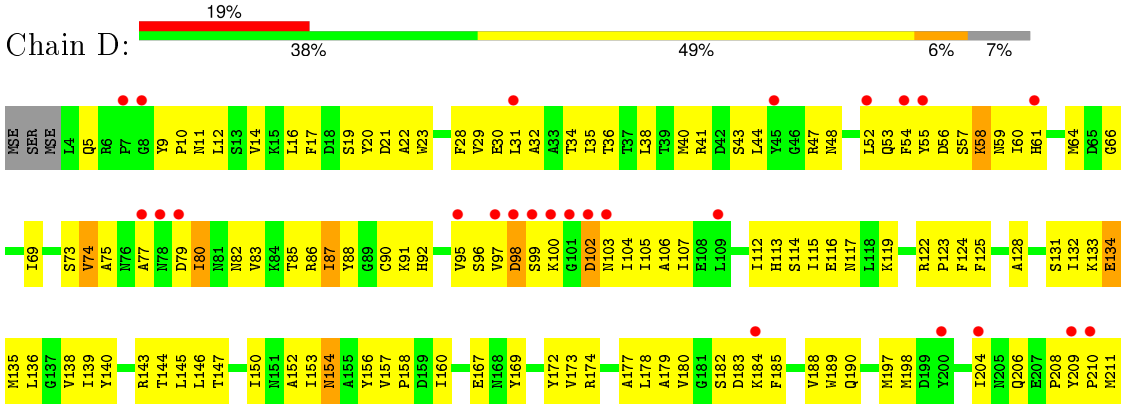
- Molecule 1: TAIL-ASSOCIATED LYSOZYME

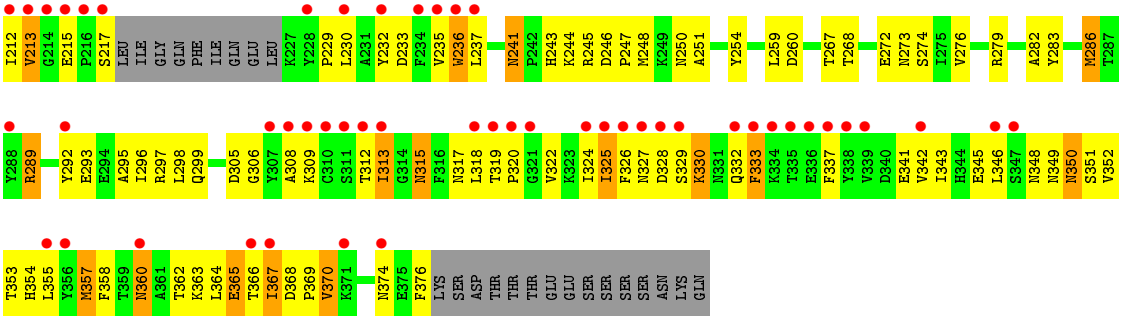
Chain A:



- Molecule 2: BASEPLATE STRUCTURAL PROTEIN GP27

Chain D:




I212 V213 G214 E215 P216 S217 LEU ILE GLY GLN PHE ILE GLN GLU LEU K227 Y228 P229 L230 A231 Y232 D233 F234 V235 W236 L237 N241 P242 H243 K244 R245 D246 P247 N248 K249 N250 A251 Y254 L259 D260 T267 T268 E272 N273 S274 I275 V276 R279 A282 Y283 N286 T287
Y288 R289 Y292 E293 E294 A295 I296 R297 L298 Q299 D305 G306 Y307 A308 K309 G310 S311 T312 I313 G314 N315 F316 N317 L318 T319 P320 G321 V322 K323 I324 I325 F326 N327 D328 S329 K330 N331 Q332 F333 K334 T335 E336 F337 Y338 V339 D340 E341 V342 I343 H344 E345 L346 S347 N348 N349 N350 S351 V352
T353 H354 L355 Y356 M357 F358 T359 N360 A361 T362 K363 L364 E365 T366 I367 D368 P369 V370 K371 N374 E375 F376 LYS SER ASP THR THR THR GLU GLU SER SER SER SER ASN LYS GLN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	139.26Å 139.26Å 382.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.90 49.72 – 2.90	Depositor EDS
% Data completeness (in resolution range)	5.1 (50.00-2.90) 98.9 (49.72-2.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	7.57 (at 2.91Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.211 , 0.280 0.209 , 0.276	Depositor DCC
R_{free} test set	1602 reflections (5.32%)	DCC
Wilson B-factor (Å^2)	52.2	Xtriage
Anisotropy	0.794	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 76.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 31766 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	7614	wwPDB-VP
Average B, all atoms (Å^2)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.73% 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

Bond lengths and bond angles in the following residue types are not validated in this section: K, PO4

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	0.39	0/4391	0.65	1/5950 (0.0%)
2	D	0.33	0/2965	0.59	0/3997
All	All	0.36	0/7356	0.63	1/9947 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	575	GLY	N-CA-C	5.25	126.21	113.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4309	0	4202	237	1
2	D	2912	0	2835	227	0
3	A	1	0	0	0	0
4	A	3	0	0	0	1
5	A	307	0	0	6	0
5	D	82	0	0	5	0
All	All	7614	0	7037	460	2

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 32.

All (460) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:LYS:HE2	1:A:89:LYS:H	1.16	1.10
1:A:184:GLU:HG2	1:A:203:GLY:HA3	1.36	1.03
1:A:89:LYS:CE	1:A:89:LYS:H	1.72	1.03
1:A:416:HIS:CD2	1:A:418:THR:HB	1.95	1.01
1:A:221:LEU:HD11	1:A:236:ILE:HD11	1.40	1.01
1:A:330:ILE:HD12	1:A:336:LEU:HD12	1.43	0.99
1:A:416:HIS:HD2	1:A:418:THR:HB	1.27	0.98
1:A:89:LYS:N	1:A:89:LYS:HE2	1.78	0.97
2:D:330:LYS:HE3	2:D:330:LYS:HA	1.52	0.91
2:D:95:VAL:HA	2:D:105:ILE:HG22	1.54	0.90
1:A:127:ASN:ND2	1:A:129:THR:HG23	1.87	0.90
1:A:127:ASN:HD21	1:A:129:THR:HG23	1.37	0.89
2:D:315:ASN:HD21	2:D:317:ASN:HD22	1.19	0.88
1:A:307:ALA:HB1	1:A:331:ILE:HD11	1.55	0.88
2:D:286:MSE:HE3	2:D:286:MSE:HA	1.56	0.88
1:A:221:LEU:HD12	1:A:229:ILE:HG13	1.53	0.87
1:A:256:ILE:HA	1:A:286:VAL:HG21	1.55	0.87
1:A:31:VAL:HB	1:A:34:LEU:HD11	1.57	0.86
1:A:133:ASN:HD21	1:A:392:THR:H	1.22	0.84
2:D:11:ASN:H	2:D:74:VAL:HG23	1.41	0.83
1:A:48:PRO:HG2	1:A:51:LYS:HD3	1.62	0.81
1:A:270:ASN:ND2	1:A:271:ARG:H	1.76	0.81
1:A:31:VAL:HB	1:A:34:LEU:CD1	2.11	0.81
2:D:75:ALA:HB2	2:D:83:VAL:HG12	1.65	0.79
2:D:87:ILE:H	2:D:87:ILE:HD12	1.45	0.79
2:D:79:ASP:OD1	2:D:82:ASN:HB3	1.83	0.79
2:D:11:ASN:N	2:D:74:VAL:HG23	1.97	0.79
1:A:266:TRP:NE1	1:A:274:GLN:HG2	1.99	0.78
2:D:169:TYR:O	2:D:173:VAL:HG23	1.83	0.78
2:D:188:VAL:HG12	2:D:197:MSE:HG2	1.67	0.76
2:D:54:PHE:O	2:D:104:ILE:HD12	1.86	0.76
2:D:315:ASN:HD21	2:D:317:ASN:ND2	1.83	0.76
2:D:16:LEU:HD22	2:D:31:LEU:HD21	1.66	0.75
2:D:325:ILE:HD13	2:D:326:PHE:N	2.02	0.75
1:A:221:LEU:O	1:A:225:VAL:HG12	1.87	0.74
2:D:237:LEU:H	2:D:237:LEU:HD22	1.51	0.74
2:D:36:THR:HB	2:D:53:GLN:HG3	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:416:HIS:HD2	1:A:418:THR:H	1.37	0.72
1:A:172:PRO:HG3	1:A:272:SER:OG	1.90	0.72
2:D:96:SER:OG	2:D:104:ILE:HG23	1.90	0.72
2:D:212:ILE:HG22	2:D:327:ASN:HB2	1.72	0.72
2:D:251:ALA:HB2	2:D:273:ASN:HB2	1.72	0.72
2:D:80:ILE:H	2:D:80:ILE:HD13	1.55	0.71
1:A:214:MET:HG2	1:A:232:ASN:O	1.90	0.71
2:D:10:PRO:HB2	2:D:74:VAL:HG21	1.73	0.71
2:D:11:ASN:HD21	2:D:80:ILE:HG22	1.55	0.71
1:A:127:ASN:HD22	1:A:128:ASP:N	1.87	0.70
1:A:209:GLN:HG3	1:A:210:PRO:HD2	1.72	0.70
1:A:200:ILE:HG12	1:A:201:GLY:H	1.55	0.70
2:D:134:GLU:O	2:D:138:VAL:HG23	1.92	0.70
2:D:337:PHE:HB2	2:D:357:MSE:HE2	1.74	0.70
1:A:232:ASN:O	1:A:234:GLY:N	2.25	0.69
1:A:416:HIS:CD2	1:A:418:THR:H	2.09	0.69
1:A:418:THR:HG22	1:A:420:THR:H	1.56	0.69
2:D:208:PRO:O	2:D:210:PRO:HD3	1.93	0.69
2:D:360:ASN:H	2:D:360:ASN:HD22	1.41	0.69
1:A:470:ARG:HH11	1:A:470:ARG:HG3	1.58	0.68
1:A:409:GLN:HA	1:A:409:GLN:HE21	1.57	0.68
1:A:184:GLU:CG	1:A:203:GLY:HA3	2.18	0.67
1:A:273:ARG:NH1	1:A:334:GLY:HA3	2.09	0.67
2:D:324:ILE:HD12	2:D:357:MSE:HE3	1.77	0.67
2:D:135:MSE:O	2:D:139:ILE:HG12	1.94	0.67
1:A:232:ASN:HB3	1:A:233:PRO:CD	2.25	0.67
1:A:239:GLU:O	1:A:243:THR:HG23	1.95	0.67
1:A:370:ASN:HD21	1:A:372:SER:CB	2.08	0.66
1:A:344:LYS:HA	1:A:344:LYS:HE2	1.78	0.66
1:A:330:ILE:CD1	1:A:336:LEU:HD12	2.24	0.66
2:D:325:ILE:HD13	2:D:326:PHE:H	1.60	0.66
2:D:250:ASN:HD21	2:D:272:GLU:HB2	1.62	0.65
1:A:418:THR:HG23	1:A:435:VAL:HG21	1.78	0.65
1:A:221:LEU:HD11	1:A:236:ILE:CD1	2.22	0.65
1:A:37:PRO:HG2	1:A:38:GLN:NE2	2.12	0.65
2:D:133:LYS:HG2	2:D:150:ILE:HG21	1.79	0.65
2:D:360:ASN:N	2:D:360:ASN:HD22	1.94	0.64
1:A:176:MET:O	1:A:180:LEU:HD23	1.97	0.64
2:D:14:VAL:HG11	2:D:52:LEU:HD11	1.77	0.64
2:D:367:ILE:O	2:D:367:ILE:HG22	1.97	0.64
1:A:495:THR:O	1:A:496:ILE:HD13	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:TYR:HB2	1:A:332:LEU:HB2	1.80	0.63
1:A:15:VAL:HG13	1:A:27:VAL:HB	1.80	0.63
1:A:409:GLN:HA	1:A:409:GLN:NE2	2.14	0.63
2:D:97:VAL:HG23	2:D:103:ASN:HD22	1.62	0.63
1:A:22:LEU:HD12	1:A:26:ARG:CZ	2.29	0.63
1:A:81:ARG:HH22	1:A:102:GLY:H	1.47	0.62
2:D:16:LEU:CD2	2:D:31:LEU:HD21	2.29	0.62
2:D:48:ASN:OD1	2:D:190:GLN:HB2	1.98	0.62
1:A:133:ASN:HD21	1:A:392:THR:N	1.97	0.62
2:D:174:ARG:NH1	2:D:188:VAL:HG23	2.15	0.61
2:D:345:GLU:O	2:D:352:VAL:HG12	2.00	0.61
1:A:522:VAL:HG11	1:A:526:GLN:NE2	2.14	0.61
1:A:195:GLU:HG2	1:A:197:TYR:CE2	2.34	0.61
1:A:182:ARG:HG2	1:A:182:ARG:HH11	1.64	0.61
1:A:343:VAL:O	1:A:343:VAL:HG13	2.01	0.61
2:D:58:LYS:HE3	2:D:58:LYS:O	1.99	0.61
2:D:97:VAL:HA	2:D:103:ASN:HB2	1.82	0.61
1:A:270:ASN:ND2	1:A:271:ARG:N	2.47	0.61
1:A:392:THR:HG23	1:A:402:GLU:HG2	1.82	0.61
1:A:77:VAL:HG21	1:A:121:TYR:CE1	2.37	0.60
2:D:97:VAL:O	2:D:98:ASP:HB2	2.00	0.60
1:A:131:VAL:HB	1:A:138:VAL:HG12	1.82	0.60
2:D:90:CYS:HB2	2:D:107:ILE:HD11	1.83	0.60
1:A:30:ARG:HB2	1:A:52:LEU:HD21	1.82	0.60
2:D:17:PHE:CD1	2:D:23:TRP:HA	2.37	0.60
2:D:31:LEU:HD22	2:D:31:LEU:N	2.17	0.60
2:D:143:ARG:HH21	2:D:143:ARG:HG3	1.67	0.60
2:D:174:ARG:HH11	2:D:188:VAL:HG23	1.67	0.59
1:A:133:ASN:HD22	1:A:390:VAL:HG12	1.67	0.59
1:A:243:THR:HG21	5:A:780:HOH:O	2.01	0.59
2:D:12:LEU:HD11	2:D:14:VAL:HG23	1.84	0.59
1:A:148:GLN:O	1:A:152:LEU:HD13	2.02	0.59
2:D:364:LEU:HD13	2:D:365:GLU:N	2.17	0.59
1:A:392:THR:OG1	1:A:402:GLU:HG2	2.02	0.59
1:A:320:THR:HB	1:A:324:ALA:HB2	1.83	0.59
2:D:73:SER:HB2	2:D:85:THR:HG23	1.84	0.59
2:D:40:MSE:HE3	2:D:86:ARG:HH21	1.68	0.58
2:D:173:VAL:HG13	2:D:177:ALA:HB2	1.84	0.58
2:D:112:ILE:O	2:D:116:GLU:HG3	2.03	0.58
2:D:97:VAL:HA	2:D:103:ASN:CB	2.33	0.58
1:A:48:PRO:CG	1:A:51:LYS:HD3	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:360:ASN:H	2:D:360:ASN:ND2	2.02	0.58
2:D:41:ARG:HG2	2:D:343:ILE:HG12	1.86	0.58
1:A:328:THR:O	1:A:331:ILE:HG23	2.04	0.58
2:D:235:VAL:HG12	2:D:236:TRP:N	2.18	0.58
1:A:470:ARG:NH1	1:A:470:ARG:HG3	2.18	0.58
2:D:232:TYR:HD1	2:D:233:ASP:OD1	1.87	0.58
2:D:80:ILE:CD1	2:D:80:ILE:H	2.17	0.58
2:D:41:ARG:HG2	2:D:343:ILE:HG23	1.85	0.58
2:D:160:ILE:HD12	2:D:160:ILE:O	2.04	0.58
2:D:20:TYR:O	2:D:23:TRP:HB3	2.04	0.57
1:A:370:ASN:C	1:A:370:ASN:HD22	2.07	0.57
1:A:200:ILE:HD13	1:A:236:ILE:HD12	1.86	0.57
1:A:132:LEU:O	1:A:390:VAL:HG11	2.05	0.57
1:A:425:SER:HB2	1:A:426:PRO:HD2	1.85	0.57
1:A:25:GLY:HA3	1:A:73:VAL:HG12	1.87	0.57
2:D:283:TYR:O	2:D:286:MSE:HB2	2.05	0.57
1:A:273:ARG:HG3	1:A:334:GLY:HA2	1.87	0.57
1:A:123:ARG:HD2	1:A:124:ARG:HH12	1.68	0.57
2:D:117:ASN:O	2:D:119:LYS:HG3	2.04	0.57
2:D:43:SER:HB3	2:D:47:ARG:HB3	1.87	0.57
2:D:91:LYS:HA	2:D:115:ILE:HD13	1.86	0.57
1:A:370:ASN:HD21	1:A:372:SER:HB3	1.69	0.56
1:A:436:ASP:CG	1:A:437:ASN:H	2.09	0.56
1:A:176:MET:HE1	1:A:279:ASN:N	2.20	0.56
2:D:318:LEU:CD2	2:D:355:LEU:HD11	2.35	0.56
1:A:170:ASP:HA	1:A:270:ASN:HD21	1.69	0.56
2:D:208:PRO:HB2	2:D:325:ILE:HB	1.87	0.56
2:D:112:ILE:HB	2:D:140:TYR:OH	2.05	0.56
2:D:185:PHE:CD2	2:D:297:ARG:HA	2.40	0.56
2:D:342:VAL:HG23	2:D:354:HIS:O	2.06	0.56
1:A:220:VAL:O	1:A:224:GLN:HG3	2.04	0.56
1:A:307:ALA:CB	1:A:331:ILE:HD11	2.33	0.56
2:D:318:LEU:HD23	2:D:355:LEU:HD21	1.87	0.56
1:A:537:LYS:HD3	1:A:537:LYS:C	2.26	0.56
1:A:82:VAL:CG2	1:A:96:VAL:HG13	2.35	0.56
2:D:286:MSE:CE	2:D:286:MSE:HA	2.31	0.56
1:A:157:ASN:HA	1:A:375:LEU:HG	1.88	0.56
2:D:211:MSE:HE1	2:D:312:THR:HB	1.87	0.56
2:D:366:THR:O	2:D:369:PRO:HD3	2.06	0.56
1:A:315:LEU:O	1:A:319:GLN:HG2	2.06	0.56
1:A:236:ILE:HG23	1:A:240:GLU:HB2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:ARG:NH2	1:A:229:ILE:HD13	2.22	0.55
2:D:57:SER:HB3	2:D:102:ASP:OD2	2.06	0.55
1:A:232:ASN:O	1:A:233:PRO:C	2.43	0.55
1:A:424:VAL:HA	1:A:429:ARG:O	2.07	0.55
2:D:133:LYS:CG	2:D:150:ILE:HG21	2.36	0.55
2:D:237:LEU:HD21	2:D:309:LYS:HG2	1.88	0.55
2:D:17:PHE:CE1	2:D:28:PHE:HB3	2.41	0.55
1:A:429:ARG:HG2	1:A:429:ARG:HH11	1.71	0.55
1:A:58:ILE:HG12	1:A:97:LEU:CD2	2.36	0.55
1:A:206:ILE:HG12	1:A:221:LEU:HD23	1.89	0.55
1:A:225:VAL:HG21	1:A:240:GLU:OE1	2.06	0.55
2:D:254:TYR:HB2	2:D:276:VAL:HG12	1.89	0.55
1:A:256:ILE:HG23	1:A:257:LYS:N	2.22	0.54
1:A:270:ASN:HD22	1:A:271:ARG:H	1.52	0.54
1:A:213:ASP:O	1:A:217:ILE:HG13	2.08	0.54
1:A:221:LEU:HD12	1:A:229:ILE:CG1	2.32	0.54
1:A:392:THR:CG2	1:A:402:GLU:HG2	2.38	0.54
1:A:416:HIS:CD2	1:A:417:PRO:HD2	2.42	0.54
2:D:279:ARG:CZ	2:D:286:MSE:HG2	2.38	0.54
2:D:189:TRP:CD1	2:D:320:PRO:HG2	2.43	0.54
1:A:50:GLU:CD	1:A:50:GLU:H	2.11	0.54
1:A:370:ASN:ND2	1:A:372:SER:H	2.05	0.53
2:D:184:LYS:HE3	2:D:367:ILE:HD12	1.89	0.53
2:D:97:VAL:HG23	2:D:103:ASN:ND2	2.23	0.53
1:A:34:LEU:HD12	1:A:34:LEU:H	1.73	0.53
2:D:96:SER:HG	2:D:104:ILE:HG23	1.73	0.53
1:A:58:ILE:HG12	1:A:97:LEU:HD23	1.90	0.53
1:A:486:GLU:HG2	5:A:801:HOH:O	2.09	0.53
2:D:237:LEU:CD2	2:D:237:LEU:H	2.21	0.53
2:D:245:ARG:HD3	2:D:305:ASP:OD1	2.08	0.53
2:D:11:ASN:HD22	2:D:75:ALA:HB3	1.74	0.53
2:D:43:SER:CB	2:D:47:ARG:HB3	2.38	0.53
2:D:157:VAL:HG13	2:D:172:TYR:HE2	1.73	0.53
1:A:265:VAL:O	1:A:269:VAL:HG22	2.09	0.53
2:D:178:LEU:HD23	2:D:293:GLU:HB3	1.90	0.53
1:A:373:ARG:HA	1:A:373:ARG:HE	1.74	0.53
2:D:217:SER:HB2	5:D:463:HOH:O	2.09	0.53
2:D:61:HIS:CD2	2:D:95:VAL:HG11	2.44	0.52
2:D:16:LEU:HA	2:D:69:ILE:O	2.09	0.52
2:D:250:ASN:ND2	2:D:272:GLU:HB2	2.23	0.52
1:A:81:ARG:HH22	1:A:102:GLY:N	2.05	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:367:ILE:HG13	5:D:431:HOH:O	2.09	0.52
1:A:22:LEU:HB3	1:A:24:LEU:HD22	1.91	0.52
1:A:263:GLY:N	1:A:264:PRO:HD2	2.25	0.52
2:D:87:ILE:HD12	2:D:87:ILE:N	2.21	0.52
1:A:176:MET:HG3	1:A:180:LEU:CD2	2.39	0.52
1:A:59:GLN:HB3	1:A:60:PRO:HD2	1.90	0.52
1:A:82:VAL:HG21	1:A:96:VAL:CG1	2.40	0.52
2:D:241:ASN:C	2:D:241:ASN:HD22	2.13	0.52
2:D:330:LYS:CA	2:D:330:LYS:HE3	2.34	0.52
2:D:346:LEU:HD23	2:D:346:LEU:N	2.24	0.52
1:A:254:ARG:HG2	1:A:254:ARG:HH11	1.75	0.52
1:A:292:PHE:HB3	1:A:295:MET:HB3	1.91	0.52
1:A:31:VAL:CB	1:A:34:LEU:HD11	2.36	0.52
1:A:402:GLU:OE1	1:A:411:ARG:NH1	2.43	0.51
2:D:12:LEU:HD11	2:D:14:VAL:CG2	2.40	0.51
2:D:38:LEU:HD13	2:D:52:LEU:HG	1.93	0.51
1:A:123:ARG:HD2	1:A:124:ARG:NH1	2.25	0.51
2:D:157:VAL:CG1	2:D:172:TYR:HE2	2.24	0.51
2:D:53:GLN:HB3	2:D:106:ALA:HB2	1.93	0.51
1:A:176:MET:O	1:A:180:LEU:CD2	2.57	0.51
1:A:60:PRO:C	1:A:62:THR:H	2.13	0.51
1:A:85:HIS:CD2	1:A:97:LEU:HD11	2.46	0.51
1:A:199:THR:HG22	1:A:200:ILE:N	2.26	0.51
2:D:346:LEU:HB3	2:D:351:SER:CB	2.41	0.50
1:A:77:VAL:CG2	1:A:121:TYR:CE1	2.94	0.50
1:A:238:MET:O	1:A:242:THR:HG22	2.11	0.50
1:A:378:GLU:OE1	1:A:433:LYS:HG3	2.11	0.50
1:A:395:THR:OG1	1:A:399:HIS:HB2	2.11	0.50
2:D:136:LEU:HD13	2:D:150:ILE:HD11	1.94	0.50
2:D:30:GLU:C	2:D:31:LEU:HD22	2.32	0.50
1:A:522:VAL:HG11	1:A:526:GLN:HE21	1.75	0.50
2:D:211:MSE:HB2	2:D:326:PHE:CE1	2.47	0.50
2:D:312:THR:CG2	2:D:353:THR:HB	2.42	0.50
1:A:332:LEU:HD22	1:A:332:LEU:O	2.11	0.50
2:D:80:ILE:HD13	2:D:80:ILE:N	2.26	0.50
2:D:174:ARG:HG3	2:D:188:VAL:HG22	1.94	0.50
2:D:213:VAL:O	2:D:213:VAL:HG22	2.12	0.50
2:D:268:THR:HG23	2:D:299:GLN:NE2	2.27	0.50
1:A:200:ILE:HG12	1:A:201:GLY:N	2.23	0.49
2:D:133:LYS:HE3	2:D:152:ALA:HB3	1.94	0.49
1:A:154:THR:H	1:A:182:ARG:NH2	2.09	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:GLY:O	1:A:128:ASP:HB2	2.12	0.49
2:D:345:GLU:HB3	2:D:352:VAL:CG1	2.43	0.49
1:A:423:GLU:OE1	1:A:429:ARG:NH2	2.46	0.49
1:A:60:PRO:HG2	1:A:62:THR:HG22	1.94	0.49
2:D:11:ASN:H	2:D:74:VAL:CG2	2.19	0.49
1:A:207:MET:SD	1:A:211:VAL:HG21	2.53	0.49
1:A:553:LYS:NZ	1:A:553:LYS:HB2	2.27	0.49
1:A:370:ASN:ND2	1:A:370:ASN:C	2.66	0.49
1:A:225:VAL:HG11	1:A:229:ILE:HD11	1.95	0.49
1:A:270:ASN:O	1:A:274:GLN:HB2	2.12	0.49
1:A:315:LEU:HD13	1:A:315:LEU:O	2.13	0.49
1:A:256:ILE:HA	1:A:286:VAL:CG2	2.36	0.48
2:D:11:ASN:ND2	2:D:80:ILE:HG22	2.26	0.48
1:A:25:GLY:CA	1:A:73:VAL:HG12	2.43	0.48
1:A:499:LYS:NZ	5:A:599:HOH:O	2.45	0.48
1:A:202:ILE:HG22	1:A:202:ILE:O	2.13	0.48
1:A:18:ARG:NH1	1:A:77:VAL:HG23	2.28	0.48
2:D:185:PHE:CE2	2:D:297:ARG:HA	2.48	0.48
1:A:172:PRO:HB3	1:A:336:LEU:HD22	1.94	0.48
1:A:38:GLN:H	1:A:38:GLN:CD	2.16	0.48
1:A:58:ILE:HG13	1:A:97:LEU:HA	1.95	0.48
2:D:215:GLU:H	2:D:329:SER:HB2	1.77	0.48
2:D:173:VAL:HG13	2:D:177:ALA:CB	2.43	0.48
1:A:182:ARG:HG2	1:A:182:ARG:NH1	2.29	0.48
2:D:313:ILE:N	2:D:313:ILE:HD12	2.27	0.48
2:D:179:ALA:HB1	2:D:182:SER:HB3	1.95	0.48
1:A:133:ASN:ND2	1:A:390:VAL:HG12	2.28	0.48
2:D:17:PHE:CD1	2:D:28:PHE:HB3	2.48	0.48
1:A:127:ASN:ND2	1:A:129:THR:H	2.11	0.48
2:D:158:PRO:HD3	2:D:286:MSE:HE1	1.95	0.48
1:A:162:PRO:HG2	1:A:165:GLU:HG3	1.96	0.48
2:D:12:LEU:HA	2:D:74:VAL:HB	1.96	0.48
2:D:58:LYS:HB3	2:D:60:ILE:HG13	1.96	0.48
1:A:337:GLU:OE1	1:A:343:VAL:HG12	2.14	0.48
2:D:248:MSE:HG2	2:D:298:LEU:O	2.13	0.48
1:A:18:ARG:NH1	1:A:78:GLU:OE2	2.47	0.47
2:D:40:MSE:HG2	2:D:88:TYR:OH	2.14	0.47
1:A:175:SER:OG	1:A:178:GLU:HG3	2.14	0.47
1:A:236:ILE:HG23	1:A:240:GLU:CB	2.45	0.47
1:A:22:LEU:HD12	1:A:26:ARG:NH2	2.30	0.47
2:D:75:ALA:HB2	2:D:83:VAL:HA	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:346:LEU:HB2	2:D:350:ASN:O	2.15	0.47
1:A:209:GLN:HB3	1:A:211:VAL:HG23	1.97	0.47
1:A:60:PRO:C	1:A:62:THR:N	2.67	0.47
2:D:144:THR:O	2:D:147:THR:HG22	2.15	0.47
1:A:127:ASN:C	1:A:127:ASN:HD22	2.18	0.47
2:D:119:LYS:NZ	5:D:392:HOH:O	2.47	0.47
1:A:375:LEU:HD22	1:A:455:LYS:HG2	1.97	0.47
1:A:239:GLU:O	1:A:242:THR:HG23	2.15	0.47
2:D:5:GLN:HG3	2:D:9:TYR:CD1	2.50	0.47
1:A:28:ARG:HD3	1:A:49:THR:O	2.15	0.47
1:A:362:ASP:N	1:A:363:PRO:CD	2.78	0.47
1:A:498:VAL:HG11	1:A:502:VAL:HG23	1.97	0.47
1:A:538:VAL:HG11	1:A:542:VAL:HG12	1.96	0.47
2:D:16:LEU:HD23	2:D:16:LEU:H	1.79	0.47
2:D:237:LEU:N	2:D:237:LEU:HD22	2.27	0.47
1:A:214:MET:HG3	1:A:218:ASN:ND2	2.30	0.47
1:A:7:ASN:HD22	1:A:7:ASN:HA	1.48	0.47
1:A:81:ARG:HB3	1:A:100:TYR:CZ	2.50	0.46
1:A:564:GLN:HG3	1:A:566:THR:HG22	1.96	0.46
1:A:323:ARG:HA	1:A:326:ARG:HH11	1.80	0.46
1:A:321:LYS:O	1:A:322:GLY:C	2.54	0.46
1:A:252:MET:CE	1:A:253:GLN:HG3	2.45	0.46
1:A:92:THR:HB	2:D:282:ALA:CB	2.45	0.46
2:D:374:ASN:C	2:D:376:PHE:H	2.17	0.46
2:D:260:ASP:OD1	2:D:289:ARG:NH2	2.48	0.46
1:A:207:MET:O	1:A:207:MET:HG3	2.14	0.46
2:D:318:LEU:HB3	2:D:355:LEU:HD21	1.98	0.46
2:D:254:TYR:HE2	2:D:274:SER:HB2	1.81	0.46
1:A:92:THR:HB	2:D:282:ALA:HB3	1.96	0.46
2:D:114:SER:HA	2:D:167:GLU:OE2	2.16	0.46
2:D:125:PHE:CE2	2:D:134:GLU:HG3	2.50	0.46
2:D:153:ILE:HG12	2:D:197:MSE:HB3	1.98	0.46
2:D:41:ARG:CG	2:D:343:ILE:HG23	2.46	0.46
2:D:91:LYS:HD3	2:D:91:LYS:O	2.16	0.46
1:A:383:TYR:O	1:A:384:LYS:HG3	2.15	0.46
1:A:416:HIS:HD2	1:A:418:THR:N	2.11	0.46
1:A:409:GLN:CA	1:A:409:GLN:NE2	2.77	0.46
2:D:54:PHE:CE1	2:D:105:ILE:HD11	2.50	0.45
1:A:214:MET:HG3	1:A:218:ASN:HD21	1.82	0.45
2:D:122:ARG:HG3	2:D:123:PRO:O	2.17	0.45
2:D:56:ASP:HA	5:D:413:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:HIS:NE2	1:A:97:LEU:HD11	2.32	0.45
1:A:9:ASN:HD22	1:A:9:ASN:HA	1.53	0.45
2:D:154:ASN:CG	2:D:180:VAL:HG21	2.37	0.45
1:A:456:THR:HG22	1:A:457:ASN:N	2.31	0.45
2:D:32:ALA:O	2:D:35:ILE:HG22	2.17	0.45
1:A:214:MET:CG	1:A:232:ASN:O	2.61	0.45
2:D:236:TRP:HH2	2:D:332:GLN:O	1.99	0.45
2:D:90:CYS:CB	2:D:107:ILE:HD11	2.47	0.45
2:D:143:ARG:NH2	2:D:143:ARG:HG3	2.30	0.45
1:A:368:ILE:HG13	1:A:368:ILE:O	2.16	0.45
2:D:345:GLU:HB3	2:D:352:VAL:HG13	1.99	0.45
2:D:131:SER:O	2:D:135:MSE:HG3	2.17	0.45
1:A:303:ASP:OD1	1:A:306:LYS:HB2	2.17	0.45
2:D:363:LYS:HG2	5:D:435:HOH:O	2.16	0.45
2:D:10:PRO:HG3	2:D:346:LEU:HD12	1.99	0.45
2:D:156:TYR:O	2:D:177:ALA:HA	2.17	0.45
1:A:337:GLU:HG2	1:A:342:GLU:HA	1.99	0.45
2:D:174:ARG:NH1	2:D:188:VAL:O	2.50	0.45
2:D:251:ALA:CB	2:D:273:ASN:HB2	2.46	0.45
2:D:19:SER:H	2:D:22:ALA:HB3	1.80	0.45
2:D:250:ASN:O	2:D:273:ASN:HB2	2.17	0.44
1:A:73:VAL:HG12	1:A:73:VAL:O	2.17	0.44
2:D:91:LYS:CA	2:D:115:ILE:HD13	2.47	0.44
2:D:319:THR:O	2:D:322:VAL:HG12	2.16	0.44
2:D:360:ASN:N	2:D:360:ASN:ND2	2.62	0.44
2:D:198:MSE:HE1	2:D:206:GLN:HE22	1.82	0.44
1:A:17:ASP:HB3	1:A:28:ARG:HB2	1.98	0.44
2:D:244:LYS:O	2:D:247:PRO:HD2	2.17	0.44
2:D:279:ARG:HG3	2:D:289:ARG:O	2.17	0.44
1:A:61:ILE:HD12	1:A:61:ILE:C	2.37	0.44
2:D:66:GLY:O	2:D:90:CYS:HB3	2.18	0.44
2:D:296:ILE:HD11	2:D:369:PRO:HD2	1.98	0.44
2:D:295:ALA:O	2:D:299:GLN:HG3	2.18	0.44
2:D:328:ASP:HB2	2:D:333:PHE:CE2	2.53	0.44
1:A:416:HIS:HD2	1:A:418:THR:CB	2.13	0.44
2:D:167:GLU:CD	2:D:167:GLU:H	2.21	0.44
1:A:31:VAL:O	1:A:35:HIS:HB2	2.18	0.44
2:D:43:SER:HA	2:D:341:GLU:HB3	2.00	0.44
2:D:189:TRP:NE1	2:D:320:PRO:HG2	2.33	0.44
1:A:418:THR:HG22	1:A:419:GLY:N	2.33	0.44
1:A:200:ILE:HG21	1:A:236:ILE:HD12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:ASP:C	1:A:172:PRO:HD3	2.38	0.44
1:A:99:THR:HG22	1:A:100:TYR:N	2.33	0.44
1:A:370:ASN:HD21	1:A:372:SER:HB2	1.79	0.44
2:D:213:VAL:HG13	2:D:213:VAL:O	2.16	0.44
1:A:253:GLN:HB2	1:A:253:GLN:HE21	1.61	0.43
1:A:295:MET:HE2	1:A:331:ILE:CD1	2.48	0.43
2:D:35:ILE:O	2:D:348:ASN:ND2	2.51	0.43
2:D:20:TYR:CZ	2:D:143:ARG:HA	2.54	0.43
1:A:320:THR:HG22	1:A:323:ARG:HB3	1.99	0.43
1:A:541:THR:HG23	5:A:848:HOH:O	2.18	0.43
2:D:95:VAL:HG13	2:D:105:ILE:CG2	2.48	0.43
2:D:35:ILE:HD11	2:D:38:LEU:HB2	2.00	0.43
2:D:125:PHE:HE2	2:D:134:GLU:HG3	1.82	0.43
1:A:242:THR:HG23	1:A:243:THR:H	1.83	0.43
2:D:235:VAL:HG12	2:D:236:TRP:H	1.83	0.43
2:D:246:ASP:HB2	2:D:247:PRO:HD3	1.99	0.43
1:A:439:TYR:HB3	1:A:441:ILE:CD1	2.49	0.43
2:D:174:ARG:CG	2:D:188:VAL:HG22	2.48	0.43
2:D:60:ILE:HG22	2:D:64:MSE:HG3	2.00	0.43
1:A:82:VAL:HG22	1:A:83:TYR:N	2.34	0.43
1:A:48:PRO:HB2	1:A:50:GLU:OE2	2.19	0.43
2:D:47:ARG:NH1	2:D:47:ARG:CB	2.82	0.43
1:A:299:MET:HG3	1:A:304:TRP:HZ3	1.84	0.43
1:A:270:ASN:O	1:A:274:GLN:N	2.52	0.42
2:D:28:PHE:HD1	2:D:29:VAL:N	2.17	0.42
2:D:236:TRP:CD1	2:D:308:ALA:HB2	2.54	0.42
1:A:43:ASP:O	2:D:122:ARG:NE	2.52	0.42
1:A:332:LEU:HD13	1:A:333:THR:HG23	1.99	0.42
2:D:21:ASP:C	2:D:23:TRP:N	2.73	0.42
2:D:369:PRO:O	2:D:370:VAL:C	2.57	0.42
2:D:212:ILE:HG13	2:D:230:LEU:HD13	2.01	0.42
1:A:242:THR:O	1:A:245:PHE:N	2.51	0.42
2:D:184:LYS:HE3	2:D:367:ILE:CG2	2.49	0.42
2:D:143:ARG:HB3	2:D:146:LEU:HD12	2.01	0.42
2:D:17:PHE:CD2	2:D:17:PHE:N	2.88	0.42
1:A:216:GLN:O	1:A:219:LYS:HB3	2.20	0.42
2:D:306:GLY:O	2:D:358:PHE:HA	2.20	0.42
1:A:209:GLN:HE21	1:A:209:GLN:HB2	1.64	0.42
2:D:324:ILE:HB	2:D:357:MSE:CE	2.50	0.42
1:A:36:PRO:HB2	1:A:38:GLN:OE1	2.20	0.42
2:D:292:TYR:CZ	2:D:296:ILE:HG13	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:ASP:OD2	1:A:216:GLN:HG3	2.20	0.42
2:D:204:ILE:C	2:D:206:GLN:H	2.23	0.42
1:A:11:PHE:CD1	1:A:11:PHE:C	2.93	0.42
2:D:136:LEU:CD1	2:D:150:ILE:HD11	2.49	0.42
1:A:58:ILE:HD12	1:A:58:ILE:C	2.40	0.42
1:A:278:GLU:O	1:A:281:ALA:HB3	2.19	0.42
2:D:318:LEU:HD23	2:D:355:LEU:HD11	2.02	0.42
1:A:296:LEU:HA	1:A:296:LEU:HD12	1.89	0.42
2:D:209:TYR:OH	2:D:229:PRO:HG2	2.19	0.42
1:A:255:ASP:HB3	1:A:286:VAL:HG11	2.02	0.42
2:D:97:VAL:HG22	2:D:98:ASP:N	2.35	0.42
2:D:56:ASP:OD2	2:D:60:ILE:HG13	2.20	0.42
1:A:277:LEU:HD23	1:A:280:MET:HE3	2.01	0.41
1:A:286:VAL:HG12	5:A:692:HOH:O	2.21	0.41
1:A:326:ARG:O	1:A:330:ILE:HG12	2.21	0.41
1:A:416:HIS:CG	1:A:417:PRO:HD2	2.54	0.41
2:D:349:ASN:OD1	2:D:350:ASN:HB2	2.21	0.41
1:A:184:GLU:HA	5:A:749:HOH:O	2.19	0.41
2:D:23:TRP:HZ3	2:D:145:LEU:CD1	2.33	0.41
2:D:47:ARG:HB3	2:D:47:ARG:HH11	1.85	0.41
2:D:57:SER:CB	2:D:102:ASP:OD2	2.69	0.41
2:D:57:SER:C	2:D:59:ASN:N	2.74	0.41
1:A:21:PRO:HD3	1:A:54:TRP:CZ2	2.55	0.41
2:D:128:ALA:O	2:D:132:ILE:HG13	2.20	0.41
1:A:323:ARG:HA	1:A:326:ARG:NH1	2.36	0.41
1:A:242:THR:O	1:A:245:PHE:HB3	2.21	0.41
1:A:78:GLU:CD	1:A:78:GLU:H	2.24	0.41
1:A:265:VAL:HG22	1:A:300:LEU:HD23	2.03	0.41
1:A:300:LEU:C	1:A:302:GLY:H	2.24	0.41
2:D:154:ASN:O	2:D:180:VAL:HG23	2.20	0.41
1:A:456:THR:CG2	1:A:457:ASN:N	2.84	0.41
2:D:208:PRO:O	2:D:210:PRO:CD	2.67	0.41
1:A:232:ASN:HB3	1:A:233:PRO:HD3	2.03	0.41
2:D:133:LYS:HE3	2:D:152:ALA:CB	2.51	0.41
1:A:176:MET:CE	1:A:180:LEU:HD21	2.51	0.41
2:D:34:THR:HB	2:D:55:TYR:O	2.21	0.41
1:A:385:GLY:HA2	1:A:406:THR:OG1	2.21	0.41
1:A:323:ARG:CA	1:A:326:ARG:HH11	2.34	0.40
1:A:176:MET:HG3	1:A:180:LEU:HD21	2.02	0.40
1:A:26:ARG:HD3	2:D:259:LEU:HD21	2.02	0.40
1:A:421:TYR:CE1	1:A:433:LYS:HB2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:113:HIS:HB3	2:D:139:ILE:HG21	2.03	0.40
2:D:235:VAL:O	2:D:308:ALA:HB1	2.21	0.40
2:D:179:ALA:CB	2:D:182:SER:HB3	2.51	0.40
2:D:12:LEU:CD1	2:D:14:VAL:HG23	2.51	0.40
2:D:235:VAL:CG1	2:D:236:TRP:N	2.84	0.40
2:D:254:TYR:CE2	2:D:274:SER:HB2	2.56	0.40
2:D:241:ASN:ND2	2:D:241:ASN:C	2.74	0.40
1:A:252:MET:CE	1:A:278:GLU:HB3	2.51	0.40
1:A:407:PRO:C	1:A:409:GLN:H	2.25	0.40
2:D:368:ASP:N	2:D:369:PRO:CD	2.84	0.40
2:D:157:VAL:HG13	2:D:172:TYR:CE2	2.53	0.40
1:A:137:GLU:O	1:A:141:ASP:N	2.48	0.40
2:D:41:ARG:NH2	2:D:341:GLU:OE2	2.54	0.40

All (2) 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)
4:A:586:PO4:P	4:A:586:PO4:O2[2_555]	1.48	0.72
1:A:584:HIS:OXT	1:A:584:HIS:OXT[4_555]	1.87	0.33

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	551/584 (94%)	512 (93%)	31 (6%)	8 (2%)	13 42
2	D	360/391 (92%)	295 (82%)	52 (14%)	13 (4%)	4 18
All	All	911/975 (93%)	807 (89%)	83 (9%)	21 (2%)	8 30

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	575	GLY
2	D	77	ALA
2	D	213	VAL
1	A	232	ASN
2	D	98	ASP
2	D	99	SER
2	D	362	THR
2	D	367	ILE
2	D	370	VAL
1	A	301	ALA
2	D	243	HIS
1	A	110	ARG
1	A	384	LYS
2	D	100	LYS
2	D	124	PHE
2	D	92	HIS
1	A	322	GLY
2	D	313	ILE
1	A	200	ILE
1	A	202	ILE
2	D	74	VAL

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	472/494 (96%)	435 (92%)	37 (8%)	16	41
2	D	324/333 (97%)	303 (94%)	21 (6%)	21	52
All	All	796/827 (96%)	738 (93%)	58 (7%)	17	45

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ASN
1	A	9	ASN
1	A	24	LEU

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Mol	Chain	Res	Type
1	A	34	LEU
1	A	50	GLU
1	A	59	GLN
1	A	62	THR
1	A	89	LYS
1	A	127	ASN
1	A	129	THR
1	A	152	LEU
1	A	184	GLU
1	A	195	GLU
1	A	209	GLN
1	A	242	THR
1	A	296	LEU
1	A	300	LEU
1	A	327	VAL
1	A	335	ASN
1	A	370	ASN
1	A	373	ARG
1	A	375	LEU
1	A	388	PRO
1	A	393	MET
1	A	397	SER
1	A	411	ARG
1	A	418	THR
1	A	429	ARG
1	A	442	THR
1	A	457	ASN
1	A	486	GLU
1	A	495	THR
1	A	519	THR
1	A	522	VAL
1	A	550	TRP
1	A	554	MET
1	A	566	THR
2	D	44	LEU
2	D	58	LYS
2	D	80	ILE
2	D	87	ILE
2	D	102	ASP
2	D	134	GLU
2	D	154	ASN
2	D	183	ASP

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Mol	Chain	Res	Type
2	D	236	TRP
2	D	241	ASN
2	D	267	THR
2	D	286	MSE
2	D	289	ARG
2	D	315	ASN
2	D	325	ILE
2	D	330	LYS
2	D	333	PHE
2	D	350	ASN
2	D	357	MSE
2	D	360	ASN
2	D	365	GLU

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	6	ASN
1	A	7	ASN
1	A	9	ASN
1	A	59	GLN
1	A	85	HIS
1	A	93	ASN
1	A	127	ASN
1	A	133	ASN
1	A	173	ASN
1	A	209	GLN
1	A	253	GLN
1	A	270	ASN
1	A	335	ASN
1	A	370	ASN
1	A	409	GLN
1	A	416	HIS
1	A	443	ASN
1	A	457	ASN
1	A	526	GLN
1	A	533	ASN
2	D	11	ASN
2	D	26	ASN
2	D	53	GLN
2	D	61	HIS
2	D	67	ASN

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Mol	Chain	Res	Type
2	D	103	ASN
2	D	154	ASN
2	D	190	GLN
2	D	241	ASN
2	D	273	ASN
2	D	303	GLN
2	D	315	ASN
2	D	332	GLN
2	D	348	ASN
2	D	354	HIS
2	D	360	ASN
2	D	374	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	PO4	A	586	-	0,2,4	0.00	-	0,1,6	0.00	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PO4	A	586	-	-	0/0/0/0	0/0/0/0

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	586	PO4	0	1

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

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	A	557/584 (95%)	0.12	7 (1%) 79 78	22, 45, 71, 103	0
2	D	349/391 (89%)	1.05	75 (21%) 1 0	49, 85, 120, 138	0
All	All	906/975 (92%)	0.48	82 (9%) 11 7	22, 59, 111, 138	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	216	PRO	5.7
2	D	367	ILE	5.2
2	D	99	SER	5.1
2	D	355	LEU	4.8
2	D	103	ASN	4.7
2	D	346	LEU	4.7
2	D	215	GLU	4.6
2	D	217	SER	4.6
2	D	318	LEU	4.5
2	D	230	LEU	4.4
2	D	100	LYS	4.3
2	D	97	VAL	4.2
2	D	310	CYS	4.2
2	D	95	VAL	4.1
2	D	312	THR	4.1
2	D	329	SER	4.1
1	A	6	ASN	4.0
2	D	98	ASP	3.9
2	D	347	SER	3.9
2	D	337	PHE	3.8
2	D	333	PHE	3.8
2	D	214	GLY	3.8
2	D	338	TYR	3.8
2	D	308	ALA	3.7

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Mol	Chain	Res	Type	RSRZ
2	D	228	TYR	3.7
2	D	234	PHE	3.7
2	D	326	PHE	3.7
2	D	78	ASN	3.6
2	D	339	VAL	3.5
2	D	325	ILE	3.4
1	A	7	ASN	3.3
2	D	324	ILE	3.3
2	D	313	ILE	3.2
2	D	209	TYR	3.2
2	D	210	PRO	3.2
1	A	269	VAL	3.1
2	D	45	TYR	3.1
2	D	7	PRO	2.9
2	D	212	ILE	2.9
2	D	61	HIS	2.8
2	D	235	VAL	2.8
2	D	334	LYS	2.8
2	D	213	VAL	2.8
2	D	311	SER	2.7
2	D	8	GLY	2.7
2	D	204	ILE	2.7
2	D	336	GLU	2.7
2	D	319	THR	2.6
2	D	335	THR	2.6
2	D	55	TYR	2.6
2	D	200	TYR	2.6
2	D	342	VAL	2.6
2	D	292	TYR	2.5
1	A	9	ASN	2.4
2	D	327	ASN	2.4
2	D	307	TYR	2.4
2	D	232	TYR	2.4
2	D	356	TYR	2.4
2	D	332	GLN	2.4
1	A	236	ILE	2.3
2	D	79	ASP	2.3
1	A	62	THR	2.3
2	D	320	PRO	2.3
2	D	102	ASP	2.3
2	D	309	LYS	2.3
2	D	54	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
2	D	360	ASN	2.2
2	D	321	GLY	2.2
2	D	184	LYS	2.2
2	D	366	THR	2.2
2	D	77	ALA	2.2
2	D	101	GLY	2.2
2	D	31	LEU	2.1
2	D	52	LEU	2.1
2	D	374	ASN	2.1
2	D	109	LEU	2.1
2	D	236	TRP	2.1
2	D	288	TYR	2.0
2	D	371	LYS	2.0
2	D	328	ASP	2.0
2	D	237	LEU	2.0
1	A	84	GLY	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
3	K	A	585	1/1	0.91	0.15	-	48,48,48,48	1
4	PO4	A	586	3/5	0.99	0.30	-	24,24,25,95	2

6.5 Other polymers (i)

There are no such residues in this entry.