

Full wwPDB X-ray Structure Validation Report (i)

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PDB ID	:	1K28
Title	:	The Structure of the Bacteriophage T4 Cell-Puncturing Device
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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 https://www.wwpdb.org/validation/2017/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	:	1.8.5 (274361), CSD as 541 be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
$\operatorname{CCP4}$:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R _{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172(2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (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 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 <=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	18%		49%	6% 7%



2 Entry composition (i)

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	А	557	Total 4309	C 2672	N 763	O 853	S 21	0	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	576	SER	-	EXPRESSION TAG	UNP P16009
А	577	VAL	-	EXPRESSION TAG	UNP P16009
А	578	ASP	-	EXPRESSION TAG	UNP P16009
А	579	HIS	-	EXPRESSION TAG	UNP P16009
А	580	HIS	-	EXPRESSION TAG	UNP P16009
А	581	HIS	-	EXPRESSION TAG	UNP P16009
A	582	HIS	-	EXPRESSION TAG	UNP P16009
А	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 2912	C 1858	N 478	O 559	S 2	Se 15	0	0	0

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



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	А	1	Total K 1 1	0	0

• Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	А	1	Total 3	O 2	Р 1	0	0



• Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	307	Total O 307 307	0	0
5	D	82	TotalO8282	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 the various outlier classes 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







4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants	139.26Å 139.26Å 382.00Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
Bosolution(A)	50.00 - 2.90	Depositor
Resolution (A)	49.72 - 2.90	EDS
% Data completeness	5.1(50.00-2.90)	Depositor
(in resolution range)	98.9(49.72-2.90)	EDS
R _{merge}	0.08	Depositor
R _{sym}	0.08	Depositor
$< I/\sigma(I) > 1$	$7.57 (at 2.91 \text{\AA})$	Xtriage
Refinement program	CNS 1.0	Depositor
D D.	0.211 , 0.280	Depositor
Π, Π_{free}	0.212 , 0.277	DCC
R_{free} test set	1602 reflections $(5.04%)$	wwPDB-VP
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
L-test for twinning ²	$ \langle L \rangle = 0.49, \langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	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.

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.



 $^{^1 {\}rm Intensities}$ estimated from amplitudes.

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: 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).

Mal	Chain	Bond lengths		Bond angles	
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	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	\mathbf{Res}	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
1	А	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 (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	А	4309	0	4202	237	1
2	D	2912	0	2835	227	0
3	А	1	0	0	0	0
4	А	3	0	0	0	1
5	А	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	Clash
Atom-1	Atom-2	${f distance} \ ({ m \AA})$	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:221:LEU:HD11	1:A:236:ILE:HD11	1.40	1.01
1:A:416:HIS:CD2	1:A:418:THR:HB	1.95	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



	A construction of the cons	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	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
1:A:214:MET:HG2	1:A:232:ASN:O	1.90	0.71
2:D:80:ILE:H	2:D:80:ILE:HD13	1.55	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
2:D:208:PRO:O	2:D:210:PRO:HD3	1.93	0.69
1:A:418:THR:HG22	1:A:420:THR:H	1.56	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:135:MSE:O	2:D:139:ILE:HG12	1.94	0.67
2:D:324:ILE:HD12	2:D:357:MSE:HE3	1.77	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: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
1:A:418:THR:HG23	1:A:435:VAL:HG21	1.78	0.65
2:D:133:LYS:HG2	2:D:150:ILE:HG21	1.79	0.65
1:A:176:MET:O	1:A:180:LEU:HD23	1.97	0.64
2:D:360:ASN:N	2:D:360:ASN:HD22	1.94	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



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	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
1:A:22:LEU:HD12	1:A:26:ARG:CZ	2.29	0.63
2:D:97:VAL:HG23	2:D:103:ASN:HD22	1.62	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
1:A:522:VAL:HG11	1:A:526:GLN:NE2	2.14	0.61
2:D:345:GLU:O	2:D:352:VAL:HG12	2.00	0.61
1:A:182:ARG:HG2	1:A:182:ARG:HH11	1.64	0.61
1:A:195:GLU:HG2	1:A:197:TYR:CE2	2.34	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
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
2:D:97:VAL:O	2:D:98:ASP:HB2	2.00	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:143:ARG:HH21	2:D:143:ARG:HG3	1.67	0.60
2:D:31:LEU:HD22	2:D:31:LEU:N	2.17	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
1:A:148:GLN:O	1:A:152:LEU:HD13	2.02	0.59
2:D:12:LEU:HD11	2:D:14:VAL:HG23	1.84	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:112:ILE:O	2:D:116:GLU:HG3	2.03	0.58
2:D:173:VAL:HG13	2:D:177:ALA:HB2	1.84	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



		Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap (Å)
2:D:41:ARG:HG2	2:D:343:ILE:HG12	1.86	0.58
2:D:360:ASN:H	2:D:360:ASN:ND2	2.02	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:160:ILE:HD12	2:D:160:ILE:O	2.04	0.58
2:D:41:ARG:HG2	2:D:343:ILE:HG23	1.85	0.58
2:D:80:ILE:CD1	2:D:80:ILE:H	2.17	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:25:GLY:HA3	1:A:73:VAL:HG12	1.87	0.57
1:A:425:SER:HB2	1:A:426:PRO:HD2	1.85	0.57
1:A:123:ARG:HD2	1:A:124:ARG:HH12	1.68	0.57
1:A:273:ARG:HG3	1:A:334:GLY:HA2	1.87	0.57
2:D:283:TYR:O	2:D:286:MSE:HB2	2.05	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: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:208:PRO:HB2	2:D:325:ILE:HB	1.87	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
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:318:LEU:HD23	2:D:355:LEU:HD21	1.87	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
1:A:315:LEU:O	1:A:319:GLN:HG2	2.06	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:236:ILE:HG23	1:A:240:GLU:HB2	1.87	0.55



		Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	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:213:ASP:O	1:A:217:ILE:HG13	2.08	0.54
1:A:270:ASN:HD22	1:A:271:ARG:H	1.52	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:189:TRP:CD1	2:D:320:PRO:HG2	2.43	0.54
2:D:279:ARG:CZ	2:D:286:MSE:HG2	2.38	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
1:A:486:GLU:HG2	5:A:801:HOH:O	2.09	0.53
1:A:58:ILE:HG12	1:A:97:LEU:HD23	1.90	0.53
2:D:96:SER:HG	2:D:104:ILE:HG23	1.73	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:157:VAL:HG13	2:D:172:TYR:HE2	1.73	0.53
2:D:43:SER:CB	2:D:47:ARG:HB3	2.38	0.53
1:A:265:VAL:O	1:A:269:VAL:HG22	2.09	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:178:LEU:HD23	2:D:293:GLU:HB3	1.90	0.53
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
2:D:61:HIS:CD2	2:D:95:VAL:HG11	2.44	0.52
1:A:81:ARG:HH22	1:A:102:GLY:N	2.05	0.52



Atom 1	Atom D	Interatomic	Clash
Atom-1	Atom-2	${ m distance}~({ m \AA})$	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
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
2:D:87:ILE:N	2:D:87:ILE:HD12	2.21	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
1:A:254:ARG:HG2	1:A:254:ARG:HH11	1.75	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: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
1:A:176:MET:O	1:A:180:LEU:CD2	2.57	0.51
2:D:53:GLN:HB3	2:D:106:ALA:HB2	1.93	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:395:THR:OG1	1:A:399:HIS:HB2	2.11	0.50
1:A:378:GLU:OE1	1:A:433:LYS:HG3	2.11	0.50
2:D:136:LEU:HD13	2:D:150:ILE:HD11	1.94	0.50
1:A:522:VAL:HG11	1:A:526:GLN:HE21	1.75	0.50
2:D:30:GLU:C	2:D:31:LEU:HD22	2.32	0.50
2:D:312:THR:CG2	2:D:353:THR:HB	2.42	0.50
2:D:211:MSE:HB2	2:D:326:PHE:CE1	2.47	0.50
1:A:332:LEU:HD22	1:A:332:LEU:O	2.11	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
2:D:80:ILE:HD13	2:D:80:ILE:N	2.26	0.50
1:A:200:ILE:HG12	1:A:201:GLY:N	2.23	0.49
1:A:154:THR:H	1:A:182:ARG:NH2	2.09	0.49
2:D:133:LYS:HE3	2:D:152:ALA:HB3	1.94	0.49



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:102:GLY:O	1:A:128:ASP:HB2	2.12	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:345:GLU:HB3	2:D:352:VAL:CG1	2.43	0.49
1:A:207:MET:SD	1:A:211:VAL:HG21	2.53	0.49
2:D:11:ASN:H	2:D:74:VAL:CG2	2.19	0.49
1:A:553:LYS:NZ	1:A:553:LYS:HB2	2.27	0.49
1:A:370:ASN:C	1:A:370:ASN:ND2	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:202:ILE:HG22	1:A:202:ILE:O	2.13	0.48
1:A:256:ILE:HA	1:A:286:VAL:CG2	2.36	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
2:D:11:ASN:ND2	2:D:80:ILE:HG22	2.26	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
1:A:182:ARG:NH1	1:A:182:ARG:HG2	2.29	0.48
2:D:173:VAL:HG13	2:D:177:ALA:CB	2.43	0.48
2:D:179:ALA:HB1	2:D:182:SER:HB3	1.95	0.48
2:D:313:ILE:HD12	2:D:313:ILE:N	2.27	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
1:A:162:PRO:HG2	1:A:165:GLU:HG3	1.96	0.48
2:D:158:PRO:HD3	2:D:286:MSE:HE1	1.95	0.48
2:D:58:LYS:HB3	2:D:60:ILE:HG13	1.96	0.48
2:D:12:LEU:HA	2:D:74:VAL:HB	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:175:SER:OG	1:A:178:GLU:HG3	2.14	0.47
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: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



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
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:346:LEU:HB2	2:D:350:ASN:O	2.15	0.47
2:D:144:THR:O	2:D:147:THR:HG22	2.15	0.47
1:A:127:ASN:HD22	1:A:127:ASN:C	2.18	0.47
1:A:375:LEU:HD22	1:A:455:LYS:HG2	1.97	0.47
2:D:119:LYS:NZ	5:D:392:HOH:O	2.47	0.47
1:A:239:GLU:O	1:A:242:THR:HG23	2.15	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
2:D:5:GLN:HG3	2:D:9:TYR:CD1	2.50	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
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
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:564:GLN:HG3	1:A:566:THR:HG22	1.96	0.46
1:A:81:ARG:HB3	1:A:100:TYR:CZ	2.50	0.46
1:A:252:MET:CE	1:A:253:GLN:HG3	2.45	0.46
1:A:321:LYS:O	1:A:322:GLY:C	2.54	0.46
1:A:323:ARG:HA	1:A:326:ARG:HH11	1.80	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:114:SER:HA	2:D:167:GLU:OE2	2.16	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:125:PHE:CE2	2:D:134:GLU:HG3	2.50	0.46
1:A:383:TYR:O	1:A:384:LYS:HG3	2.15	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:409:GLN:CA	1:A:409:GLN:NE2	2.77	0.46
1:A:416:HIS:HD2	1:A:418:THR:N	2.11	0.46
1:A:214:MET:HG3	1:A:218:ASN:HD21	1.82	0.45
2:D:54:PHE:CE1	2:D:105:ILE:HD11	2.50	0.45
2:D:122:ARG:HG3	2:D:123:PRO:O	2.17	0.45
1:A:85:HIS:NE2	1:A:97:LEU:HD11	2.32	0.45



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	${ m distance}~({ m \AA})$	overlap (Å)
1:A:9:ASN:HD22	1:A:9:ASN:HA	1.53	0.45
2:D:56:ASP:HA	5:D:413:HOH:O	2.16	0.45
1:A:456:THR:HG22	1:A:457:ASN:N	2.31	0.45
2:D:154:ASN:CG	2:D:180:VAL:HG21	2.37	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:32:ALA:O	2:D:35:ILE:HG22	2.17	0.45
1:A:368:ILE:HG13	1:A:368:ILE:O	2.16	0.45
2:D:90:CYS:CB	2:D:107:ILE:HD11	2.47	0.45
2:D:143:ARG:HG3	2:D:143:ARG:NH2	2.30	0.45
2:D:345:GLU:HB3	2:D:352:VAL:HG13	1.99	0.45
1:A:303:ASP:OD1	1:A:306:LYS:HB2	2.17	0.45
2:D:131:SER:O	2:D:135:MSE:HG3	2.17	0.45
2:D:363:LYS:HG2	5:D:435:HOH:O	2.16	0.45
1:A:337:GLU:HG2	1:A:342:GLU:HA	1.99	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
2:D:174:ARG:NH1	2:D:188:VAL:O	2.50	0.45
2:D:19:SER:H	2:D:22:ALA:HB3	1.80	0.45
2:D:251:ALA:CB	2:D:273:ASN:HB2	2.46	0.45
1:A:73:VAL:O	1:A:73:VAL:HG12	2.17	0.44
2:D:250:ASN:O	2:D:273:ASN:HB2	2.17	0.44
2:D:319:THR:O	2:D:322:VAL:HG12	2.16	0.44
2:D:91:LYS:CA	2:D:115:ILE:HD13	2.47	0.44
2:D:198:MSE:HE1	2:D:206:GLN:HE22	1.82	0.44
2:D:360:ASN:N	2:D:360:ASN:ND2	2.62	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
1:A:61:ILE:HD12	1:A:61:ILE:C	2.37	0.44
2:D:279:ARG:HG3	2:D:289:ARG:O	2.17	0.44
2:D:295:ALA:O	2:D:299:GLN:HG3	2.18	0.44
2:D:296:ILE:HD11	2:D:369:PRO:HD2	1.98	0.44
2:D:328:ASP:HB2	2:D:333:PHE:CE2	2.53	0.44
2:D:66:GLY:O	2:D:90:CYS:HB3	2.18	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:189:TRP:NE1	2:D:320:PRO:HG2	2.33	0.44
2:D:43:SER:HA	2:D:341:GLU:HB3	2.00	0.44
1:A:99:THR:HG22	1:A:100:TYR:N	2.33	0.44
1:A:170:ASP:C	1:A:172:PRO:HD3	2.38	0.44



		Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap (Å)
1:A:200:ILE:HG21	1:A:236:ILE:HD12	1.99	0.44
1:A:370:ASN:HD21	1:A:372:SER:HB2	1.79	0.44
1:A:418:THR:HG22	1:A:419:GLY:N	2.33	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:20:TYR:CZ	2:D:143:ARG:HA	2.54	0.43
2:D:35:ILE:O	2:D:348:ASN:ND2	2.51	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
1:A:242:THR:HG23	1:A:243:THR:H	1.83	0.43
2:D:95:VAL:HG13	2:D:105:ILE:CG2	2.48	0.43
2:D:125:PHE:HE2	2:D:134:GLU:HG3	1.82	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
2:D:35:ILE:HD11	2:D:38:LEU:HB2	2.00	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:299:MET:HG3	1:A:304:TRP:HZ3	1.84	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:270:ASN:O	1:A:274:GLN:N	2.52	0.42
1:A:43:ASP:O	2:D:122:ARG:NE	2.52	0.42
2:D:236:TRP:CD1	2:D:308:ALA:HB2	2.54	0.42
2:D:28:PHE:HD1	2:D:29:VAL:N	2.17	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
1:A:216:GLN:O	1:A:219:LYS:HB3	2.20	0.42
1:A:242:THR:O	1:A:245:PHE:N	2.51	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
2:D:184:LYS:HE3	2:D:367:ILE:CG2	2.49	0.42
2:D:212:ILE:HG13	2:D:230:LEU:HD13	2.01	0.42
2:D:306:GLY:O	2:D:358:PHE:HA	2.20	0.42
1:A:11:PHE:CD1	1:A:11:PHE:C	2.93	0.42
1:A:209:GLN:HE21	1:A:209:GLN:HB2	1.64	0.42
1:A:213:ASP:OD2	1:A:216:GLN:HG3	2.20	0.42
1:A:36:PRO:HB2	1:A:38:GLN:OE1	2.20	0.42



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:D:204:ILE:C	2:D:206:GLN:H	2.23	0.42
2:D:292:TYR:CZ	2:D:296:ILE:HG13	2.54	0.42
2:D:324:ILE:HB	2:D:357:MSE:CE	2.50	0.42
2:D:136:LEU:CD1	2:D:150:ILE:HD11	2.49	0.42
1:A:278:GLU:O	1:A:281:ALA:HB3	2.19	0.42
1:A:58:ILE:HD12	1:A:58:ILE:C	2.40	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
2:D:318:LEU:HD23	2:D:355:LEU:HD11	2.02	0.42
1:A:255:ASP:HB3	1:A:286:VAL:HG11	2.02	0.42
2:D:56:ASP:OD2	2:D:60:ILE:HG13	2.20	0.42
2:D:97:VAL:HG22	2:D:98:ASP:N	2.35	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
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
2:D:57:SER:C	2:D:59:ASN:N	2.74	0.41
1:A:242:THR:O	1:A:245:PHE:HB3	2.21	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
1:A:323:ARG:HA	1:A:326:ARG:NH1	2.36	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
1:A:78:GLU:CD	1:A:78:GLU:H	2.24	0.41
1:A:176:MET:CE	1:A:180:LEU:HD21	2.51	0.41
1:A:232:ASN:HB3	1:A:233:PRO:HD3	2.03	0.41
1:A:385:GLY:HA2	1:A:406:THR:OG1	2.21	0.41
2:D:133:LYS:HE3	2:D:152:ALA:CB	2.51	0.41
2:D:208:PRO:O	2:D:210:PRO:CD	2.67	0.41
2:D:34:THR:HB	2:D:55:TYR:O	2.21	0.41
1:A:176:MET:HG3	1:A:180:LEU:HD21	2.02	0.40
1:A:323:ARG:CA	1:A:326:ARG:HH11	2.34	0.40
1:A:421:TYR:CE1	1:A:433:LYS:HB2	2.56	0.40
1:A:26:ARG:HD3	2:D:259:LEU:HD21	2.02	0.40



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:D:113:HIS:HB3	2:D:139:ILE:HG21	2.03	0.40
2:D:179:ALA:CB	2:D:182:SER:HB3	2.51	0.40
2:D:235:VAL:O	2:D:308:ALA:HB1	2.21	0.40
1:A:252:MET:CE	1:A:278:GLU: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:241:ASN:ND2	2:D:241:ASN:C	2.74	0.40
2:D:254:TYR:CE2	2:D:274:SER:HB2	2.56	0.40
1:A:137:GLU:O	1:A:141:ASP:N	2.48	0.40
1:A:407:PRO:C	1:A:409:GLN:H	2.25	0.40
2:D:157:VAL:HG13	2:D:172:TYR:CE2	2.53	0.40
2:D:368:ASP:N	2:D:369:PRO:CD	2.84	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	$\begin{array}{c} {\rm Interatomic}\\ {\rm distance}~({\rm \AA}) \end{array}$	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	Percer	ntiles
1	А	551/584~(94%)	512 (93%)	31~(6%)	8 (2%)	10	34
2	D	360/391~(92%)	295~(82%)	52 (14%)	13~(4%)	3	14
All	All	911/975~(93%)	807~(89%)	83~(9%)	21 (2%)	6	23

All (21) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	А	575	GLY
2	D	77	ALA
2	D	213	VAL
1	А	232	ASN
2	D	98	ASP
2	D	99	SER
2	D	362	THR
2	D	367	ILE
2	D	370	VAL
1	А	301	ALA
2	D	243	HIS
1	А	110	ARG
1	А	384	LYS
2	D	100	LYS
2	D	124	PHE
2	D	92	HIS
1	А	322	GLY
2	D	313	ILE
1	А	200	ILE
1	А	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	А	472/494~(96%)	435~(92%)	37~(8%)	12 34
2	D	324/333~(97%)	303~(94%)	21~(6%)	17 45
All	All	796/827~(96%)	738~(93%)	58 (7%)	14 38

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

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



Mol	Chain	Res	Type
1	А	34	LEU
1	А	50	GLU
1	А	59	GLN
1	А	62	THR
1	А	89	LYS
1	А	127	ASN
1	А	129	THR
1	А	152	LEU
1	А	184	GLU
1	А	195	GLU
1	А	209	GLN
1	A	242	THR
1	А	296	LEU
1	A	300	LEU
1	A	327	VAL
1	A	335	ASN
1	А	370	ASN
1	А	373	ARG
1	А	375	LEU
1	А	388	PRO
1	А	393	MET
1	А	397	SER
1	А	411	ARG
1	А	418	THR
1	А	429	ARG
1	А	442	THR
1	А	457	ASN
1	А	486	GLU
1	А	495	THR
1	A	519	THR
1	А	522	VAL
1	A	550	TRP
1	А	554	MET
1	Ā	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



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



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 (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)

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 Tune (Chain Dog	Pog Link	Bond lengths			Bond angles			
	туре	Chain			Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
4	PO4	А	586	-	0,2,4	0.00	-	$0,\!1,\!6$	0.00	-



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	А	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 (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, 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	$\mathbf{OWAB}(\mathbf{\AA}^2)$	Q<0.9
1	А	557/584~(95%)	0.11	6 (1%) 80 80	22, 45, 71, 103	0
2	D	349/391~(89%)	1.02	71 (20%) 1 0	49, 85, 120, 138	0
All	All	906/975~(92%)	0.46	77 (8%) 10 8	22, 59, 111, 138	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	216	PRO	5.5
2	D	367	ILE	5.1
2	D	99	SER	4.9
2	D	355	LEU	4.7
2	D	346	LEU	4.6
2	D	103	ASN	4.5
2	D	215	GLU	4.5
2	D	217	SER	4.4
2	D	318	LEU	4.4
2	D	230	LEU	4.4
2	D	100	LYS	4.2
2	D	97	VAL	4.2
2	D	95	VAL	4.1
2	D	310	CYS	4.0
2	D	329	SER	4.0
2	D	312	THR	3.9
1	А	6	ASN	3.8
2	D	337	PHE	3.8
2	D	347	SER	3.8
2	D	98	ASP	3.8
2	D	214	GLY	3.7
2	D	308	ALA	3.7
2	D	338	TYR	3.7
2	D	333	PHE	3.7



2

2

2

2

D

D

D

2	D	326	PHE	3.6
2	D	234	PHE	3.6
2	D	339	VAL	3.5
2	D	78	ASN	3.5
2	D	325	ILE	3.3
2	D	324	ILE	3.2
2	D	313	ILE	3.2
2	D	209	TYR	3.2
1	А	7	ASN	3.1
1	А	269	VAL	3.0
2	D	45	TYR	3.0
2	D	210	PRO	3.0
2	D	212	ILE	2.9
2	D	7	PRO	2.9
2	D	213	VAL	2.8
2	D	334	LYS	2.8
2	D	235	VAL	2.8
2	D	61	HIS	2.8
2	D	311	SER	2.7
2	D	8	GLY	2.7
2	D	336	GLU	2.6
2	D	204	ILE	2.6
2	D	319	THR	2.6
2	D	342	VAL	2.5
2	D	55	TYR	2.5
2	D	335	THR	2.5
2	D	200	TYR	2.5
2	D	292	TYR	2.4
2	D	307	TYR	2.4
2	D	232	TYR	2.4
2	D	356	TYR	2.4
1	А	9	ASN	2.4
1	А	236	ILE	2.3
2	D	327	ASN	2.3
2	D	332	GLN	2.3
2	D	79	ASP	2.2
1	А	62	THR	2.2
2	D	54	PHE	2.2

Continued from previous page...

228

Type

TYR

RSRZ

3.7

Mol Chain Res

D

ASP Continued on next page...

LYS

GLY

2.2

2.2

2.2

309

101

102



	•	<u> </u>		
Mol	Chain	\mathbf{Res}	Type	RSRZ
2	D	320	PRO	2.2
2	D	321	GLY	2.2
2	D	77	ALA	2.2
2	D	31	LEU	2.2
2	D	360	ASN	2.2
2	D	52	LEU	2.1
2	D	184	LYS	2.1
2	D	366	THR	2.1
2	D	109	LEU	2.0
2	D	236	TRP	2.0
2	D	374	ASN	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. 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	$\mathbf{B} extsf{-}\mathbf{B} extsf{-}\mathbf{factors}(\mathbf{A}^2)$	Q<0.9
3	K	А	585	1/1	0.91	0.15	$48,\!48,\!48,\!48$	1
4	PO4	А	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.

