Full wwPDB X-ray Structure Validation Report

Aug 14, 2023 – 10:43 PM EDT

PDB ID	:	1R0C
Title	:	Products in the T State of Aspartate Transcarbamylase: Crystal Structure of the Phosphate and N-carbamyl-L-aspartate Ligated Enzyme
Authors	:	Huang, J.; Lipscomb, W.N.
Deposited on	:	2003-09-19
Resolution	:	2.37 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:

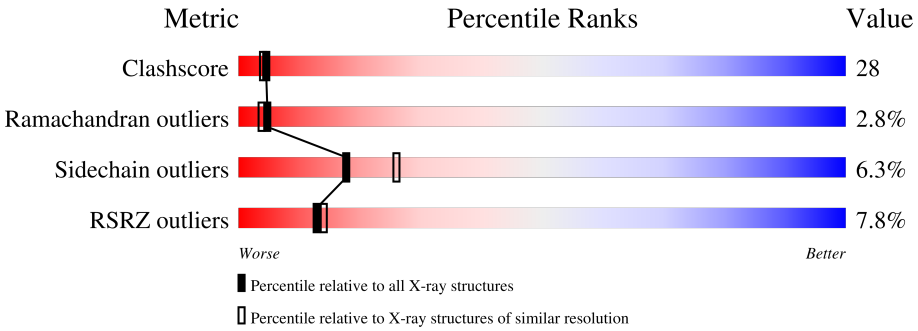
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.37 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))
Clashscore	141614	6082 (2.40-2.36)
Ramachandran outliers	138981	5973 (2.40-2.36)
Sidechain outliers	138945	5975 (2.40-2.36)
RSRZ outliers	127900	5397 (2.40-2.36)

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 <=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	310	3% 60% 33% 6%
1	G	310	3% 61% 32% 6%
2	B	153	18% 44% 50% 5%
2	H	153	16% 50% 46%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PO4	G	3002	-	-	X	-
4	NCD	G	2002	-	-	-	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 7821 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.

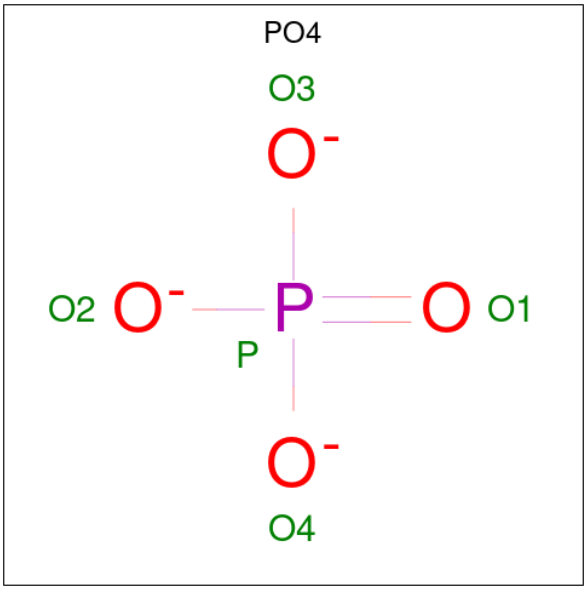
- Molecule 1 is a protein called Aspartate carbamoyltransferase catalytic chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	310	Total	C	N	O	S	0	0	0
			2415	1527	423	456	9			
1	G	310	Total	C	N	O	S	0	0	0
			2415	1527	423	456	9			

- Molecule 2 is a protein called Aspartate carbamoyltransferase regulatory chain.

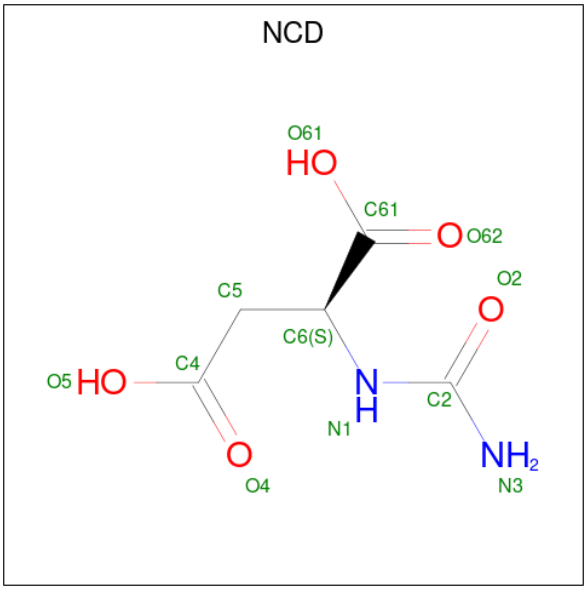
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	153	Total	C	N	O	S	0	0	0
			1201	752	213	230	6			
2	H	153	Total	C	N	O	S	0	0	0
			1201	752	213	230	6			

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O P 5 4 1	0	0
3	G	1	Total O P 5 4 1	0	0

- Molecule 4 is N-CARBAMOYL-L-ASPARTATE (three-letter code: NCD) (formula: $C_5H_8N_2O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 12 5 2 5	0	0
4	G	1	Total C N O 12 5 2 5	0	0

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Zn 1 1	0	0
5	H	1	Total Zn 1 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	197	Total O 197 197	0	0

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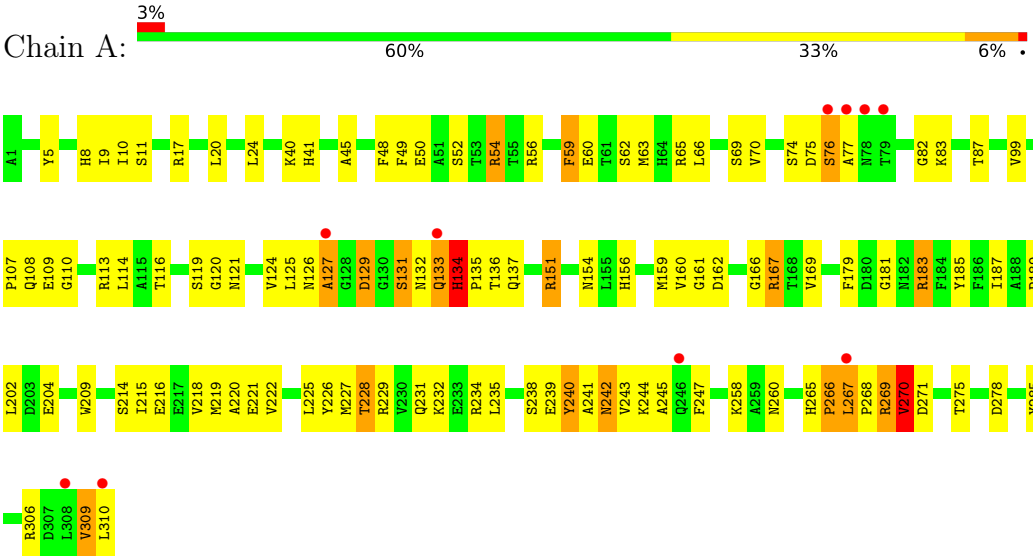
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	79	Total O 79 79	0	0
6	G	185	Total O 185 185	0	0
6	H	92	Total O 92 92	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

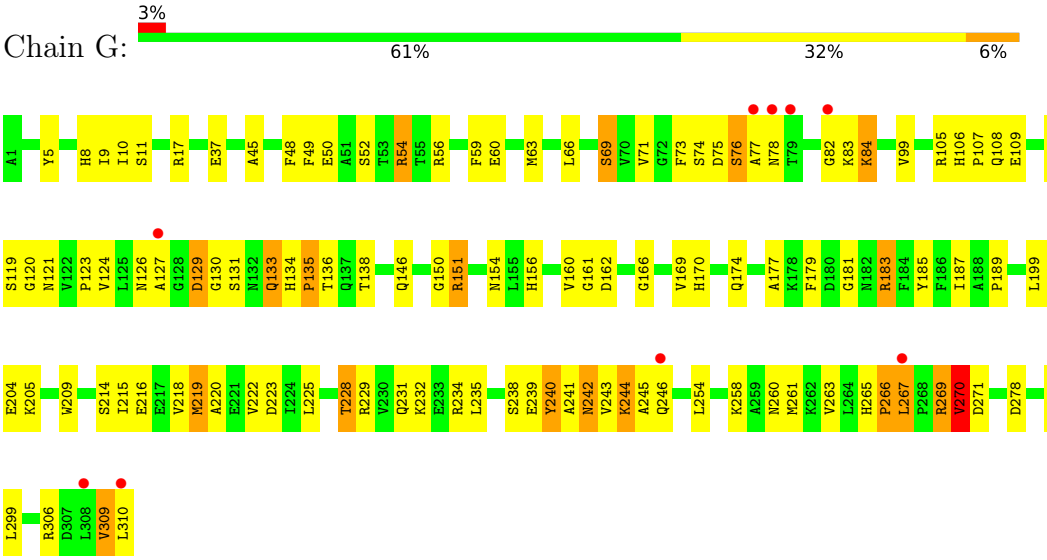
• Molecule 1: Aspartate carbamoyltransferase catalytic chain

Chain A:



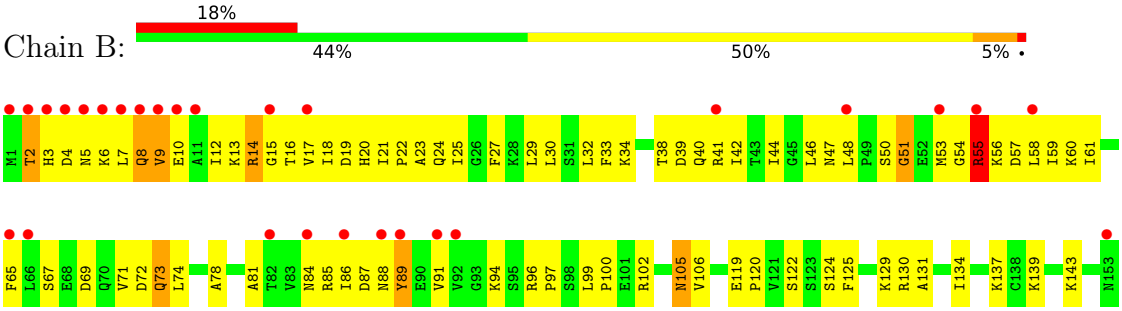
• Molecule 1: Aspartate carbamoyltransferase catalytic chain

Chain G:



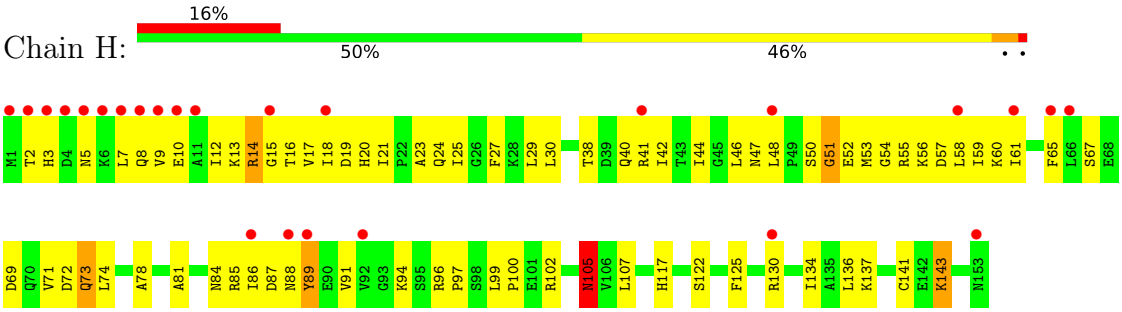
• Molecule 2: Aspartate carbamoyltransferase regulatory chain

Chain B:



• Molecule 2: Aspartate carbamoyltransferase regulatory chain

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	128.78Å 128.78Å 198.02Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.37 48.59 – 2.40	Depositor EDS
% Data completeness (in resolution range)	95.0 (50.00-2.37) 91.2 (48.59-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	2.06 (at 2.39Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.226 , 0.274 0.226 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	36.8	Xtriage
Anisotropy	0.024	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 36.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.476 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	7821	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.71% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: NCD, PO4, 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	0.38	0/2461	0.71	3/3339 (0.1%)
1	G	0.39	0/2461	0.73	4/3339 (0.1%)
2	B	0.32	0/1219	0.60	0/1647
2	H	0.31	0/1219	0.61	0/1647
All	All	0.36	0/7360	0.69	7/9972 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	135	PRO	CA-N-CD	-12.58	93.89	111.50
1	A	267	LEU	N-CA-C	7.77	131.99	111.00
1	G	267	LEU	N-CA-C	7.28	130.67	111.00
1	G	266	PRO	N-CA-C	-6.00	96.51	112.10
1	A	266	PRO	N-CA-C	-5.95	96.63	112.10
1	A	119	SER	N-CA-C	-5.21	96.92	111.00
1	G	119	SER	N-CA-C	-5.00	97.49	111.00

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	2415	0	2422	124	0
1	G	2415	0	2422	142	0
2	B	1201	0	1219	83	0
2	H	1201	0	1219	78	0
3	A	5	0	0	0	0
3	G	5	0	0	2	0
4	A	12	0	6	1	0
4	G	12	0	6	1	0
5	B	1	0	0	0	0
5	H	1	0	0	0	0
6	A	197	0	0	6	0
6	B	79	0	0	5	0
6	G	185	0	0	12	0
6	H	92	0	0	7	0
All	All	7821	0	7294	413	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 28.

All (413) 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:G:60:GLU:HA	1:G:63:MET:CE	1.83	1.07
1:G:11:SER:HA	1:G:133:GLN:HG3	1.09	1.05
1:G:11:SER:CA	1:G:133:GLN:HG3	1.86	1.05
1:A:201:MET:CE	1:A:202:LEU:HD23	1.89	1.02
1:A:11:SER:HA	1:A:133:GLN:HG3	1.38	1.01
1:G:60:GLU:HA	1:G:63:MET:HE3	1.41	1.01
1:G:309:VAL:HG12	1:G:310:LEU:H	1.31	0.95
1:A:309:VAL:HG12	1:A:310:LEU:H	1.33	0.92
2:H:2:THR:HG22	2:H:3:HIS:H	1.34	0.92
1:A:60:GLU:HA	1:A:63:MET:CE	2.00	0.91
1:A:60:GLU:HA	1:A:63:MET:HE3	1.55	0.89
1:G:60:GLU:HA	1:G:63:MET:HE2	1.59	0.84
1:G:269:ARG:O	1:G:270:VAL:HG13	1.76	0.84
1:A:162:ASP:H	1:A:228:THR:HG21	1.43	0.83
1:A:201:MET:HE1	1:A:202:LEU:HD23	1.61	0.82
1:A:229:ARG:HE	1:A:231:GLN:NE2	1.77	0.82
2:H:53:MET:HG2	2:H:54:GLY:N	1.92	0.82
1:G:106:HIS:HD2	1:G:108:GLN:H	1.25	0.82
2:B:5:ASN:HB2	2:H:7:LEU:HD13	1.59	0.82
1:A:11:SER:CA	1:A:133:GLN:HG3	2.08	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:133:GLN:O	1:G:135:PRO:HD2	1.81	0.80
1:G:229:ARG:HE	1:G:231:GLN:NE2	1.78	0.80
1:G:133:GLN:HA	1:G:133:GLN:OE1	1.82	0.80
1:G:17:ARG:NH2	1:G:179:PHE:HA	1.98	0.79
2:H:14:ARG:HB2	6:H:1022:HOH:O	1.82	0.79
1:A:106:HIS:HD2	1:A:108:GLN:H	1.32	0.78
2:B:20:HIS:HA	2:B:56:LYS:HD2	1.65	0.78
2:B:8:GLN:O	2:B:9:VAL:HG23	1.84	0.78
1:A:162:ASP:H	1:A:228:THR:CG2	1.97	0.78
1:A:215:ILE:HD12	1:A:215:ILE:H	1.48	0.78
2:H:20:HIS:HA	2:H:56:LYS:HD2	1.65	0.77
1:A:162:ASP:N	1:A:228:THR:HG21	2.00	0.77
2:H:53:MET:HG2	2:H:54:GLY:H	1.48	0.77
1:G:127:ALA:O	1:G:134:HIS:CD2	2.37	0.76
2:B:102:ARG:HB2	6:B:1012:HOH:O	1.85	0.76
1:A:201:MET:CE	1:A:202:LEU:CD2	2.64	0.76
1:G:162:ASP:H	1:G:228:THR:HG21	1.51	0.76
1:A:160:VAL:HB	1:A:227:MET:HE2	1.68	0.76
1:G:133:GLN:C	1:G:135:PRO:HD2	2.06	0.76
2:H:58:LEU:HD21	2:H:60:LYS:HE3	1.68	0.75
1:A:133:GLN:OE1	1:A:133:GLN:HA	1.86	0.74
1:G:240:TYR:HE1	1:G:244:LYS:HD2	1.51	0.74
1:A:129:ASP:OD2	1:A:132:ASN:ND2	2.20	0.74
1:A:161:GLY:HA3	1:A:228:THR:HG22	1.71	0.73
1:G:201:MET:HE2	1:G:202:LEU:HA	1.70	0.73
1:G:162:ASP:N	1:G:228:THR:HG21	2.04	0.73
2:B:44:ILE:HB	2:H:44:ILE:HB	1.69	0.72
1:G:215:ILE:HD12	1:G:215:ILE:H	1.53	0.72
1:A:17:ARG:NH2	1:A:179:PHE:HA	2.05	0.72
1:A:189:PRO:HB3	1:A:243:VAL:HG11	1.71	0.71
1:G:120:GLY:O	1:G:121:ASN:HB2	1.88	0.71
2:H:12:ILE:HG22	2:H:13:LYS:H	1.55	0.71
1:A:201:MET:HE1	1:A:202:LEU:CD2	2.19	0.71
2:B:5:ASN:HB2	2:H:7:LEU:CD1	2.20	0.71
1:G:162:ASP:H	1:G:228:THR:CG2	2.04	0.70
2:H:12:ILE:HG22	2:H:13:LYS:N	2.05	0.70
2:H:65:PHE:HB3	2:H:85:ARG:HH21	1.56	0.70
1:A:133:GLN:O	1:A:135:PRO:CD	2.40	0.69
1:G:189:PRO:HB3	1:G:243:VAL:HG11	1.73	0.68
2:B:32:LEU:HD22	2:B:106:VAL:HG13	1.75	0.68
1:A:309:VAL:HG12	1:A:310:LEU:N	2.08	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:58:LEU:HD21	2:B:60:LYS:HE3	1.76	0.68
1:A:60:GLU:HA	1:A:63:MET:HE2	1.74	0.68
2:B:72:ASP:HB3	2:B:100:PRO:HG3	1.75	0.68
1:A:269:ARG:O	1:A:270:VAL:HG13	1.94	0.67
1:G:127:ALA:O	1:G:134:HIS:HD2	1.77	0.67
1:G:161:GLY:HA3	1:G:228:THR:HG22	1.77	0.67
1:G:183:ARG:HG3	1:G:183:ARG:HH11	1.60	0.67
1:G:234:ARG:HG2	1:G:234:ARG:HH11	1.60	0.66
2:B:12:ILE:HG22	2:B:13:LYS:N	2.11	0.66
1:A:120:GLY:O	1:A:121:ASN:HB2	1.95	0.66
1:A:54:ARG:HB3	4:A:2001:NCD:O62	1.96	0.66
1:A:215:ILE:HD12	1:A:215:ILE:N	2.10	0.65
2:B:17:VAL:HG13	2:B:60:LYS:HG2	1.78	0.65
2:H:13:LYS:HE2	6:H:1022:HOH:O	1.96	0.65
1:G:258:LYS:HE3	1:G:260:ASN:HD21	1.61	0.65
1:G:17:ARG:HH21	1:G:179:PHE:HA	1.62	0.65
1:G:240:TYR:HD1	1:G:241:ALA:N	1.95	0.65
1:A:258:LYS:HE3	1:A:260:ASN:HD21	1.61	0.64
1:A:269:ARG:O	1:A:270:VAL:HG22	1.97	0.64
1:G:265:HIS:ND1	1:G:266:PRO:O	2.26	0.64
2:B:65:PHE:HB3	2:B:85:ARG:HH21	1.61	0.64
2:B:105:ASN:OD1	2:B:122:SER:HB3	1.97	0.63
1:A:131:SER:O	1:A:131:SER:OG	2.12	0.63
1:G:201:MET:HE2	1:G:202:LEU:HD23	1.80	0.63
1:G:177:ALA:HB1	1:G:201:MET:HE1	1.78	0.63
1:A:48:PHE:CD1	1:A:56:ARG:HG3	2.34	0.63
1:A:50:GLU:HB2	1:A:107:PRO:HD3	1.81	0.63
2:B:78:ALA:HB1	2:B:81:ALA:HB2	1.81	0.63
1:A:240:TYR:HD1	1:A:241:ALA:N	1.97	0.63
1:G:199:LEU:HD13	1:G:209:TRP:CH2	2.34	0.63
1:A:183:ARG:HG3	1:A:183:ARG:HH11	1.65	0.62
2:B:39:ASP:HB3	2:H:55:ARG:NH1	2.14	0.62
1:A:235:LEU:HD22	1:A:239:GLU:CD	2.21	0.62
1:G:60:GLU:HG2	1:G:63:MET:CE	2.30	0.61
1:G:309:VAL:HG12	1:G:310:LEU:N	2.09	0.61
1:A:48:PHE:CE1	1:A:56:ARG:HG3	2.35	0.61
1:G:245:ALA:HB1	6:G:3079:HOH:O	2.00	0.61
1:G:76:SER:HB2	1:G:78:ASN:ND2	2.16	0.61
2:H:25:ILE:O	2:H:29:LEU:HG	2.00	0.61
1:G:60:GLU:HG2	1:G:63:MET:HE1	1.82	0.60
1:A:60:GLU:HG2	1:A:63:MET:CE	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:78:ALA:HB1	2:H:81:ALA:HB2	1.84	0.60
1:A:11:SER:CB	1:A:133:GLN:HG3	2.31	0.60
1:A:240:TYR:HE1	1:A:244:LYS:HD2	1.67	0.60
1:A:87:THR:HB	2:B:119:GLU:OE1	2.01	0.60
2:B:61:ILE:HD12	2:B:61:ILE:N	2.17	0.60
1:G:113:ARG:O	1:G:116:THR:HB	2.00	0.60
1:A:133:GLN:O	1:A:135:PRO:HD2	2.02	0.60
1:G:109:GLU:HG3	1:G:130:GLY:O	2.02	0.59
1:G:54:ARG:HB3	4:G:2002:NCD:O62	2.02	0.59
1:G:243:VAL:O	1:G:245:ALA:N	2.35	0.59
2:H:72:ASP:HB3	2:H:100:PRO:HG3	1.83	0.59
2:B:99:LEU:HD21	2:B:134:ILE:HD12	1.84	0.59
1:G:183:ARG:HG3	1:G:183:ARG:NH1	2.17	0.59
1:G:48:PHE:CE1	1:G:56:ARG:HG3	2.38	0.58
2:H:65:PHE:CB	2:H:85:ARG:HH21	2.16	0.58
2:H:17:VAL:HG13	2:H:60:LYS:HG2	1.85	0.58
1:G:11:SER:CB	1:G:133:GLN:HG3	2.32	0.58
2:B:48:LEU:O	2:B:56:LYS:HG2	2.04	0.58
1:G:60:GLU:CG	1:G:63:MET:CE	2.82	0.58
1:G:76:SER:HB2	1:G:78:ASN:HD21	1.69	0.58
2:B:2:THR:HG23	2:B:3:HIS:N	2.18	0.58
1:A:234:ARG:HG2	1:A:234:ARG:HH11	1.68	0.57
1:A:166:GLY:O	1:A:169:VAL:HG22	2.04	0.57
1:A:109:GLU:HA	1:A:129:ASP:HB2	1.85	0.57
1:A:133:GLN:O	1:A:135:PRO:HD3	2.04	0.57
1:G:243:VAL:C	1:G:245:ALA:H	2.07	0.57
2:B:96:ARG:HG3	2:B:97:PRO:CD	2.34	0.57
2:B:7:LEU:HD11	2:H:10:GLU:HA	1.86	0.57
2:H:99:LEU:HD21	2:H:134:ILE:HD12	1.87	0.57
1:A:238:SER:O	1:A:242:ASN:HB2	2.04	0.57
2:B:13:LYS:HB3	2:B:89:TYR:CG	2.40	0.57
2:B:25:ILE:O	2:B:29:LEU:HG	2.04	0.57
1:G:129:ASP:O	1:G:130:GLY:C	2.40	0.57
1:A:269:ARG:C	1:A:270:VAL:HG22	2.25	0.56
1:G:134:HIS:HD2	6:G:3010:HOH:O	1.88	0.56
1:G:82:GLY:O	1:G:84:LYS:N	2.39	0.56
1:G:154:ASN:HA	1:G:181:GLY:O	2.05	0.56
1:G:201:MET:HE3	1:G:205:LYS:HD2	1.85	0.56
1:G:215:ILE:HD12	1:G:215:ILE:N	2.19	0.56
2:B:53:MET:HG2	2:B:54:GLY:N	2.20	0.56
2:B:7:LEU:C	2:B:9:VAL:H	2.09	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:214:SER:OG	1:G:216:GLU:HG2	2.05	0.56
1:A:215:ILE:H	1:A:215:ILE:CD1	2.17	0.56
2:B:22:PRO:HB2	2:B:25:ILE:HG13	1.85	0.56
1:A:120:GLY:O	1:A:121:ASN:CB	2.53	0.56
1:G:50:GLU:HB2	1:G:107:PRO:HD3	1.88	0.56
2:H:61:ILE:N	2:H:61:ILE:HD12	2.20	0.56
1:A:49:PHE:HA	1:A:75:ASP:HB3	1.87	0.55
1:G:5:TYR:CZ	1:G:306:ARG:HG3	2.42	0.55
1:G:238:SER:O	1:G:242:ASN:HB2	2.05	0.55
1:A:60:GLU:HG2	1:A:63:MET:HE1	1.88	0.55
1:G:129:ASP:OD1	1:G:129:ASP:N	2.38	0.55
2:H:2:THR:HG22	2:H:3:HIS:N	2.14	0.55
1:A:9:ILE:HG21	1:A:299:LEU:HD21	1.87	0.55
1:A:268:PRO:HG2	6:A:3084:HOH:O	2.06	0.55
2:B:65:PHE:CB	2:B:85:ARG:HH21	2.20	0.55
1:G:235:LEU:HD22	1:G:239:GLU:CD	2.27	0.55
1:A:5:TYR:CZ	1:A:306:ARG:HG3	2.41	0.55
2:B:72:ASP:C	2:B:74:LEU:H	2.09	0.55
1:G:60:GLU:CA	1:G:63:MET:HE2	2.35	0.55
2:H:12:ILE:CG2	2:H:13:LYS:H	2.19	0.55
1:G:225:LEU:HD23	1:G:263:VAL:HG22	1.89	0.54
1:G:60:GLU:CA	1:G:63:MET:CE	2.73	0.54
2:H:27:PHE:HA	2:H:30:LEU:HD12	1.90	0.54
1:G:240:TYR:CD1	1:G:241:ALA:N	2.74	0.54
1:A:183:ARG:HG3	1:A:183:ARG:NH1	2.21	0.54
1:A:265:HIS:ND1	1:A:266:PRO:O	2.25	0.54
2:B:12:ILE:HG22	2:B:13:LYS:H	1.72	0.54
2:H:7:LEU:C	2:H:9:VAL:H	2.11	0.54
1:G:134:HIS:CE1	3:G:3002:PO4:O1	2.61	0.54
1:G:134:HIS:HE1	3:G:3002:PO4:O1	1.91	0.53
1:G:201:MET:HE2	1:G:202:LEU:CA	2.36	0.53
2:H:7:LEU:O	2:H:9:VAL:N	2.41	0.53
1:G:49:PHE:HA	1:G:75:ASP:HB3	1.90	0.53
2:H:72:ASP:C	2:H:74:LEU:H	2.11	0.53
1:G:109:GLU:HA	1:G:129:ASP:HB2	1.90	0.53
1:G:120:GLY:O	1:G:121:ASN:CB	2.56	0.53
1:G:69:SER:HB2	6:G:3026:HOH:O	2.07	0.53
1:A:17:ARG:HH21	1:A:179:PHE:HA	1.72	0.53
1:G:189:PRO:HB3	1:G:243:VAL:CG1	2.39	0.53
1:A:56:ARG:NH1	6:A:3125:HOH:O	2.41	0.53
1:A:156:HIS:HD2	1:A:185:TYR:OH	1.92	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:15:GLY:O	2:H:86:ILE:HB	2.08	0.53
1:G:160:VAL:HG22	1:G:187:ILE:HB	1.91	0.52
1:A:240:TYR:CD1	1:A:241:ALA:N	2.75	0.52
2:B:42:ILE:HB	2:H:46:LEU:HB2	1.91	0.52
2:H:50:SER:O	2:H:51:GLY:C	2.47	0.52
2:B:67:SER:O	2:B:71:VAL:HG23	2.08	0.52
2:B:96:ARG:HG3	2:B:97:PRO:HD2	1.91	0.52
1:G:269:ARG:C	1:G:270:VAL:HG22	2.29	0.52
1:G:76:SER:O	1:G:77:ALA:HB3	2.10	0.52
1:G:109:GLU:OE2	1:G:131:SER:HB3	2.09	0.52
2:H:84:ASN:OD1	2:H:94:LYS:HG3	2.09	0.52
2:H:13:LYS:HB3	2:H:89:TYR:CG	2.45	0.52
1:G:105:ARG:HB2	1:G:127:ALA:HB3	1.92	0.52
1:G:166:GLY:O	1:G:169:VAL:CG2	2.59	0.51
1:A:126:ASN:O	1:A:127:ALA:C	2.44	0.51
1:G:106:HIS:CD2	1:G:108:GLN:H	2.15	0.51
1:A:225:LEU:HG	1:A:227:MET:HE3	1.92	0.51
2:H:102:ARG:HB3	6:H:1014:HOH:O	2.09	0.51
1:A:159:MET:HG2	1:A:226:TYR:HB3	1.91	0.51
1:A:200:ASP:O	1:A:204:GLU:HG3	2.10	0.51
1:G:246:GLN:HA	6:G:3136:HOH:O	2.11	0.51
2:B:91:VAL:HG23	2:B:91:VAL:O	2.11	0.51
1:A:189:PRO:HB3	1:A:243:VAL:CG1	2.40	0.51
2:B:18:ILE:HG22	2:B:21:ILE:HD11	1.93	0.51
1:A:45:ALA:HB2	1:A:99:VAL:HG11	1.92	0.51
2:B:15:GLY:O	2:B:86:ILE:HB	2.11	0.51
1:G:8:HIS:HB3	1:G:10:ILE:HD13	1.93	0.51
2:H:18:ILE:HG22	2:H:21:ILE:HD11	1.93	0.51
1:A:133:GLN:OE1	1:A:133:GLN:CA	2.57	0.51
2:B:87:ASP:OD1	2:B:88:ASN:N	2.44	0.51
1:G:134:HIS:CD2	6:G:3010:HOH:O	2.63	0.51
2:H:48:LEU:O	2:H:56:LYS:HG2	2.11	0.51
1:A:129:ASP:OD1	1:A:129:ASP:N	2.42	0.50
1:G:11:SER:HA	1:G:133:GLN:CG	2.05	0.50
1:A:154:ASN:HA	1:A:181:GLY:O	2.10	0.50
1:A:151:ARG:NH1	1:A:154:ASN:O	2.44	0.50
1:G:200:ASP:O	1:G:204:GLU:HG3	2.11	0.50
2:H:87:ASP:OD1	2:H:88:ASN:N	2.45	0.50
1:G:8:HIS:CE1	1:G:123:PRO:HA	2.46	0.50
2:H:12:ILE:CG2	2:H:13:LYS:N	2.72	0.50
1:G:243:VAL:C	1:G:245:ALA:N	2.65	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:ARG:NE	1:A:231:GLN:NE2	2.55	0.50
1:A:269:ARG:HG2	1:A:270:VAL:N	2.27	0.50
2:B:60:LYS:C	2:B:61:ILE:HD12	2.32	0.50
2:B:130:ARG:HG3	6:B:1052:HOH:O	2.11	0.50
1:G:66:LEU:CD2	1:G:297:GLN:HE21	2.25	0.49
1:G:183:ARG:NH1	6:G:3182:HOH:O	2.44	0.49
1:G:11:SER:CB	1:G:133:GLN:CG	2.90	0.49
1:G:215:ILE:H	1:G:215:ILE:CD1	2.24	0.49
2:H:51:GLY:HA3	6:H:1018:HOH:O	2.12	0.49
2:H:91:VAL:O	2:H:91:VAL:HG23	2.12	0.49
1:A:126:ASN:O	1:A:127:ALA:O	2.30	0.49
2:H:87:ASP:C	2:H:89:TYR:N	2.66	0.49
2:H:130:ARG:HG3	6:H:1078:HOH:O	2.11	0.49
1:G:133:GLN:OE1	1:G:133:GLN:CA	2.56	0.49
2:B:129:LYS:HD2	2:B:130:ARG:H	1.78	0.49
1:G:240:TYR:CE1	1:G:244:LYS:HD2	2.39	0.49
2:H:96:ARG:HG3	2:H:97:PRO:HD2	1.95	0.49
1:A:8:HIS:HB3	1:A:10:ILE:HD13	1.94	0.48
1:A:229:ARG:HE	1:A:231:GLN:HE21	1.54	0.48
2:H:125:PHE:HA	2:H:137:LYS:O	2.13	0.48
1:A:59:PHE:O	1:A:62:SER:HB2	2.13	0.48
1:A:270:VAL:O	1:A:271:ASP:CB	2.61	0.48
2:B:7:LEU:HD22	2:H:5:ASN:HB3	1.95	0.48
2:B:20:HIS:HA	2:B:56:LYS:CD	2.41	0.48
1:G:136:THR:HG22	1:G:299:LEU:HD22	1.95	0.48
1:G:48:PHE:CD1	1:G:56:ARG:HG3	2.49	0.48
1:A:160:VAL:HG22	1:A:187:ILE:HB	1.94	0.48
2:B:16:THR:OG1	2:B:65:PHE:HA	2.14	0.48
1:G:244:LYS:HG2	1:G:244:LYS:O	2.12	0.48
2:H:53:MET:CG	2:H:54:GLY:N	2.71	0.48
2:H:67:SER:O	2:H:71:VAL:HG23	2.13	0.48
1:A:189:PRO:CB	1:A:243:VAL:HG11	2.42	0.48
1:A:82:GLY:O	1:A:83:LYS:C	2.52	0.48
2:H:18:ILE:CG2	2:H:21:ILE:HD11	2.44	0.48
2:H:69:ASP:O	2:H:73:GLN:HG2	2.13	0.48
1:A:76:SER:O	1:A:77:ALA:HB3	2.14	0.47
1:A:265:HIS:O	1:A:266:PRO:C	2.53	0.47
2:B:48:LEU:C	6:B:1020:HOH:O	2.52	0.47
2:H:105:ASN:OD1	2:H:122:SER:HB3	2.14	0.47
2:B:39:ASP:HB3	2:H:55:ARG:HH12	1.78	0.47
1:G:126:ASN:O	1:G:127:ALA:C	2.51	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:VAL:HG22	1:A:125:LEU:HB2	1.96	0.47
1:G:189:PRO:CB	1:G:243:VAL:HG11	2.42	0.47
1:A:214:SER:OG	1:A:216:GLU:HG2	2.14	0.47
1:G:177:ALA:CB	1:G:201:MET:HE1	2.44	0.47
2:H:55:ARG:HA	6:H:1017:HOH:O	2.15	0.47
2:H:60:LYS:C	2:H:61:ILE:HD12	2.35	0.47
2:B:12:ILE:CG2	2:B:13:LYS:N	2.76	0.47
2:B:54:GLY:O	2:B:55:ARG:C	2.52	0.47
2:B:130:ARG:HG3	2:B:131:ALA:H	1.80	0.47
1:G:116:THR:HG22	6:G:3059:HOH:O	2.15	0.47
1:G:232:LYS:HA	1:G:240:TYR:HD2	1.78	0.47
1:A:113:ARG:O	1:A:116:THR:HB	2.14	0.47
2:H:117:HIS:HD2	6:H:1074:HOH:O	1.98	0.47
1:G:106:HIS:HD2	1:G:108:GLN:N	2.04	0.47
1:G:201:MET:CE	1:G:205:LYS:HD2	2.45	0.47
2:B:46:LEU:HB2	2:H:42:ILE:HB	1.97	0.46
1:G:240:TYR:CD1	1:G:240:TYR:C	2.89	0.46
1:A:40:LYS:HG2	1:A:41:HIS:CD2	2.49	0.46
2:B:8:GLN:O	2:B:9:VAL:CG2	2.60	0.46
2:B:87:ASP:C	2:B:89:TYR:N	2.69	0.46
1:G:126:ASN:ND2	1:G:129:ASP:OD1	2.38	0.46
1:G:201:MET:CE	1:G:202:LEU:HD23	2.44	0.46
2:B:69:ASP:O	2:B:73:GLN:HG2	2.15	0.46
1:G:60:GLU:CG	1:G:63:MET:HE1	2.43	0.46
2:B:18:ILE:CG2	2:B:21:ILE:HD11	2.45	0.46
2:B:59:ILE:HG22	2:B:61:ILE:CD1	2.46	0.46
1:A:10:ILE:HD11	1:A:124:VAL:HG23	1.98	0.46
1:G:8:HIS:CD2	1:G:116:THR:HG23	2.51	0.46
1:G:151:ARG:NH1	1:G:154:ASN:O	2.48	0.46
2:B:5:ASN:CB	2:H:7:LEU:HD13	2.38	0.46
2:H:16:THR:OG1	2:H:65:PHE:HA	2.16	0.46
1:A:59:PHE:CZ	1:A:136:THR:HG21	2.51	0.46
1:G:10:ILE:HD11	1:G:124:VAL:CG2	2.46	0.46
1:G:73:PHE:HD1	1:G:75:ASP:H	1.62	0.46
1:G:229:ARG:HE	1:G:231:GLN:HE21	1.57	0.45
1:G:240:TYR:O	1:G:241:ALA:C	2.54	0.45
2:H:50:SER:O	2:H:52:GLU:O	2.34	0.45
1:A:60:GLU:CG	1:A:63:MET:CE	2.95	0.45
1:G:170:HIS:O	1:G:174:GLN:HG3	2.16	0.45
1:G:45:ALA:HA	1:G:71:VAL:O	2.17	0.45
1:G:166:GLY:O	1:G:169:VAL:HG22	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:223:ASP:O	1:G:261:MET:HA	2.17	0.45
1:G:228:THR:HG23	1:G:229:ARG:N	2.32	0.45
1:A:106:HIS:CD2	1:A:107:PRO:HD2	2.51	0.45
1:A:218:VAL:O	1:A:220:ALA:N	2.50	0.45
1:A:199:LEU:HD13	1:A:209:TRP:CH2	2.52	0.45
1:A:66:LEU:CD2	1:A:297:GLN:HE21	2.30	0.44
1:G:219:MET:HE3	1:G:254:LEU:HD23	1.99	0.44
2:B:23:ALA:O	2:B:24:GLN:HB2	2.18	0.44
2:H:23:ALA:O	2:H:24:GLN:HB2	2.18	0.44
2:H:20:HIS:H	2:H:56:LYS:NZ	2.15	0.44
1:G:229:ARG:NE	1:G:231:GLN:NE2	2.58	0.44
1:G:134:HIS:N	6:G:3011:HOH:O	2.51	0.44
1:A:269:ARG:NH2	1:A:278:ASP:OD1	2.50	0.44
2:B:47:ASN:ND2	2:H:40:GLN:O	2.51	0.44
1:G:218:VAL:O	1:G:220:ALA:N	2.51	0.44
1:A:106:HIS:CD2	1:A:108:GLN:H	2.23	0.44
1:A:166:GLY:O	1:A:169:VAL:CG2	2.66	0.44
2:B:41:ARG:HA	2:H:47:ASN:HB2	1.99	0.44
1:G:138:THR:HA	6:G:3025:HOH:O	2.16	0.44
2:H:21:ILE:HB	2:H:57:ASP:HB2	1.99	0.44
1:A:201:MET:HE3	1:A:202:LEU:HD23	1.90	0.43
2:H:87:ASP:C	2:H:89:TYR:H	2.20	0.43
1:A:110:GLY:HA2	6:A:3022:HOH:O	2.19	0.43
2:B:59:ILE:HG22	2:B:61:ILE:HD11	2.00	0.43
1:G:126:ASN:O	1:G:127:ALA:O	2.37	0.43
2:H:7:LEU:C	2:H:9:VAL:N	2.71	0.43
2:H:72:ASP:CB	2:H:100:PRO:HG3	2.48	0.43
1:G:234:ARG:HH11	1:G:234:ARG:CG	2.29	0.43
2:H:19:ASP:CG	2:H:56:LYS:HZ1	2.21	0.43
2:B:102:ARG:NH1	2:B:124:SER:OG	2.51	0.43
2:B:125:PHE:HA	2:B:137:LYS:O	2.19	0.43
1:A:232:LYS:HA	1:A:240:TYR:HD2	1.83	0.43
2:B:27:PHE:HA	2:B:30:LEU:HD12	2.00	0.43
1:G:166:GLY:O	1:G:169:VAL:HG23	2.19	0.43
2:B:12:ILE:CG2	2:B:13:LYS:H	2.30	0.43
1:G:246:GLN:O	1:G:246:GLN:HG3	2.19	0.43
1:A:65:ARG:HD3	1:A:65:ARG:HA	1.81	0.42
1:G:9:ILE:C	1:G:10:ILE:HD12	2.38	0.42
1:G:56:ARG:NH1	6:G:3119:HOH:O	2.51	0.42
1:A:126:ASN:ND2	1:A:129:ASP:OD1	2.41	0.42
1:A:240:TYR:O	1:A:241:ALA:C	2.57	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:269:ARG:O	1:G:270:VAL:CG1	2.58	0.42
2:B:7:LEU:O	2:B:9:VAL:N	2.52	0.42
1:A:105:ARG:HB2	1:A:127:ALA:HB3	2.00	0.42
2:H:99:LEU:HA	2:H:100:PRO:HD3	1.91	0.42
1:A:106:HIS:HE1	6:A:3049:HOH:O	2.03	0.42
1:G:218:VAL:O	1:G:219:MET:C	2.58	0.42
2:H:107:LEU:HD13	2:H:136:LEU:HD13	2.00	0.42
2:B:22:PRO:HB2	2:B:25:ILE:CG1	2.49	0.42
2:B:38:THR:OG1	2:B:40:GLN:HG2	2.19	0.42
2:H:99:LEU:CD2	2:H:134:ILE:HD12	2.48	0.42
1:A:240:TYR:CD1	1:A:240:TYR:C	2.93	0.42
1:A:243:VAL:HG12	1:A:247:PHE:HE2	1.84	0.42
2:B:99:LEU:HA	2:B:100:PRO:HD3	1.83	0.42
1:G:234:ARG:HG2	1:G:234:ARG:NH1	2.32	0.42
1:A:113:ARG:HD2	6:B:1002:HOH:O	2.19	0.42
1:A:243:VAL:C	1:A:245:ALA:N	2.72	0.42
2:H:53:MET:CG	2:H:54:GLY:H	2.25	0.42
1:A:10:ILE:HD11	1:A:124:VAL:CG2	2.50	0.42
2:B:55:ARG:HB3	6:B:1020:HOH:O	2.19	0.42
2:B:58:LEU:CD2	2:B:60:LYS:HE3	2.48	0.42
2:B:84:ASN:OD1	2:B:94:LYS:HG3	2.20	0.42
1:G:66:LEU:HG	1:G:297:GLN:HE21	1.84	0.42
1:G:134:HIS:HB2	6:G:3125:HOH:O	2.19	0.42
1:A:270:VAL:O	1:A:271:ASP:HB2	2.20	0.42
2:B:21:ILE:HB	2:B:57:ASP:HB2	2.01	0.42
1:G:45:ALA:HB2	1:G:99:VAL:HG11	2.01	0.42
2:H:20:HIS:O	2:H:81:ALA:HA	2.20	0.42
2:B:33:PHE:O	2:B:34:LYS:C	2.58	0.41
2:B:99:LEU:CD2	2:B:134:ILE:HD12	2.49	0.41
1:G:146:GLN:O	1:G:150:GLY:N	2.52	0.41
1:G:239:GLU:O	1:G:243:VAL:HG23	2.19	0.41
1:G:269:ARG:O	1:G:270:VAL:HG22	2.20	0.41
2:H:59:ILE:HG22	2:H:61:ILE:CD1	2.49	0.41
2:B:102:ARG:HH12	2:B:139:LYS:HB2	1.86	0.41
1:G:269:ARG:NH2	1:G:278:ASP:OD1	2.53	0.41
2:B:47:ASN:HB2	2:H:41:ARG:HA	2.01	0.41
1:G:244:LYS:NZ	1:G:271:ASP:HB3	2.36	0.41
2:H:141:CYS:SG	2:H:143:LYS:HB2	2.60	0.41
2:H:72:ASP:C	2:H:74:LEU:N	2.74	0.41
1:A:60:GLU:HG2	1:A:70:VAL:HG11	2.02	0.41
2:B:119:GLU:HB3	2:B:120:PRO:HD2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:HIS:N	6:A:3011:HOH:O	2.54	0.41
1:A:134:HIS:CD2	1:A:137:GLN:HB2	2.55	0.41
1:A:160:VAL:O	1:A:228:THR:HB	2.21	0.41
1:A:269:ARG:NH2	1:A:275:THR:HA	2.35	0.41
2:B:19:ASP:CG	2:B:56:LYS:HZ1	2.23	0.41
1:A:20:LEU:O	1:A:24:LEU:HG	2.20	0.41
1:A:235:LEU:HD22	1:A:239:GLU:OE1	2.21	0.41
1:A:243:VAL:O	1:A:245:ALA:N	2.54	0.41
2:B:50:SER:OG	2:B:51:GLY:N	2.54	0.41
2:B:10:GLU:O	2:B:60:LYS:NZ	2.45	0.40
2:H:38:THR:OG1	2:H:40:GLN:HG2	2.21	0.40
1:A:9:ILE:HB	1:A:125:LEU:HD22	2.04	0.40
1:A:114:LEU:C	1:A:114:LEU:HD23	2.42	0.40
1:A:167:ARG:HD3	1:A:167:ARG:HA	1.83	0.40
1:A:234:ARG:HD2	6:A:3090:HOH:O	2.22	0.40
2:B:20:HIS:CA	2:B:56:LYS:HD2	2.45	0.40
2:B:87:ASP:C	2:B:89:TYR:H	2.23	0.40
1:G:121:ASN:N	1:G:121:ASN:HD22	2.19	0.40
1:G:133:GLN:OE1	6:G:3011:HOH:O	2.22	0.40
2:H:130:ARG:HD2	2:H:130:ARG:HA	1.87	0.40
1:A:121:ASN:N	1:A:121:ASN:HD22	2.19	0.40
2:B:17:VAL:HG21	2:B:86:ILE:HD12	2.02	0.40
2:B:18:ILE:O	2:B:58:LEU:HD12	2.22	0.40
1:G:156:HIS:HD2	1:G:185:TYR:OH	2.05	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	308/310 (99%)	274 (89%)	27 (9%)	7 (2%)	6 6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	308/310 (99%)	277 (90%)	22 (7%)	9 (3%)	4	3
2	B	151/153 (99%)	126 (83%)	19 (13%)	6 (4%)	3	2
2	H	151/153 (99%)	121 (80%)	26 (17%)	4 (3%)	5	4
All	All	918/926 (99%)	798 (87%)	94 (10%)	26 (3%)	5	4

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	219	MET
1	A	240	TYR
1	A	270	VAL
1	G	83	LYS
1	G	84	LYS
1	G	219	MET
1	G	270	VAL
2	H	51	GLY
2	B	8	GLN
1	G	76	SER
1	G	240	TYR
1	G	244	LYS
2	H	8	GLN
2	B	14	ARG
2	B	55	ARG
2	B	73	GLN
2	H	105	ASN
1	G	52	SER
1	A	52	SER
1	A	127	ALA
1	A	134	HIS
1	A	309	VAL
2	H	73	GLN
2	B	51	GLY
1	G	309	VAL
2	B	9	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	261/261 (100%)	240 (92%)	21 (8%)	12	17
1	G	261/261 (100%)	244 (94%)	17 (6%)	17	24
2	B	137/137 (100%)	129 (94%)	8 (6%)	20	30
2	H	137/137 (100%)	133 (97%)	4 (3%)	42	60
All	All	796/796 (100%)	746 (94%)	50 (6%)	18	26

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	ARG
1	A	59	PHE
1	A	69	SER
1	A	74	SER
1	A	76	SER
1	A	129	ASP
1	A	131	SER
1	A	133	GLN
1	A	134	HIS
1	A	151	ARG
1	A	167	ARG
1	A	183	ARG
1	A	201	MET
1	A	221	GLU
1	A	222	VAL
1	A	228	THR
1	A	242	ASN
1	A	267	LEU
1	A	269	ARG
1	A	270	VAL
1	A	285	TYR
2	B	2	THR
2	B	4	ASP
2	B	6	LYS
2	B	14	ARG
2	B	55	ARG
2	B	89	TYR
2	B	105	ASN
2	B	143	LYS
1	G	37	GLU

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Mol	Chain	Res	Type
1	G	54	ARG
1	G	59	PHE
1	G	69	SER
1	G	74	SER
1	G	129	ASP
1	G	133	GLN
1	G	151	ARG
1	G	183	ARG
1	G	201	MET
1	G	222	VAL
1	G	228	THR
1	G	242	ASN
1	G	267	LEU
1	G	269	ARG
1	G	270	VAL
1	G	285	TYR
2	H	14	ARG
2	H	89	TYR
2	H	105	ASN
2	H	143	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	ASN
1	A	41	HIS
1	A	106	HIS
1	A	121	ASN
1	A	156	HIS
1	A	231	GLN
1	A	242	ASN
1	A	260	ASN
1	A	297	GLN
2	B	20	HIS
2	B	47	ASN
2	B	63	ASN
2	B	88	ASN
2	B	117	HIS
1	G	13	ASN
1	G	41	HIS
1	G	78	ASN
1	G	106	HIS

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Mol	Chain	Res	Type
1	G	121	ASN
1	G	134	HIS
1	G	137	GLN
1	G	156	HIS
1	G	231	GLN
1	G	242	ASN
1	G	260	ASN
1	G	297	GLN
2	H	20	HIS
2	H	47	ASN
2	H	63	ASN
2	H	88	ASN
2	H	117	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	NCD	A	2001	-	11,11,11	1.06	0	13,14,14	1.73	4 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	PO4	G	3002	-	4,4,4	2.03	1 (25%)	6,6,6	1.79	2 (33%)
3	PO4	A	3001	-	4,4,4	2.16	1 (25%)	6,6,6	1.76	2 (33%)
4	NCD	G	2002	-	11,11,11	1.15	0	13,14,14	1.66	3 (23%)

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	NCD	A	2001	-	-	6/12/12/12	-
4	NCD	G	2002	-	-	7/12/12/12	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	3001	PO4	P-O1	4.11	1.60	1.50
3	G	3002	PO4	P-O1	3.83	1.59	1.50

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	2001	NCD	O2-C2-N3	-3.40	117.38	123.22
4	G	2002	NCD	O2-C2-N3	-3.29	117.57	123.22
4	A	2001	NCD	N3-C2-N1	2.67	122.75	116.77
3	G	3002	PO4	O3-P-O1	-2.63	101.27	110.89
4	G	2002	NCD	N3-C2-N1	2.61	122.62	116.77
3	A	3001	PO4	O3-P-O1	-2.51	101.71	110.89
4	G	2002	NCD	O61-C61-O62	-2.47	118.48	124.09
4	A	2001	NCD	O61-C61-O62	-2.36	118.73	124.09
4	A	2001	NCD	C5-C6-C61	-2.32	106.34	110.83
3	G	3002	PO4	O4-P-O1	-2.27	102.58	110.89
3	A	3001	PO4	O4-P-O1	-2.26	102.61	110.89

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	2001	NCD	C4-C5-C6-N1
4	G	2002	NCD	C4-C5-C6-C61

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Mol	Chain	Res	Type	Atoms
4	G	2002	NCD	C4-C5-C6-N1
4	A	2001	NCD	O4-C4-C5-C6
4	A	2001	NCD	O5-C4-C5-C6
4	G	2002	NCD	O4-C4-C5-C6
4	G	2002	NCD	O5-C4-C5-C6
4	A	2001	NCD	C4-C5-C6-C61
4	G	2002	NCD	C61-C6-N1-C2
4	A	2001	NCD	O2-C2-N1-C6
4	A	2001	NCD	N3-C2-N1-C6
4	G	2002	NCD	O2-C2-N1-C6
4	G	2002	NCD	N3-C2-N1-C6

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2001	NCD	1	0
3	G	3002	PO4	2	0
4	G	2002	NCD	1	0

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	310/310 (100%)	0.01	10 (3%) 47 50	20, 34, 71, 88	0
1	G	310/310 (100%)	-0.03	9 (2%) 51 53	19, 33, 71, 89	0
2	B	153/153 (100%)	1.02	28 (18%) 1 1	28, 70, 126, 139	0
2	H	153/153 (100%)	0.96	25 (16%) 1 1	26, 70, 125, 141	0
All	All	926/926 (100%)	0.32	72 (7%) 13 14	19, 40, 98, 141	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	2	THR	14.2
2	B	4	ASP	10.1
2	H	4	ASP	8.8
2	B	2	THR	8.2
2	B	5	ASN	7.1
2	H	8	GLN	6.9
2	H	1	MET	6.9
2	B	15	GLY	6.4
2	B	8	GLN	5.7
2	H	3	HIS	5.7
2	B	1	MET	5.6
2	B	7	LEU	5.4
2	H	6	LYS	5.2
2	B	6	LYS	5.1
2	H	7	LEU	5.0
2	B	3	HIS	4.5
2	B	9	VAL	4.5
2	H	9	VAL	4.5
1	A	308	LEU	4.4
2	H	5	ASN	4.3
1	A	77	ALA	4.2

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Mol	Chain	Res	Type	RSRZ
2	B	153	ASN	4.2
2	H	92	VAL	4.2
2	B	88	ASN	4.1
2	H	15	GLY	4.0
2	H	88	ASN	3.8
1	A	310	LEU	3.7
1	G	310	LEU	3.7
2	H	89	TYR	3.5
1	A	76	SER	3.3
2	B	92	VAL	3.3
2	B	11	ALA	3.3
1	G	246	GLN	3.3
2	H	65	PHE	3.3
2	B	55	ARG	3.2
2	B	65	PHE	3.2
2	H	10	GLU	3.2
1	G	78	ASN	3.2
1	G	267	LEU	3.2
2	B	58	LEU	3.1
2	H	153	ASN	3.1
2	B	10	GLU	2.9
2	H	58	LEU	2.9
1	A	78	ASN	2.9
2	B	17	VAL	2.9
2	B	66	LEU	2.9
1	A	127	ALA	2.9
1	G	308	LEU	2.8
2	H	48	LEU	2.7
1	A	246	GLN	2.7
1	G	77	ALA	2.7
2	H	11	ALA	2.7
2	B	41	ARG	2.6
2	B	89	TYR	2.6
2	B	91	VAL	2.6
2	B	53	MET	2.6
1	A	267	LEU	2.5
2	B	82	THR	2.5
1	G	127	ALA	2.5
1	A	133	GLN	2.5
2	H	66	LEU	2.4
2	B	48	LEU	2.4
2	B	86	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	82	GLY	2.3
2	H	18	ILE	2.2
2	H	61	ILE	2.2
2	H	41	ARG	2.2
2	H	86	ILE	2.1
1	G	79	THR	2.1
2	H	130	ARG	2.1
1	A	79	THR	2.0
2	B	84	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 monosaccharides 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	B-factors(Å^2)	Q<0.9
4	NCD	A	2001	12/12	0.56	0.37	73,78,79,81	0
4	NCD	G	2002	12/12	0.63	0.42	80,81,82,82	0
3	PO4	G	3002	5/5	0.94	0.12	69,69,70,71	0
3	PO4	A	3001	5/5	0.97	0.10	67,67,69,69	0
5	ZN	B	1001	1/1	1.00	0.14	30,30,30,30	0
5	ZN	H	1002	1/1	1.00	0.13	27,27,27,27	0

6.5 Other polymers (i)

There are no such residues in this entry.