



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2023 – 04:49 PM EDT

PDB ID : 2PMI
Title : Structure of the Pho85-Pho80 CDK-cyclin Complex of the Phosphate-responsive Signal Transduction Pathway with Bound ATP-gamma-S
Authors : Huang, K.; Ferrin-O'Connell, I.; Zhang, W.; Leonard, G.A.; O'Shea, E.K.; Quiocho, F.A.
Deposited on : 2007-04-23
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 ⓘ 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
buster-report : 1.1.7 (2018)
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

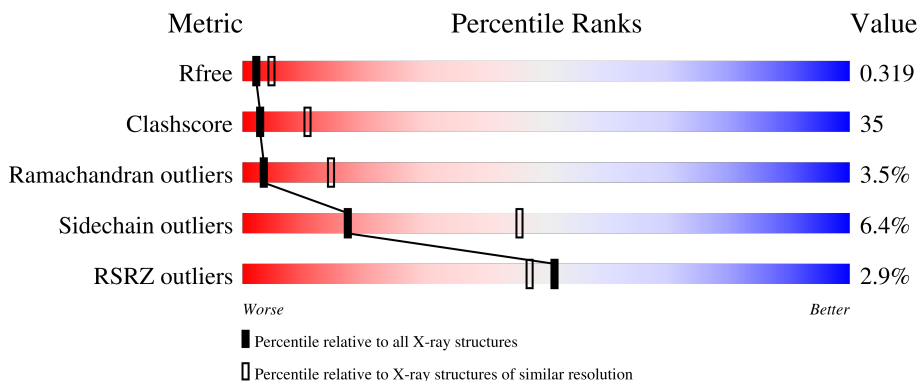
1 Overall quality at a glance

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}	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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	317	 3% 46% 38% 6% 10%
1	C	317	 4% 31% 52% 6% 10%
2	B	293	 % 33% 35% • 27%
2	D	293	 % 34% 37% • 26%

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	AGS	A	3001	X	-	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8138 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 Cyclin-dependent protein kinase PHO85.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	284	2298	1476	394	417	11	49	0	0
1	C	285	2316	1491	397	417	11	58	0	0

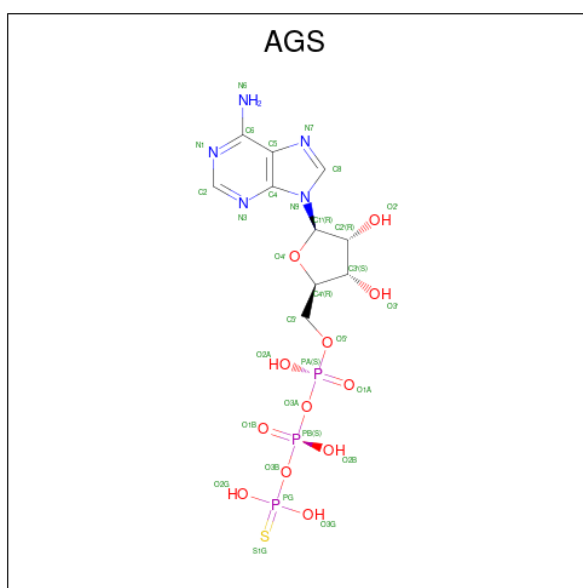
There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	306	MET	-	expression tag	UNP P17157
A	307	GLY	-	expression tag	UNP P17157
A	308	GLY	-	expression tag	UNP P17157
A	309	SER	-	expression tag	UNP P17157
A	310	ARG	-	expression tag	UNP P17157
A	311	SER	-	expression tag	UNP P17157
A	312	HIS	-	expression tag	UNP P17157
A	313	HIS	-	expression tag	UNP P17157
A	314	HIS	-	expression tag	UNP P17157
A	315	HIS	-	expression tag	UNP P17157
A	316	HIS	-	expression tag	UNP P17157
A	317	HIS	-	expression tag	UNP P17157
C	306	MET	-	expression tag	UNP P17157
C	307	GLY	-	expression tag	UNP P17157
C	308	GLY	-	expression tag	UNP P17157
C	309	SER	-	expression tag	UNP P17157
C	310	ARG	-	expression tag	UNP P17157
C	311	SER	-	expression tag	UNP P17157
C	312	HIS	-	expression tag	UNP P17157
C	313	HIS	-	expression tag	UNP P17157
C	314	HIS	-	expression tag	UNP P17157
C	315	HIS	-	expression tag	UNP P17157
C	316	HIS	-	expression tag	UNP P17157
C	317	HIS	-	expression tag	UNP P17157

- Molecule 2 is a protein called PHO85 cyclin PHO80.

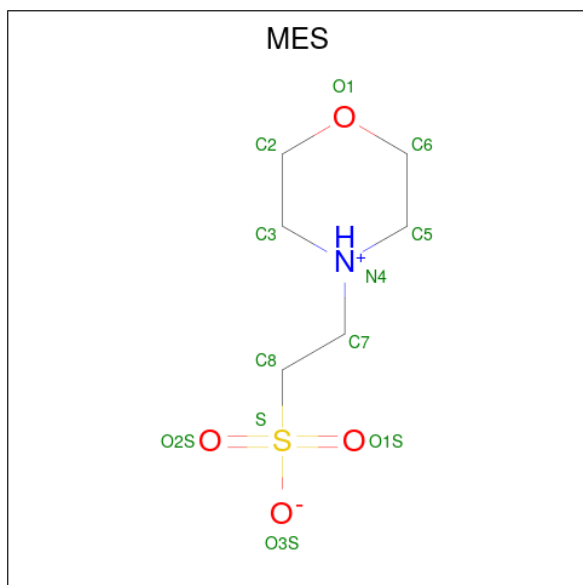
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	213	Total	C	N	O	S	13	0	0
			1722	1109	298	308	7			
2	D	216	Total	C	N	O	S	14	0	0
			1747	1124	303	313	7			

- Molecule 3 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	N	O	P			S
3	A	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		

- Molecule 4 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).

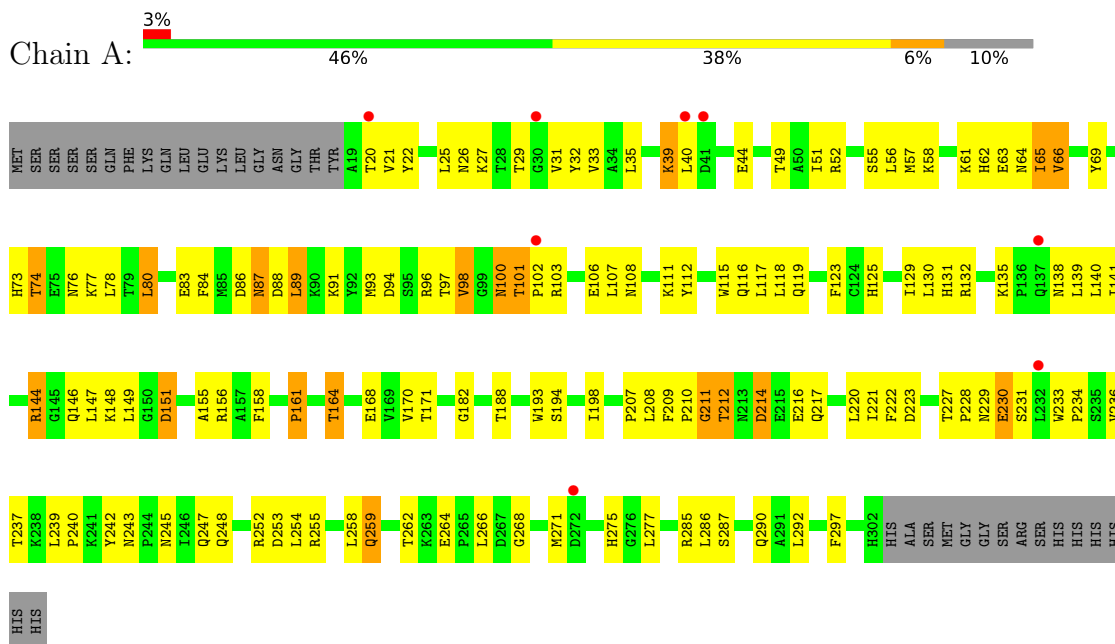


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
4	B	1	12	6	1	4	1	0	0
4	D	1	12	6	1	4	1	0	0

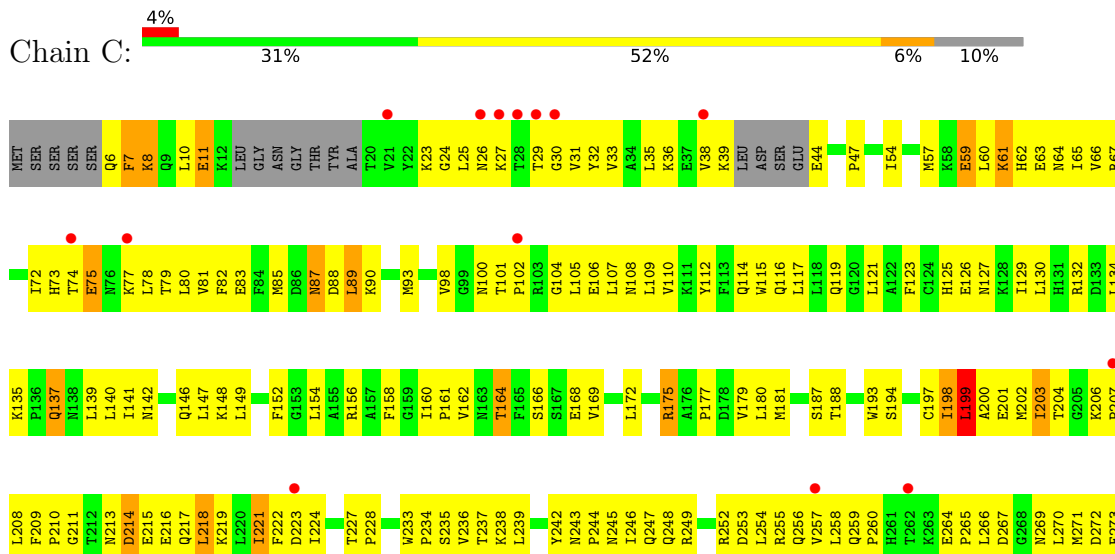
3 Residue-property plots i

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: Cyclin-dependent protein kinase PHO85

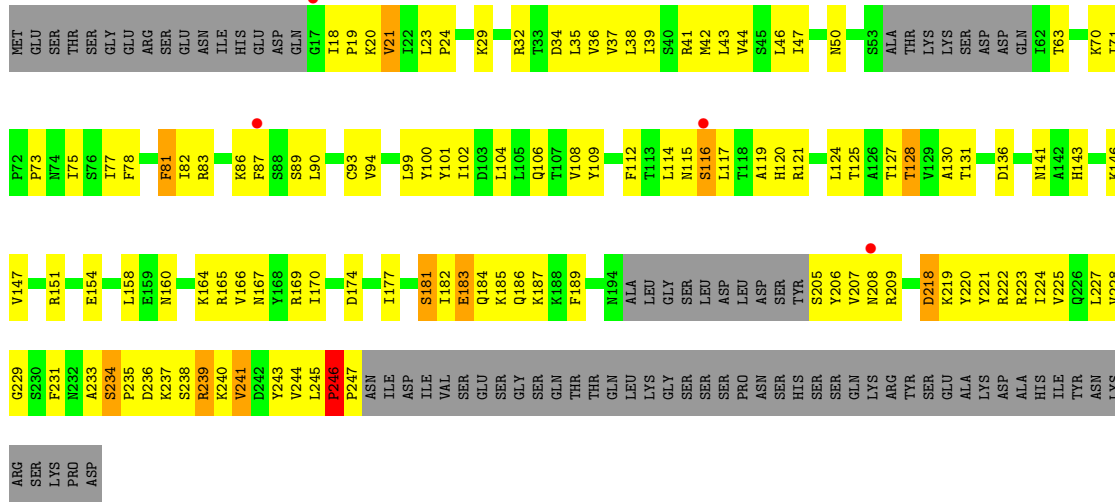


- Molecule 1: Cyclin-dependent protein kinase PHO85

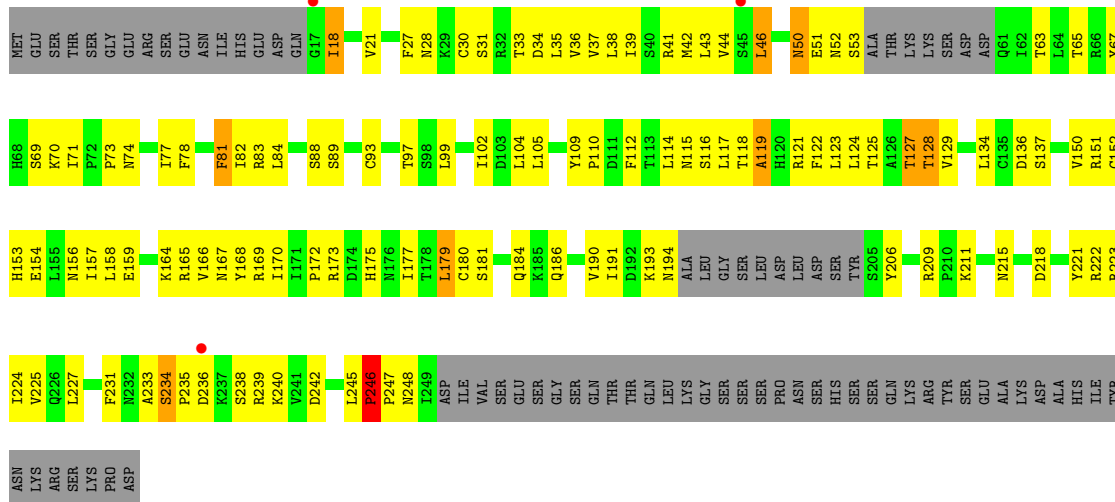




• Molecule 2: PHO85 cyclin PHO80



• Molecule 2: PHO85 cyclin PHO80



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	146.59Å 146.59Å 212.85Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	14.98 – 2.90 14.98 – 2.90	Depositor EDS
% Data completeness (in resolution range)	91.2 (14.98-2.90) 91.0 (14.98-2.90)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.42 (at 2.91Å)	Xtrriage
Refinement program	CNS	Depositor
R, R_{free}	0.289 , 0.325 0.284 , 0.319	Depositor DCC
R_{free} test set	2707 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	46.2	Xtrriage
Anisotropy	0.277	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 24.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	0.043 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	8138	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.80% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0/2354	0.62	1/3192 (0.0%)
1	C	0.34	0/2370	0.58	0/3207
2	B	0.43	0/1757	0.65	0/2380
2	D	0.43	0/1782	0.63	0/2414
All	All	0.40	0/8263	0.62	1/11193 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	286	LEU	CA-CB-CG	5.72	128.46	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2298	0	2316	125	0
1	C	2316	0	2344	211	0
2	B	1722	0	1771	134	0
2	D	1747	0	1796	114	0
3	A	31	0	12	1	0
4	B	12	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	12	0	13	2	0
All	All	8138	0	8265	562	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 35.

All (562) 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:255:ARG:HH21	1:A:259:GLN:HG2	1.14	1.09
1:A:116:GLN:NE2	1:A:147:LEU:H	1.50	1.08
1:A:39:LYS:H	1:A:39:LYS:HD3	1.17	1.05
1:A:193:TRP:HB2	1:A:285:ARG:HH11	1.23	1.03
2:D:218:ASP:HB3	2:D:222:ARG:HH22	1.28	0.98
1:C:193:TRP:HB2	1:C:285:ARG:HH21	1.30	0.92
1:A:56:LEU:HD22	1:A:129:ILE:HD13	1.52	0.91
2:B:218:ASP:HB3	2:B:222:ARG:HH12	1.36	0.91
1:A:259:GLN:HE22	1:A:266:LEU:H	1.10	0.90
1:A:116:GLN:HE22	1:A:147:LEU:H	0.93	0.89
1:C:175:ARG:HB3	1:C:180:LEU:HD21	1.53	0.89
2:D:44:VAL:HG21	2:D:235:PRO:HD3	1.54	0.89
2:D:246:PRO:HB2	2:D:247:PRO:HD3	1.54	0.88
1:C:139:LEU:HB3	1:C:147:LEU:HD11	1.57	0.87
1:C:135:LYS:HG3	1:C:137:GLN:HG2	1.53	0.87
2:D:33:THR:O	2:D:37:VAL:HG23	1.75	0.87
2:B:124:LEU:O	2:B:127:THR:HG22	1.76	0.86
1:C:101:THR:HG23	1:C:102:PRO:HD2	1.58	0.84
1:A:116:GLN:HE22	1:A:147:LEU:N	1.75	0.82
1:C:243:ASN:HB3	1:C:246:ILE:HG23	1.61	0.82
1:C:57:MET:HE2	1:C:57:MET:HA	1.62	0.82
2:B:34:ASP:O	2:B:37:VAL:HG22	1.79	0.81
1:A:193:TRP:HB2	1:A:285:ARG:NH1	1.95	0.81
2:D:109:TYR:CD2	2:D:112:PHE:HB2	2.16	0.80
1:A:87:ASN:HD22	1:A:87:ASN:H	1.27	0.80
1:C:209:PHE:CE2	1:C:221:ILE:HA	2.17	0.80
1:A:255:ARG:NH2	1:A:259:GLN:HG2	1.97	0.79
1:C:242:TYR:O	1:C:244:PRO:HD3	1.83	0.79
2:B:245:LEU:HD12	2:B:246:PRO:HD2	1.63	0.79
2:D:104:LEU:HD21	2:D:166:VAL:HG11	1.65	0.78
1:C:164:THR:HA	2:D:136:ASP:OD2	1.83	0.78
1:A:26:ASN:HB3	1:A:29:THR:O	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:74:THR:HG23	1:C:77:LYS:HB2	1.67	0.76
2:B:47:ILE:HG21	2:B:116:SER:HB3	1.68	0.76
1:A:156:ARG:HH12	1:A:164:THR:HB	1.50	0.75
1:A:212:THR:H	1:A:216:GLU:HG2	1.52	0.75
2:D:31:SER:HB3	2:D:34:ASP:OD2	1.85	0.75
2:B:73:PRO:HG2	2:B:120:HIS:HD2	1.50	0.75
2:B:41:ARG:HA	2:B:235:PRO:HG3	1.69	0.74
1:C:125:HIS:CE1	1:C:188:THR:HG23	2.21	0.74
1:C:107:LEU:HD21	1:C:266:LEU:HD23	1.68	0.74
2:B:43:LEU:HD11	2:B:102:ILE:HD11	1.69	0.73
2:B:101:TYR:OH	2:B:170:ILE:HB	1.88	0.73
2:B:223:ARG:NH1	2:B:227:LEU:HG	2.02	0.73
1:C:60:LEU:HD21	1:C:129:ILE:HD12	1.69	0.73
2:B:106:GLN:HE21	2:B:114:LEU:H	1.36	0.73
2:D:218:ASP:HB3	2:D:222:ARG:NH2	2.03	0.73
1:A:236:VAL:HG23	1:A:239:LEU:HD12	1.71	0.72
1:A:97:THR:HG21	1:A:103:ARG:HB2	1.70	0.72
2:D:123:LEU:O	2:D:127:THR:HB	1.89	0.72
2:B:233:ALA:O	2:B:234:SER:OG	2.07	0.72
2:B:218:ASP:CB	2:B:222:ARG:HH12	2.03	0.72
1:A:117:LEU:HD12	1:A:149:LEU:HD21	1.72	0.72
1:C:7:PHE:CE1	1:C:35:LEU:HD21	2.25	0.72
1:C:207:PRO:HB2	1:C:210:PRO:HG3	1.70	0.71
1:C:253:ASP:O	1:C:257:VAL:HG23	1.89	0.71
1:A:287:SER:H	1:A:290:GLN:HE21	1.39	0.70
1:C:7:PHE:HE1	1:C:35:LEU:HD21	1.57	0.70
1:C:63:GLU:O	1:C:148:LYS:HE2	1.90	0.70
1:C:181:MET:HB2	1:C:239:LEU:HD13	1.73	0.69
1:C:10:LEU:HB2	1:C:23:LYS:HB3	1.73	0.69
1:C:255:ARG:NH2	1:C:259:GLN:HE21	1.91	0.68
1:A:207:PRO:HB2	1:A:210:PRO:HG3	1.76	0.68
2:B:225:VAL:HG11	2:B:245:LEU:HB2	1.75	0.68
2:D:44:VAL:CG2	2:D:235:PRO:HD3	2.21	0.68
1:C:219:LYS:HG2	1:C:249:ARG:HH12	1.57	0.68
1:A:56:LEU:HD22	1:A:129:ILE:CD1	2.24	0.68
2:D:124:LEU:O	2:D:128:THR:HG23	1.93	0.68
1:A:106:GLU:OE2	1:A:108:ASN:HB2	1.94	0.67
1:C:279:GLN:HB2	1:C:285:ARG:HD2	1.76	0.67
1:C:237:THR:HA	1:C:242:TYR:CD1	2.30	0.67
2:D:211:LYS:HD3	2:D:215:ASN:OD1	1.94	0.67
2:D:221:TYR:O	2:D:225:VAL:HG23	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:GLY:HA3	1:A:240:PRO:HG2	1.78	0.66
1:A:209:PHE:HB3	1:A:217:GLN:NE2	2.11	0.66
1:C:114:GLN:NE2	1:C:199:LEU:HB2	2.11	0.66
2:B:20:LYS:HE3	2:B:244:VAL:HG21	1.77	0.65
1:A:168:GLU:OE1	2:D:152:CYS:N	2.28	0.65
1:C:181:MET:CE	1:C:242:TYR:HA	2.27	0.65
1:C:255:ARG:HA	1:C:271:MET:HE2	1.77	0.65
1:C:141:ILE:HA	1:C:146:GLN:O	1.97	0.64
1:C:119:GLN:NE2	1:C:292:LEU:HD13	2.13	0.64
1:C:193:TRP:CB	1:C:285:ARG:HH21	2.06	0.64
2:D:42:MET:CE	2:D:227:LEU:HD12	2.27	0.64
1:C:8:LYS:HB3	1:C:25:LEU:H	1.62	0.64
1:A:212:THR:N	1:A:216:GLU:HG2	2.13	0.63
1:C:194:SER:O	1:C:198:ILE:HG12	1.98	0.63
1:A:161:PRO:HG2	2:B:93:CYS:SG	2.39	0.63
2:D:51:GLU:C	2:D:53:SER:H	2.01	0.63
1:C:209:PHE:CB	1:C:217:GLN:HE22	2.12	0.63
1:C:255:ARG:HG2	1:C:271:MET:HE2	1.81	0.63
1:C:236:VAL:HG13	1:C:237:THR:N	2.14	0.63
2:B:20:LYS:CE	2:B:244:VAL:HG21	2.28	0.63
2:D:77:ILE:HD13	2:D:119:ALA:HB1	1.80	0.63
1:A:87:ASN:H	1:A:87:ASN:ND2	1.94	0.62
1:C:121:LEU:HG	1:C:125:HIS:CD2	2.34	0.62
1:C:209:PHE:HB3	1:C:217:GLN:HE22	1.64	0.62
1:C:130:LEU:HD12	1:C:158:PHE:CE2	2.34	0.62
2:B:38:LEU:HB3	2:B:224:ILE:HD12	1.82	0.62
1:A:29:THR:HB	1:A:31:VAL:HG12	1.81	0.62
2:B:234:SER:N	2:B:235:PRO:HD2	2.15	0.62
1:C:23:LYS:HG2	1:C:24:GLY:H	1.64	0.62
1:C:233:TRP:HB2	1:C:281:ASN:HB2	1.81	0.62
2:D:36:VAL:HG11	2:D:82:ILE:HG22	1.82	0.62
1:A:214:ASP:OD2	1:A:214:ASP:N	2.33	0.62
2:B:109:TYR:CD2	2:B:112:PHE:HB2	2.35	0.62
2:D:190:VAL:HG23	2:D:191:ILE:HG12	1.81	0.62
1:C:107:LEU:HD12	1:C:107:LEU:N	2.15	0.61
1:C:265:PRO:O	1:C:266:LEU:HD23	2.00	0.61
2:D:104:LEU:HD21	2:D:166:VAL:CG1	2.31	0.61
1:A:259:GLN:HE22	1:A:266:LEU:N	1.92	0.61
1:C:213:ASN:OD1	1:C:215:GLU:HB3	2.00	0.61
1:C:267:ASP:OD2	1:C:269:ASN:HB3	2.00	0.61
2:D:129:VAL:HG22	2:D:159:GLU:HG3	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:47:ILE:HG23	2:B:116:SER:H	1.65	0.61
2:B:231:PHE:CZ	2:B:240:LYS:HG3	2.35	0.61
2:B:37:VAL:HG23	2:B:38:LEU:N	2.16	0.61
1:C:298:ALA:C	1:C:300:TYR:H	2.03	0.61
1:A:144:ARG:HD3	1:A:144:ARG:N	2.15	0.61
2:D:42:MET:HE1	2:D:227:LEU:HB2	1.83	0.61
1:A:39:LYS:H	1:A:39:LYS:CD	1.99	0.60
2:B:77:ILE:HD12	2:B:120:HIS:CE1	2.36	0.60
1:C:72:ILE:HB	1:C:79:THR:OG1	2.00	0.60
1:A:116:GLN:NE2	1:A:147:LEU:N	2.35	0.60
1:A:57:MET:HA	1:A:57:MET:HE2	1.82	0.60
1:C:243:ASN:CB	1:C:246:ILE:HG23	2.32	0.60
1:C:107:LEU:HD21	1:C:266:LEU:CD2	2.30	0.60
1:C:39:LYS:HD3	1:C:39:LYS:C	2.21	0.60
1:A:287:SER:H	1:A:290:GLN:NE2	2.00	0.59
1:C:181:MET:HE2	1:C:242:TYR:HA	1.84	0.59
1:C:26:ASN:HB3	1:C:29:THR:O	2.01	0.59
1:C:73:HIS:CG	2:D:164:LYS:HE2	2.37	0.59
2:D:165:ARG:HG2	2:D:165:ARG:HH11	1.67	0.59
2:B:234:SER:H	2:B:235:PRO:HD2	1.67	0.59
1:C:193:TRP:HB2	1:C:285:ARG:NH2	2.12	0.59
2:D:43:LEU:HD11	2:D:102:ILE:CD1	2.32	0.59
1:C:132:ARG:HD3	1:C:154:LEU:O	2.02	0.59
2:D:181:SER:O	2:D:184:GLN:HB2	2.02	0.58
1:A:107:LEU:HB2	1:A:264:GLU:OE1	2.03	0.58
1:A:39:LYS:HD3	1:A:39:LYS:N	2.01	0.58
1:A:233:TRP:N	1:A:234:PRO:HD3	2.19	0.58
1:C:161:PRO:HG2	2:D:93:CYS:SG	2.42	0.58
2:B:82:ILE:HG13	2:B:83:ARG:N	2.18	0.58
1:C:209:PHE:HB3	1:C:217:GLN:NE2	2.18	0.58
1:C:247:GLN:O	1:C:249:ARG:HG3	2.04	0.58
1:C:125:HIS:ND1	1:C:188:THR:HG23	2.18	0.58
2:B:73:PRO:CG	2:B:120:HIS:HD2	2.17	0.58
2:B:42:MET:HE3	2:B:227:LEU:HD12	1.86	0.58
2:B:70:LYS:O	2:B:71:ILE:HG23	2.04	0.58
1:C:199:LEU:HD13	1:C:274:LEU:HD13	1.85	0.58
1:C:61:LYS:HE2	1:C:61:LYS:HA	1.86	0.58
1:C:223:ASP:O	1:C:252:ARG:HD3	2.04	0.57
2:D:233:ALA:O	2:D:234:SER:OG	2.19	0.57
1:C:221:ILE:HG13	1:C:222:PHE:HD2	1.69	0.57
1:A:107:LEU:HD13	1:A:264:GLU:CD	2.24	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:127:THR:HG22	2:D:128:THR:HG22	1.86	0.57
2:B:125:THR:OG1	2:B:158:LEU:HG	2.04	0.57
1:C:161:PRO:CG	2:D:28:ASN:HD21	2.17	0.57
1:A:194:SER:O	1:A:198:ILE:HG12	2.04	0.57
2:D:46:LEU:O	2:D:50:ASN:HB2	2.05	0.57
1:A:101:THR:HB	1:A:102:PRO:CD	2.35	0.57
2:B:160:ASN:ND2	2:B:164:LYS:NZ	2.53	0.57
1:C:172:LEU:O	1:C:175:ARG:HB2	2.05	0.57
1:C:255:ARG:HG2	1:C:271:MET:CE	2.35	0.57
1:A:66:VAL:HG21	1:A:140:LEU:HD22	1.86	0.56
1:A:87:ASN:HD22	1:A:87:ASN:N	1.92	0.56
2:B:43:LEU:HD11	2:B:102:ILE:CD1	2.35	0.56
2:B:233:ALA:HB3	2:B:235:PRO:HD2	1.87	0.56
1:A:222:PHE:CE2	1:A:228:PRO:HD3	2.40	0.56
1:A:25:LEU:HD12	1:A:25:LEU:O	2.06	0.56
1:C:117:LEU:HD13	1:C:139:LEU:HD21	1.86	0.56
1:A:125:HIS:ND1	1:A:188:THR:HB	2.21	0.56
2:B:205:SER:OG	2:B:207:VAL:HG23	2.06	0.56
1:C:297:PHE:O	1:C:299:GLU:N	2.39	0.56
1:C:85:MET:HB2	1:C:140:LEU:HD23	1.87	0.55
1:C:87:ASN:O	1:C:140:LEU:HA	2.06	0.55
2:D:127:THR:HG22	2:D:128:THR:N	2.21	0.55
1:C:38:VAL:CG1	1:C:47:PRO:HG2	2.37	0.55
2:D:206:TYR:O	2:D:209:ARG:HB3	2.07	0.55
1:A:21:VAL:HG23	1:A:35:LEU:C	2.27	0.55
1:A:33:VAL:C	1:A:84:PHE:HB2	2.27	0.55
2:B:104:LEU:HD21	2:B:166:VAL:HG13	1.89	0.55
2:D:165:ARG:HG2	2:D:165:ARG:NH1	2.22	0.55
1:A:40:LEU:HB2	1:A:76:ASN:HA	1.89	0.55
1:C:175:ARG:NE	1:C:179:VAL:HG11	2.22	0.55
1:C:10:LEU:CB	1:C:23:LYS:HB3	2.37	0.55
1:A:97:THR:HG23	1:A:97:THR:O	2.07	0.54
2:B:223:ARG:HH12	2:B:227:LEU:HG	1.69	0.54
2:B:234:SER:C	2:B:236:ASP:H	2.11	0.54
2:D:166:VAL:HG12	2:D:166:VAL:O	2.08	0.54
2:B:47:ILE:CG2	2:B:116:SER:HB3	2.37	0.54
1:C:62:HIS:HB2	1:C:123:PHE:CD2	2.43	0.54
1:A:111:LYS:HG3	1:A:297:PHE:CE1	2.43	0.54
1:C:117:LEU:HD12	1:C:149:LEU:HD21	1.89	0.54
1:C:177:PRO:HB3	1:C:221:ILE:HD11	1.89	0.54
1:A:164:THR:HA	2:B:136:ASP:OD2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:231:PHE:CE2	2:B:236:ASP:HA	2.43	0.54
1:C:6:GLN:OE1	1:C:72:ILE:HD13	2.07	0.54
2:B:82:ILE:O	2:B:86:LYS:HG2	2.08	0.53
2:D:37:VAL:O	2:D:41:ARG:HG3	2.07	0.53
1:A:125:HIS:CE1	1:A:188:THR:HB	2.43	0.53
1:C:66:VAL:HG23	1:C:149:LEU:O	2.08	0.53
2:D:168:TYR:O	2:D:170:ILE:N	2.41	0.53
1:A:63:GLU:O	1:A:148:LYS:HE2	2.08	0.53
1:C:7:PHE:HB2	1:C:25:LEU:O	2.08	0.53
1:C:107:LEU:H	1:C:107:LEU:CD1	2.21	0.53
2:D:231:PHE:CE2	2:D:236:ASP:HA	2.44	0.53
1:C:57:MET:HA	1:C:57:MET:CE	2.36	0.53
1:C:142:ASN:HD21	1:C:146:GLN:HB2	1.74	0.53
1:C:227:THR:HG21	1:C:248:GLN:HA	1.91	0.53
2:B:221:TYR:O	2:B:224:ILE:HG12	2.09	0.53
2:B:104:LEU:HD12	2:B:177:ILE:HG12	1.91	0.53
1:C:114:GLN:HE22	1:C:199:LEU:HB2	1.73	0.53
1:C:127:ASN:O	1:C:129:ILE:HG13	2.08	0.53
2:B:77:ILE:CG2	2:B:78:PHE:N	2.72	0.52
1:C:282:PRO:C	1:C:284:MET:H	2.12	0.52
2:D:167:ASN:N	2:D:167:ASN:HD22	2.06	0.52
2:B:104:LEU:HD21	2:B:166:VAL:CG1	2.39	0.52
2:D:102:ILE:HD13	2:D:114:LEU:HD22	1.91	0.52
2:D:246:PRO:O	2:D:248:ASN:N	2.36	0.52
2:D:84:LEU:O	2:D:88:SER:HB2	2.09	0.52
2:D:99:LEU:HD12	2:D:102:ILE:HD12	1.91	0.52
2:B:104:LEU:O	2:B:108:VAL:HG22	2.10	0.52
2:D:246:PRO:HB2	2:D:247:PRO:CD	2.35	0.52
1:A:73:HIS:O	1:A:74:THR:HB	2.09	0.52
1:A:138:ASN:O	1:A:139:LEU:HD23	2.08	0.52
2:B:225:VAL:O	2:B:229:GLY:HA3	2.09	0.52
1:C:121:LEU:HD13	1:C:134:LEU:HD11	1.92	0.52
1:A:97:THR:CG2	1:A:103:ARG:HB2	2.40	0.52
2:B:41:ARG:HG2	2:B:235:PRO:HG2	1.91	0.52
1:C:126:GLU:OE2	1:C:126:GLU:HA	2.09	0.52
1:C:175:ARG:CB	1:C:180:LEU:HD21	2.34	0.52
1:A:229:ASN:O	1:A:231:SER:N	2.41	0.52
2:B:46:LEU:O	2:B:50:ASN:HB2	2.10	0.52
2:B:160:ASN:ND2	2:B:164:LYS:HE3	2.24	0.52
1:C:282:PRO:O	1:C:284:MET:N	2.42	0.52
1:C:161:PRO:HG2	2:D:28:ASN:HD21	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:222:PHE:CE1	1:C:228:PRO:HD3	2.45	0.52
1:C:253:ASP:OD1	1:C:256:GLN:HG2	2.09	0.52
1:C:258:LEU:CD1	1:C:274:LEU:HD21	2.39	0.51
1:C:270:LEU:HD13	1:C:296:TRP:CE2	2.45	0.51
2:B:166:VAL:HG12	2:B:166:VAL:O	2.10	0.51
1:C:236:VAL:CG1	1:C:237:THR:N	2.73	0.51
1:C:279:GLN:HG3	1:C:284:MET:HB3	1.92	0.51
2:D:81:PHE:CG	2:D:123:LEU:HD21	2.46	0.51
1:C:26:ASN:OD1	1:C:27:LYS:N	2.43	0.51
1:C:208:LEU:HG	1:C:209:PHE:CZ	2.45	0.51
1:A:101:THR:HB	1:A:102:PRO:HD2	1.92	0.51
1:C:93:MET:CE	1:C:202:MET:HA	2.40	0.51
1:C:142:ASN:ND2	1:C:146:GLN:HB2	2.25	0.51
2:D:246:PRO:CB	2:D:247:PRO:HD3	2.35	0.51
2:B:34:ASP:O	2:B:37:VAL:CG2	2.56	0.51
1:C:106:GLU:HA	1:C:264:GLU:OE2	2.11	0.51
2:D:46:LEU:HD23	2:D:46:LEU:N	2.25	0.51
1:A:21:VAL:HG22	1:A:22:TYR:N	2.26	0.51
1:A:96:ARG:HG3	1:A:96:ARG:HH11	1.76	0.51
1:A:209:PHE:CB	1:A:217:GLN:NE2	2.73	0.51
1:A:135:LYS:HA	1:A:198:ILE:HD11	1.93	0.51
1:C:243:ASN:HB3	1:C:246:ILE:CG2	2.38	0.51
2:D:65:THR:HG22	2:D:109:TYR:OH	2.11	0.51
1:A:26:ASN:O	1:A:29:THR:O	2.29	0.50
1:A:94:ASP:O	1:A:98:VAL:N	2.43	0.50
2:B:185:LYS:C	2:B:186:GLN:HE21	2.14	0.50
2:D:77:ILE:CD1	2:D:119:ALA:HB1	2.41	0.50
2:D:150:VAL:HG23	2:D:151:ARG:O	2.11	0.50
1:C:90:LYS:HD2	1:C:137:GLN:NE2	2.26	0.50
1:A:227:THR:HG21	1:A:248:GLN:HA	1.94	0.50
2:D:42:MET:HE1	2:D:227:LEU:HD12	1.93	0.50
1:A:73:HIS:HA	1:A:78:LEU:HD12	1.93	0.50
2:B:124:LEU:O	2:B:128:THR:HG23	2.12	0.50
2:B:234:SER:N	2:B:235:PRO:CD	2.74	0.50
1:C:87:ASN:N	1:C:87:ASN:HD22	2.10	0.50
1:C:62:HIS:HB3	1:C:65:ILE:HD12	1.94	0.50
1:C:89:LEU:HD12	1:C:139:LEU:HD12	1.93	0.50
1:C:107:LEU:N	1:C:107:LEU:CD1	2.74	0.50
1:C:233:TRP:HZ3	1:C:280:LEU:HB3	1.75	0.50
2:B:42:MET:HE1	2:B:227:LEU:CB	2.42	0.50
1:C:224:ILE:O	1:C:224:ILE:HG22	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:82:ILE:HG13	2:B:83:ARG:H	1.77	0.50
2:B:184:GLN:HA	2:B:184:GLN:OE1	2.12	0.50
2:D:73:PRO:HG3	4:D:2001:MES:H22	1.94	0.50
2:B:219:LYS:HA	2:B:222:ARG:NH2	2.26	0.49
1:C:116:GLN:HE22	1:C:146:GLN:HA	1.76	0.49
1:A:66:VAL:HG13	1:A:83:GLU:HG2	1.94	0.49
1:C:59:GLU:HG3	2:D:173:ARG:NH1	2.26	0.49
1:C:299:GLU:HG3	1:C:300:TYR:CD2	2.47	0.49
1:C:83:GLU:OE2	1:C:148:LYS:HD2	2.12	0.49
2:D:35:LEU:O	2:D:39:ILE:HG13	2.11	0.49
1:C:119:GLN:HE22	1:C:292:LEU:HD13	1.78	0.49
1:A:130:LEU:N	1:A:130:LEU:HD12	2.28	0.49
2:B:42:MET:CE	2:B:227:LEU:HD12	2.42	0.49
1:A:211:GLY:HA2	1:A:216:GLU:HG2	1.93	0.49
2:D:44:VAL:HG21	2:D:235:PRO:CD	2.35	0.49
2:D:109:TYR:CD2	2:D:112:PHE:CB	2.93	0.49
2:D:109:TYR:CE2	2:D:112:PHE:HB2	2.47	0.49
1:A:65:ILE:O	1:A:66:VAL:C	2.51	0.49
1:C:106:GLU:HG3	1:C:109:LEU:H	1.78	0.49
1:C:217:GLN:O	1:C:221:ILE:HG23	2.13	0.49
1:C:73:HIS:CD2	2:D:164:LYS:HG2	2.47	0.49
1:A:209:PHE:CE2	1:A:221:ILE:HA	2.47	0.49
1:A:236:VAL:CG2	1:A:239:LEU:HD12	2.40	0.49
2:B:37:VAL:HG21	2:B:243:TYR:OH	2.13	0.49
1:C:177:PRO:HB3	1:C:221:ILE:CD1	2.43	0.49
1:C:255:ARG:HH21	1:C:259:GLN:HE21	1.56	0.49
1:C:33:VAL:HG22	1:C:82:PHE:O	2.13	0.49
1:C:237:THR:HA	1:C:242:TYR:CE1	2.47	0.49
2:B:44:VAL:HG21	2:B:235:PRO:HD3	1.94	0.48
1:C:270:LEU:HD13	1:C:296:TRP:CZ2	2.47	0.48
1:A:138:ASN:ND2	1:A:151:ASP:HB3	2.28	0.48
2:B:115:ASN:O	2:B:117:LEU:N	2.39	0.48
1:C:31:VAL:O	1:C:31:VAL:HG13	2.14	0.48
1:C:140:LEU:HD12	1:C:140:LEU:N	2.28	0.48
1:C:279:GLN:HG3	1:C:284:MET:CB	2.43	0.48
2:D:184:GLN:O	2:D:186:GLN:NE2	2.47	0.48
1:C:198:ILE:O	1:C:199:LEU:C	2.50	0.48
2:D:104:LEU:HD13	2:D:177:ILE:HG12	1.94	0.48
1:A:119:GLN:HE22	1:A:292:LEU:HD13	1.77	0.48
2:B:36:VAL:HG13	2:B:81:PHE:CD2	2.49	0.48
1:C:137:GLN:H	1:C:137:GLN:CD	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:156:ARG:CZ	1:C:162:VAL:HG23	2.44	0.48
1:C:198:ILE:O	1:C:201:GLU:N	2.45	0.48
2:B:41:ARG:HG2	2:B:235:PRO:CG	2.44	0.48
1:C:33:VAL:HG21	1:C:81:VAL:CG1	2.44	0.48
2:B:82:ILE:O	2:B:86:LYS:N	2.41	0.47
2:B:127:THR:HG23	2:B:128:THR:N	2.29	0.47
2:B:160:ASN:HD21	2:B:164:LYS:NZ	2.11	0.47
1:A:80:LEU:N	1:A:80:LEU:HD23	2.30	0.47
2:D:82:ILE:HG13	2:D:83:ARG:N	2.27	0.47
1:A:96:ARG:HG3	1:A:96:ARG:NH1	2.30	0.47
2:B:23:LEU:HD11	2:B:243:TYR:HB3	1.97	0.47
1:C:104:GLY:O	1:C:105:LEU:HD23	2.14	0.47
1:C:166:SER:HB3	1:C:175:ARG:HH21	1.79	0.47
1:C:201:GLU:HG3	1:C:206:LYS:C	2.35	0.47
1:C:216:GLU:O	1:C:219:LYS:N	2.46	0.47
2:D:97:THR:HG21	2:D:134:LEU:HD11	1.96	0.47
1:C:101:THR:HG23	1:C:102:PRO:CD	2.36	0.47
2:D:18:ILE:HD12	2:D:242:ASP:OD2	2.14	0.47
2:D:121:ARG:HG2	2:D:121:ARG:NH1	2.29	0.47
2:B:47:ILE:HG23	2:B:116:SER:N	2.28	0.47
2:B:99:LEU:HD12	2:B:102:ILE:HD12	1.96	0.47
1:A:170:VAL:HG23	1:A:171:THR:HG23	1.97	0.47
1:C:181:MET:HE1	1:C:242:TYR:HA	1.96	0.47
1:C:298:ALA:C	1:C:300:TYR:N	2.68	0.47
1:C:299:GLU:HG3	1:C:300:TYR:HD2	1.78	0.47
2:D:36:VAL:HG12	2:D:78:PHE:CE2	2.49	0.47
2:D:51:GLU:C	2:D:53:SER:N	2.68	0.47
2:D:67:TYR:O	2:D:118:THR:HA	2.15	0.47
1:C:88:ASP:HA	1:C:139:LEU:O	2.14	0.47
2:B:77:ILE:HA	2:B:120:HIS:HE1	1.80	0.47
2:B:101:TYR:HH	2:B:170:ILE:HB	1.80	0.47
2:B:151:ARG:O	2:B:154:GLU:HB2	2.14	0.47
2:D:166:VAL:HG13	2:D:180:CYS:SG	2.55	0.47
2:D:231:PHE:CE2	2:D:240:LYS:HA	2.50	0.47
1:A:131:HIS:O	1:A:132:ARG:HB2	2.15	0.46
2:B:47:ILE:HD11	2:B:119:ALA:HB2	1.96	0.46
1:C:106:GLU:O	1:C:110:VAL:HG23	2.15	0.46
1:A:87:ASN:HB2	1:A:91:LYS:HB3	1.97	0.46
2:B:143:HIS:HE1	2:D:137:SER:OG	1.99	0.46
1:C:203:ILE:HG22	1:C:204:THR:N	2.30	0.46
2:D:99:LEU:O	2:D:102:ILE:HB	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:8:LYS:HB3	1:C:25:LEU:HB2	1.98	0.46
1:C:93:MET:HE3	1:C:202:MET:HA	1.96	0.46
1:C:201:GLU:HG3	1:C:206:LYS:O	2.15	0.46
1:C:269:ASN:ND2	1:C:296:TRP:HA	2.30	0.46
2:B:207:VAL:O	2:B:208:ASN:HB2	2.15	0.46
1:C:175:ARG:HE	1:C:179:VAL:HG11	1.81	0.46
1:A:112:TYR:O	1:A:115:TRP:HB3	2.16	0.46
1:A:271:MET:HE3	1:A:271:MET:HA	1.97	0.46
2:B:18:ILE:HG21	2:B:240:LYS:HG2	1.97	0.46
1:C:62:HIS:CE1	1:C:64:ASN:HB2	2.51	0.46
1:A:211:GLY:HA2	1:A:216:GLU:CG	2.45	0.46
2:B:37:VAL:CG2	2:B:38:LEU:N	2.79	0.46
2:B:239:ARG:HE	2:B:239:ARG:CA	2.28	0.46
1:A:39:LYS:HA	1:A:77:LYS:HA	1.98	0.46
1:A:254:LEU:HD12	1:A:275:HIS:NE2	2.31	0.46
2:D:18:ILE:HG22	2:D:240:LYS:CG	2.46	0.46
1:C:273:PHE:CE2	1:C:291:ALA:HB1	2.51	0.46
2:B:239:ARG:HB3	2:B:241:VAL:HG23	1.97	0.45
1:C:248:GLN:C	1:C:249:ARG:HG3	2.36	0.45
2:D:38:LEU:HB3	2:D:224:ILE:HD12	1.97	0.45
1:A:44:GLU:HA	2:B:141:ASN:H	1.81	0.45
2:B:94:VAL:HG13	2:B:130:ALA:HB3	1.98	0.45
1:C:36:LYS:HD3	1:C:80:LEU:HD12	1.98	0.45
1:C:254:LEU:HD23	1:C:254:LEU:O	2.17	0.45
2:B:89:SER:CB	2:D:89:SER:OG	2.64	0.45
2:B:154:GLU:O	2:B:158:LEU:HB2	2.16	0.45
1:C:23:LYS:CG	1:C:24:GLY:H	2.27	0.45
2:D:234:SER:H	2:D:235:PRO:HD2	1.82	0.45
2:B:160:ASN:CG	2:B:164:LYS:HE3	2.36	0.45
2:B:246:PRO:HA	2:B:247:PRO:HD3	1.84	0.45
2:D:109:TYR:HA	2:D:110:PRO:HD2	1.72	0.45
2:B:160:ASN:ND2	2:B:164:LYS:CE	2.79	0.45
1:C:181:MET:HG2	1:C:218:LEU:HD11	1.97	0.45
2:D:43:LEU:HD11	2:D:102:ILE:HD11	1.98	0.45
2:B:37:VAL:HG23	2:B:38:LEU:H	1.81	0.45
1:C:23:LYS:HG2	1:C:24:GLY:N	2.30	0.45
1:C:201:GLU:OE1	1:C:207:PRO:HA	2.16	0.45
1:C:269:ASN:OD1	1:C:295:PRO:HB2	2.17	0.45
1:C:298:ALA:O	1:C:300:TYR:N	2.48	0.45
2:B:35:LEU:O	2:B:36:VAL:C	2.54	0.45
1:A:209:PHE:N	1:A:210:PRO:HD3	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:70:LYS:O	2:B:71:ILE:CG2	2.64	0.45
1:C:135:LYS:HG3	1:C:137:GLN:CG	2.37	0.45
1:C:294:HIS:CE1	1:C:296:TRP:H	2.33	0.45
1:A:237:THR:O	2:D:74:ASN:ND2	2.43	0.45
1:C:259:GLN:N	1:C:260:PRO:HD2	2.32	0.44
2:D:153:HIS:O	2:D:156:ASN:HB2	2.17	0.44
2:B:90:LEU:HD13	2:B:127:THR:OG1	2.18	0.44
2:B:127:THR:CG2	2:B:128:THR:N	2.80	0.44
1:C:187:SER:OG	1:C:188:THR:N	2.50	0.44
1:C:233:TRP:CD1	1:C:235:SER:HB2	2.52	0.44
2:D:167:ASN:N	2:D:167:ASN:ND2	2.65	0.44
1:A:64:ASN:HA	1:A:148:LYS:HG2	1.98	0.44
1:A:140:LEU:N	1:A:140:LEU:HD12	2.32	0.44
2:D:115:ASN:O	2:D:117:LEU:N	2.45	0.44
1:C:10:LEU:HB3	1:C:11:GLU:H	1.60	0.44
1:C:115:TRP:O	1:C:119:GLN:HB2	2.17	0.44
2:D:109:TYR:CZ	2:D:165:ARG:NE	2.86	0.44
1:A:58:LYS:HE3	2:B:167:ASN:O	2.18	0.44
2:B:20:LYS:HE2	2:B:244:VAL:HG21	2.00	0.44
2:B:23:LEU:HA	2:B:24:PRO:HD3	1.79	0.44
1:C:54:ILE:HD11	1:C:80:LEU:HD21	2.00	0.44
2:D:42:MET:HE3	2:D:227:LEU:HD12	1.96	0.44
2:B:222:ARG:HG3	2:B:222:ARG:HH11	1.82	0.44
1:C:107:LEU:HD12	1:C:107:LEU:H	1.80	0.44
1:C:193:TRP:NE1	1:C:197:CYS:SG	2.91	0.44
1:C:253:ASP:CG	1:C:256:GLN:HG2	2.37	0.44
2:B:24:PRO:HG2	2:B:29:LYS:O	2.18	0.44
2:D:168:TYR:O	2:D:170:ILE:HG13	2.18	0.44
2:B:44:VAL:CG2	2:B:235:PRO:HD3	2.47	0.43
2:D:73:PRO:CG	4:D:2001:MES:H22	2.48	0.43
2:B:143:HIS:O	2:B:147:VAL:HG23	2.17	0.43
2:B:151:ARG:HB3	1:C:168:GLU:OE2	2.18	0.43
2:B:182:ILE:O	2:B:184:GLN:N	2.51	0.43
2:D:51:GLU:O	2:D:53:SER:N	2.51	0.43
1:A:25:LEU:HD23	1:A:32:TYR:CE2	2.53	0.43
1:A:229:ASN:C	1:A:231:SER:H	2.22	0.43
1:C:209:PHE:N	1:C:210:PRO:HD3	2.33	0.43
1:C:209:PHE:HB2	1:C:217:GLN:HE22	1.82	0.43
1:C:214:ASP:OD2	1:C:214:ASP:N	2.48	0.43
2:D:127:THR:CG2	2:D:128:THR:N	2.79	0.43
2:B:18:ILE:CG2	2:B:240:LYS:HE2	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:42:MET:HE1	2:B:227:LEU:HB2	1.99	0.43
2:B:42:MET:HA	2:B:228:VAL:HG11	1.99	0.43
2:D:102:ILE:HG13	2:D:122:PHE:CE2	2.53	0.43
1:C:57:MET:HE1	1:C:152:PHE:CD1	2.54	0.43
1:C:213:ASN:O	1:C:215:GLU:N	2.52	0.43
1:C:219:LYS:O	1:C:222:PHE:N	2.51	0.43
1:C:38:VAL:HB	1:C:78:LEU:HB3	2.00	0.43
2:D:105:LEU:O	2:D:109:TYR:HB3	2.18	0.43
2:B:109:TYR:CD2	2:B:165:ARG:HD3	2.54	0.43
2:B:207:VAL:C	2:B:209:ARG:H	2.22	0.43
1:C:106:GLU:HG3	1:C:106:GLU:O	2.18	0.43
2:B:39:ILE:HG23	2:B:99:LEU:HD13	2.00	0.43
2:B:151:ARG:HH22	1:C:214:ASP:H	1.66	0.43
2:B:169:ARG:HD2	2:B:183:GLU:OE1	2.18	0.43
2:D:121:ARG:HH22	2:D:154:GLU:HG2	1.83	0.43
1:A:258:LEU:O	1:A:259:GLN:C	2.57	0.43
2:B:75:ILE:HG23	2:B:75:ILE:O	2.19	0.43
2:B:235:PRO:O	2:B:236:ASP:C	2.57	0.43
1:A:52:ARG:HD3	1:A:155:ALA:O	2.19	0.42
2:B:109:TYR:CZ	2:B:165:ARG:CZ	3.02	0.42
1:C:132:ARG:NH1	1:C:156:ARG:HB2	2.34	0.42
1:A:40:LEU:O	1:A:76:ASN:HB3	2.19	0.42
1:A:64:ASN:O	1:A:65:ILE:HG12	2.18	0.42
1:A:140:LEU:N	1:A:140:LEU:CD1	2.82	0.42
2:B:73:PRO:HG2	2:B:120:HIS:CD2	2.41	0.42
2:B:89:SER:HB3	2:D:89:SER:OG	2.19	0.42
2:B:174:ASP:HB3	2:B:209:ARG:HH11	1.84	0.42
1:A:271:MET:HE3	1:A:271:MET:CA	2.49	0.42
2:B:166:VAL:HG12	2:B:169:ARG:H	1.83	0.42
1:C:23:LYS:O	1:C:35:LEU:HD12	2.19	0.42
2:D:69:SER:O	2:D:70:LYS:C	2.58	0.42
2:B:109:TYR:CG	2:B:165:ARG:HD3	2.55	0.42
1:C:59:GLU:CG	2:D:173:ARG:HH11	2.33	0.42
1:C:109:LEU:O	1:C:112:TYR:HB3	2.19	0.42
1:C:169:VAL:HG23	1:C:172:LEU:HD23	2.02	0.42
1:C:175:ARG:HE	1:C:179:VAL:CG1	2.32	0.42
2:B:94:VAL:HG11	2:B:131:THR:OG1	2.19	0.42
2:B:181:SER:O	2:B:184:GLN:HB2	2.20	0.42
1:C:200:ALA:O	1:C:203:ILE:HB	2.19	0.42
2:D:27:PHE:O	2:D:30:CYS:HB3	2.20	0.42
1:C:221:ILE:HG13	1:C:222:PHE:CD2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:130:LEU:HD12	1:C:158:PHE:CZ	2.55	0.42
1:C:269:ASN:O	1:C:296:TRP:HB2	2.20	0.42
1:A:100:ASN:OD1	1:A:100:ASN:N	2.53	0.42
1:A:130:LEU:HD22	1:A:158:PHE:CZ	2.54	0.42
1:A:138:ASN:HD21	1:A:151:ASP:HB3	1.85	0.42
1:A:139:LEU:CD2	1:A:149:LEU:HD23	2.50	0.42
2:B:77:ILE:HG23	2:B:78:PHE:N	2.34	0.42
2:B:87:PHE:CD1	2:B:87:PHE:N	2.88	0.42
2:B:187:LYS:O	2:B:189:PHE:CD1	2.73	0.42
1:A:21:VAL:HG11	3:A:3001:AGS:O4'	2.20	0.41
2:D:121:ARG:HG2	2:D:121:ARG:HH11	1.85	0.41
2:D:125:THR:OG1	2:D:158:LEU:HG	2.19	0.41
1:A:89:LEU:HD12	1:A:139:LEU:HD12	2.02	0.41
1:A:141:ILE:HA	1:A:146:GLN:O	2.20	0.41
1:A:268:GLY:O	1:A:271:MET:HB2	2.20	0.41
2:B:237:LYS:HD2	2:B:237:LYS:O	2.20	0.41
1:C:25:LEU:HD11	1:C:32:TYR:CE2	2.55	0.41
1:C:67:ARG:H	1:C:83:GLU:HG2	1.84	0.41
1:A:27:LYS:HA	1:A:27:LYS:HD3	1.86	0.41
1:A:58:LYS:O	1:A:61:LYS:HE3	2.19	0.41
1:A:118:LEU:HD23	1:A:118:LEU:HA	1.86	0.41
1:C:83:GLU:O	1:C:83:GLU:HG3	2.19	0.41
2:D:154:GLU:O	2:D:157:ILE:HG12	2.20	0.41
1:A:51:ILE:O	1:A:55:SER:HB2	2.21	0.41
1:A:230:GLU:OE2	1:A:242:TYR:OH	2.38	0.41
2:D:97:THR:HG22	2:D:97:THR:O	2.20	0.41
1:C:175:ARG:HG2	1:C:175:ARG:HH11	1.85	0.41
1:A:26:ASN:CG	1:A:29:THR:H	2.22	0.41
2:D:190:VAL:HG23	2:D:191:ILE:N	2.35	0.41
1:A:208:LEU:O	1:A:209:PHE:CD2	2.72	0.41
1:A:223:ASP:HB3	1:A:252:ARG:NH2	2.35	0.41
2:D:109:TYR:HD2	2:D:112:PHE:HB2	1.78	0.41
1:A:93:MET:O	1:A:96:ARG:HB3	2.20	0.41
2:B:100:TYR:HD1	2:B:220:TYR:CZ	2.39	0.41
1:C:211:GLY:HA3	1:C:217:GLN:OE1	2.21	0.41
1:C:223:ASP:OD1	1:C:249:ARG:NH1	2.54	0.41
1:C:236:VAL:C	1:C:238:LYS:H	2.23	0.41
2:D:115:ASN:C	2:D:117:LEU:H	2.23	0.41
1:A:62:HIS:HB2	1:A:123:PHE:CD2	2.56	0.41
1:A:101:THR:CB	1:A:102:PRO:CD	2.99	0.41
1:A:243:ASN:ND2	2:D:71:ILE:HD13	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:100:TYR:HA	2:B:220:TYR:CE1	2.56	0.41
2:B:117:LEU:HD12	2:B:117:LEU:HA	1.95	0.41
2:B:146:LYS:HE3	2:B:146:LYS:HB2	1.95	0.41
1:C:74:THR:O	1:C:75:GLU:C	2.60	0.41
1:C:160:ILE:HD12	2:D:172:PRO:HG2	2.03	0.41
1:C:208:LEU:HG	1:C:209:PHE:CE1	2.55	0.41
2:D:18:ILE:HG22	2:D:240:LYS:HG3	2.02	0.41
2:D:77:ILE:O	2:D:81:PHE:HB2	2.21	0.41
2:D:97:THR:HG21	2:D:134:LEU:CD1	2.51	0.41
1:A:33:VAL:HG12	1:A:69:TYR:HE2	1.86	0.41
1:A:57:MET:HA	1:A:57:MET:CE	2.51	0.41
1:A:87:ASN:ND2	1:A:87:ASN:N	2.56	0.41
2:B:187:LYS:O	2:B:189:PHE:HD1	2.04	0.41
2:B:206:TYR:O	2:B:209:ARG:HB3	2.21	0.41
2:B:218:ASP:N	2:B:218:ASP:OD1	2.54	0.41
1:C:233:TRP:N	1:C:234:PRO:HD3	2.35	0.41
1:C:255:ARG:HA	1:C:271:MET:CE	2.49	0.41
1:C:233:TRP:CZ3	1:C:280:LEU:HB3	2.54	0.40
1:A:211:GLY:HA2	1:A:220:LEU:HD11	2.03	0.40
2:B:124:LEU:O	2:B:128:THR:CG2	2.70	0.40
1:C:255:ARG:HE	1:C:255:ARG:HB3	1.58	0.40
1:C:277:LEU:N	1:C:277:LEU:HD12	2.36	0.40
2:D:175:HIS:O	2:D:179:LEU:HD12	2.22	0.40
2:B:21:VAL:H	2:B:21:VAL:HG12	1.67	0.40
2:B:35:LEU:HD23	2:B:35:LEU:HA	1.86	0.40
1:C:132:ARG:HH11	1:C:156:ARG:HB2	1.85	0.40
1:C:199:LEU:O	1:C:202:MET:HB2	2.21	0.40
1:C:239:LEU:HB2	1:C:242:TYR:HB2	2.04	0.40
1:C:243:ASN:ND2	1:C:246:ILE:HG22	2.36	0.40
1:A:130:LEU:N	1:A:130:LEU:CD1	2.85	0.40
2:D:222:ARG:HG3	2:D:222:ARG:HH21	1.86	0.40
2:D:235:PRO:O	2:D:238:SER:HB2	2.22	0.40
1:A:51:ILE:O	1:A:55:SER:CB	2.70	0.40
1:C:29:THR:C	1:C:31:VAL:H	2.25	0.40
1:C:160:ILE:CD1	2:D:172:PRO:HG2	2.51	0.40
1:C:278:LEU:HD23	1:C:278:LEU:HA	1.89	0.40
2:D:193:LYS:O	2:D:194:ASN:HB3	2.21	0.40
2:D:223:ARG:HE	2:D:227:LEU:HD21	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	282/317 (89%)	232 (82%)	39 (14%)	11 (4%)	3	12
1	C	279/317 (88%)	218 (78%)	49 (18%)	12 (4%)	2	10
2	B	207/293 (71%)	169 (82%)	32 (16%)	6 (3%)	4	18
2	D	210/293 (72%)	177 (84%)	28 (13%)	5 (2%)	6	22
All	All	978/1220 (80%)	796 (81%)	148 (15%)	34 (4%)	3	14

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	86	ASP
2	B	234	SER
2	B	238	SER
1	C	8	LYS
1	C	98	VAL
1	C	100	ASN
1	C	198	ILE
1	C	298	ALA
2	D	234	SER
2	D	246	PRO
1	A	65	ILE
1	A	74	THR
1	A	151	ASP
1	A	230	GLU
2	B	19	PRO
1	C	214	ASP
1	C	283	ASP
1	C	299	GLU
1	A	101	THR
1	A	247	GLN
2	B	116	SER
1	C	75	GLU

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Mol	Chain	Res	Type
1	C	199	LEU
2	D	52	ASN
2	D	116	SER
2	D	119	ALA
1	A	66	VAL
2	B	183	GLU
1	C	203	ILE
1	A	259	GLN
2	B	246	PRO
1	C	30	GLY
1	A	211	GLY
1	A	161	PRO

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	256/284 (90%)	239 (93%)	17 (7%)	16	44
1	C	258/284 (91%)	240 (93%)	18 (7%)	15	41
2	B	199/271 (73%)	188 (94%)	11 (6%)	21	53
2	D	202/271 (74%)	189 (94%)	13 (6%)	17	45
All	All	915/1110 (82%)	856 (94%)	59 (6%)	17	45

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	THR
1	A	39	LYS
1	A	49	THR
1	A	80	LEU
1	A	87	ASN
1	A	88	ASP
1	A	89	LEU
1	A	98	VAL
1	A	100	ASN

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Mol	Chain	Res	Type
1	A	144	ARG
1	A	164	THR
1	A	212	THR
1	A	214	ASP
1	A	245	ASN
1	A	253	ASP
1	A	262	THR
1	A	277	LEU
2	B	21	VAL
2	B	32	ARG
2	B	63	THR
2	B	81	PHE
2	B	121	ARG
2	B	128	THR
2	B	181	SER
2	B	218	ASP
2	B	239	ARG
2	B	241	VAL
2	B	246	PRO
1	C	7	PHE
1	C	11	GLU
1	C	44	GLU
1	C	59	GLU
1	C	61	LYS
1	C	87	ASN
1	C	89	LEU
1	C	108	ASN
1	C	137	GLN
1	C	164	THR
1	C	175	ARG
1	C	199	LEU
1	C	218	LEU
1	C	221	ILE
1	C	245	ASN
1	C	272	ASP
1	C	285	ARG
1	C	286	LEU
2	D	18	ILE
2	D	21	VAL
2	D	46	LEU
2	D	50	ASN
2	D	63	THR

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Mol	Chain	Res	Type
2	D	81	PHE
2	D	127	THR
2	D	128	THR
2	D	169	ARG
2	D	179	LEU
2	D	239	ARG
2	D	245	LEU
2	D	246	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	87	ASN
1	A	116	GLN
1	A	119	GLN
1	A	138	ASN
1	A	245	ASN
1	A	259	GLN
1	A	279	GLN
1	A	290	GLN
2	B	50	ASN
2	B	79	ASN
2	B	92	HIS
2	B	106	GLN
2	B	120	HIS
2	B	141	ASN
2	B	143	HIS
2	B	153	HIS
2	B	156	ASN
2	B	160	ASN
2	B	167	ASN
2	B	186	GLN
1	C	87	ASN
1	C	116	GLN
1	C	119	GLN
1	C	217	GLN
1	C	245	ASN
1	C	259	GLN
1	C	279	GLN
1	C	290	GLN
2	D	28	ASN
2	D	50	ASN

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Mol	Chain	Res	Type
2	D	61	GLN
2	D	79	ASN
2	D	92	HIS
2	D	141	ASN
2	D	156	ASN
2	D	167	ASN
2	D	194	ASN
2	D	226	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 ligands are modelled in this entry.

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	MES	B	1001	-	12,12,12	1.13	1 (8%)	14,16,16	1.22	1 (7%)
4	MES	D	2001	-	12,12,12	1.03	1 (8%)	14,16,16	1.07	1 (7%)
3	AGS	A	3001	-	26,33,33	1.35	4 (15%)	26,52,52	1.85	7 (26%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MES	B	1001	-	-	0/6/14/14	0/1/1/1
4	MES	D	2001	-	-	0/6/14/14	0/1/1/1
3	AGS	A	3001	-	1/1/7/7	9/17/38/38	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	3001	AGS	O4'-C1'	3.85	1.46	1.41
4	B	1001	MES	C8-S	3.30	1.82	1.77
4	D	2001	MES	C8-S	2.87	1.81	1.77
3	A	3001	AGS	C8-N7	-2.51	1.30	1.34
3	A	3001	AGS	PG-O3G	2.12	1.61	1.54
3	A	3001	AGS	PG-O2G	2.07	1.61	1.54

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	3001	AGS	N3-C2-N1	-5.71	119.75	128.68
3	A	3001	AGS	O4'-C4'-C5'	3.22	119.95	109.37
4	B	1001	MES	O1S-S-C8	2.91	110.42	106.92
3	A	3001	AGS	O5'-C5'-C4'	2.54	117.74	108.99
3	A	3001	AGS	C4-C5-N7	-2.42	106.88	109.40
3	A	3001	AGS	PA-O3A-PB	-2.31	124.91	132.83
3	A	3001	AGS	C2-N1-C6	2.13	122.40	118.75
3	A	3001	AGS	O2A-PA-O1A	-2.12	101.78	112.24
4	D	2001	MES	O1S-S-C8	2.03	109.36	106.92

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	3001	AGS	C3'

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	3001	AGS	C5'-O5'-PA-O2A
3	A	3001	AGS	C5'-O5'-PA-O3A
3	A	3001	AGS	O4'-C4'-C5'-O5'
3	A	3001	AGS	C3'-C4'-C5'-O5'

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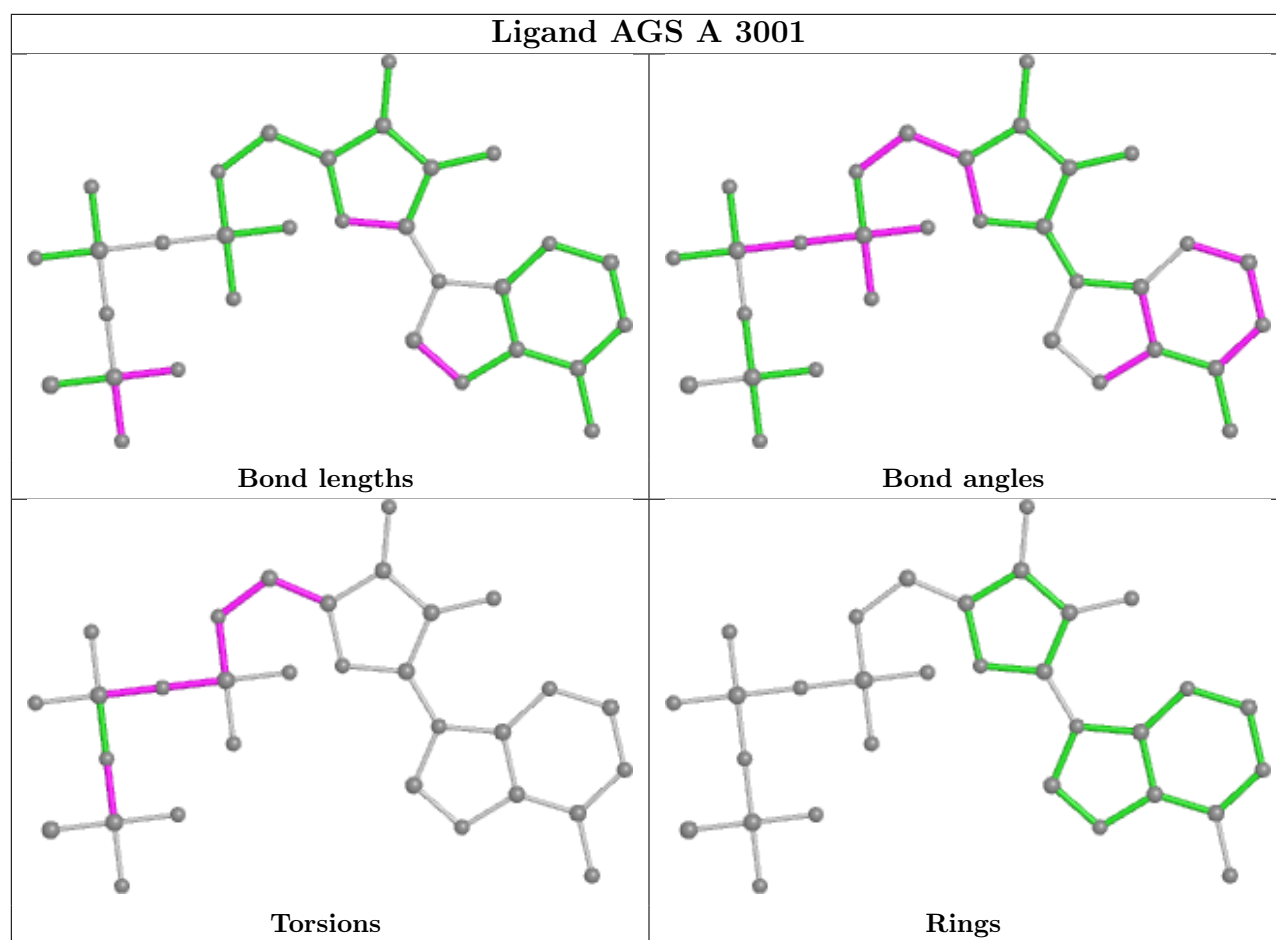
Mol	Chain	Res	Type	Atoms
3	A	3001	AGS	C5'-O5'-PA-O1A
3	A	3001	AGS	C4'-C5'-O5'-PA
3	A	3001	AGS	PB-O3A-PA-O2A
3	A	3001	AGS	PB-O3B-PG-O2G
3	A	3001	AGS	PA-O3A-PB-O2B

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	2001	MES	2	0
3	A	3001	AGS	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	284/317 (89%)	0.26	8 (2%) 53 49	14, 39, 79, 107	13 (4%)
1	C	285/317 (89%)	0.50	14 (4%) 29 26	27, 64, 108, 131	17 (5%)
2	B	213/293 (72%)	0.24	4 (1%) 66 65	16, 37, 62, 78	6 (2%)
2	D	216/293 (73%)	0.26	3 (1%) 75 75	16, 38, 67, 107	4 (1%)
All	All	998/1220 (81%)	0.32	29 (2%) 51 47	14, 44, 92, 131	40 (4%)

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	102	PRO	6.9
1	C	30	GLY	4.7
1	C	26	ASN	3.9
1	C	21	VAL	3.8
1	C	27	LYS	3.6
1	C	29	THR	3.3
1	A	232	LEU	3.1
2	B	17	GLY	3.0
1	A	102	PRO	3.0
1	C	77	LYS	3.0
1	C	223	ASP	2.8
2	D	17	GLY	2.7
1	A	40	LEU	2.7
2	D	45	SER	2.6
1	A	30	GLY	2.5
2	B	208	ASN	2.5
2	B	116	SER	2.5
1	C	74	THR	2.4
1	C	207	PRO	2.4
1	A	41	ASP	2.4
1	C	38	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	257	VAL	2.3
1	A	20	THR	2.3
1	A	272	ASP	2.2
2	B	87	PHE	2.2
1	C	28	THR	2.1
1	A	137	GLN	2.1
1	C	262	THR	2.1
2	D	236	ASP	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](#)

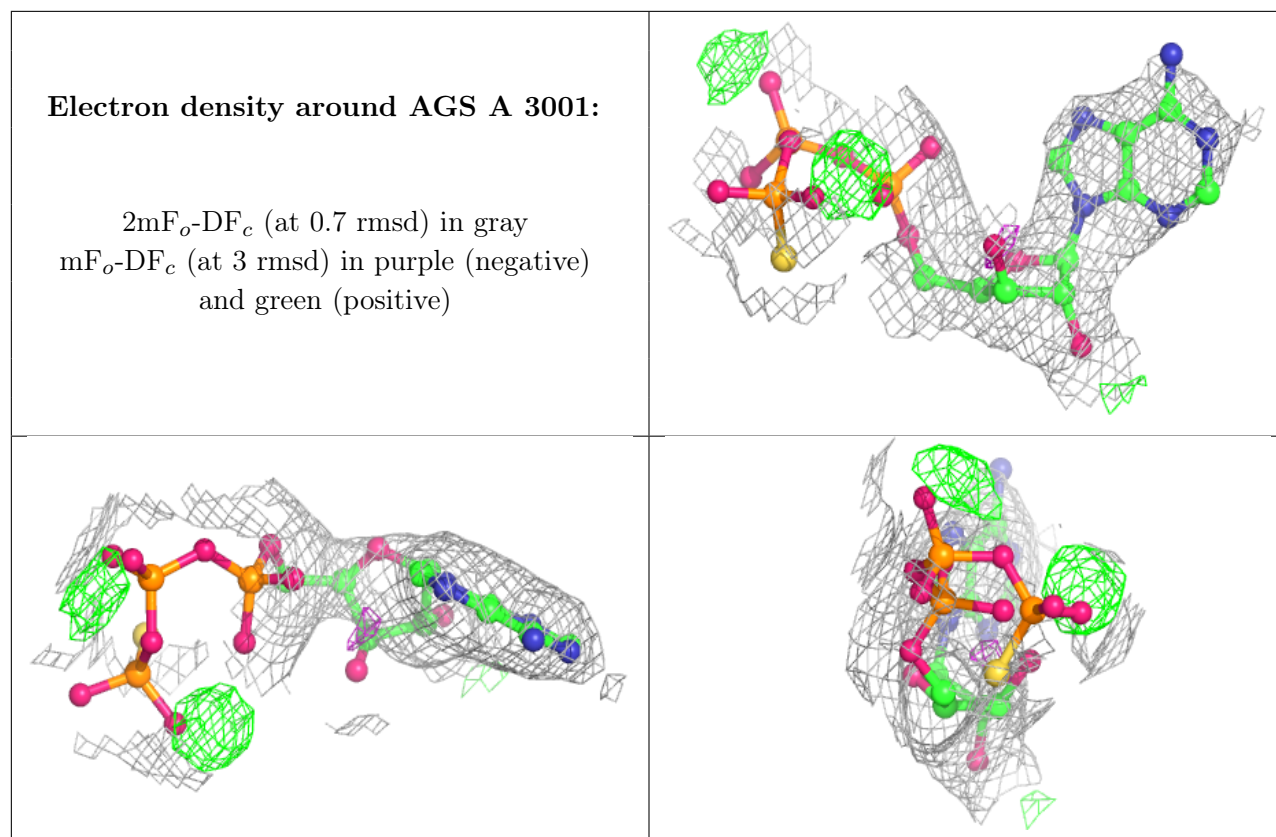
There are no monosaccharides in this entry.

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	AGS	A	3001	31/31	0.78	0.24	71,97,115,118	0
4	MES	B	1001	12/12	0.95	0.25	56,61,68,70	0
4	MES	D	2001	12/12	0.98	0.23	43,47,49,53	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.