Full wwPDB X-ray Structure Validation Report ⓘ

Jun 13, 2024 – 11:11 AM EDT

PDB ID	:	1P1Z
Title	:	X-RAY CRYSTAL STRUCTURE OF THE LECTIN-LIKE NATURAL KILLER CELL RECEPTOR LY-49C BOUND TO ITS MHC CLASS I LIGAND H-2Kb
Authors	:	Dimasi, N.; Natarajan, K.; Rangjin, G.; Dam, J.; Margulies, D.H.; Mariuzza, R.A.
Deposited on	:	2003-04-14
Resolution	:	3.26 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:

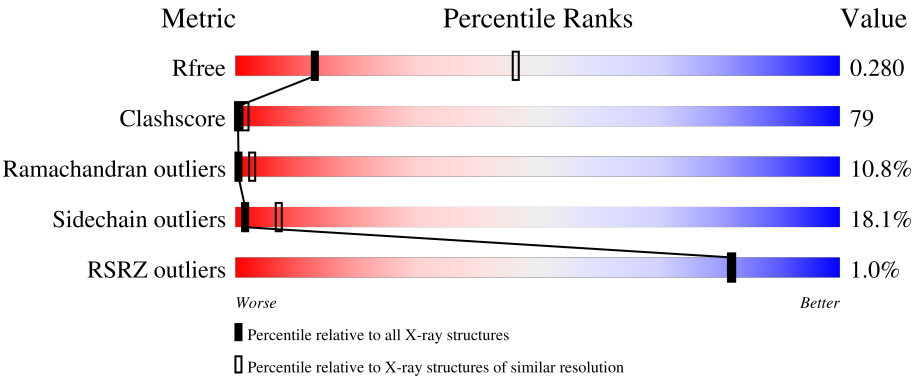
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 3.26 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	1191 (3.30-3.22)
Clashscore	141614	1251 (3.30-3.22)
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)
RSRZ outliers	127900	1154 (3.30-3.22)

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	274	19% 56% 15% • 7%
2	B	99	% 25% 57% 15% ••
3	P	8	62% 38%
4	D	120	2% 14% 59% 20% 5% •

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 3926 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 H-2 class I histocompatibility antigen, K-B alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	255	Total	C	N	O	S	0	0	0
			2072	1312	361	390	9			

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	97	Total	C	N	O	S	0	0	0
			803	515	136	146	6			

- Molecule 3 is a protein called Ovalbumin peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	P	8	Total	C	N	O	0	0	0
			68	45	10	13			

- Molecule 4 is a protein called LY49-C antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	118	Total	C	N	O	S	0	0	0
			983	637	161	174	11			

There is a discrepancy between the modelled and reference sequences:

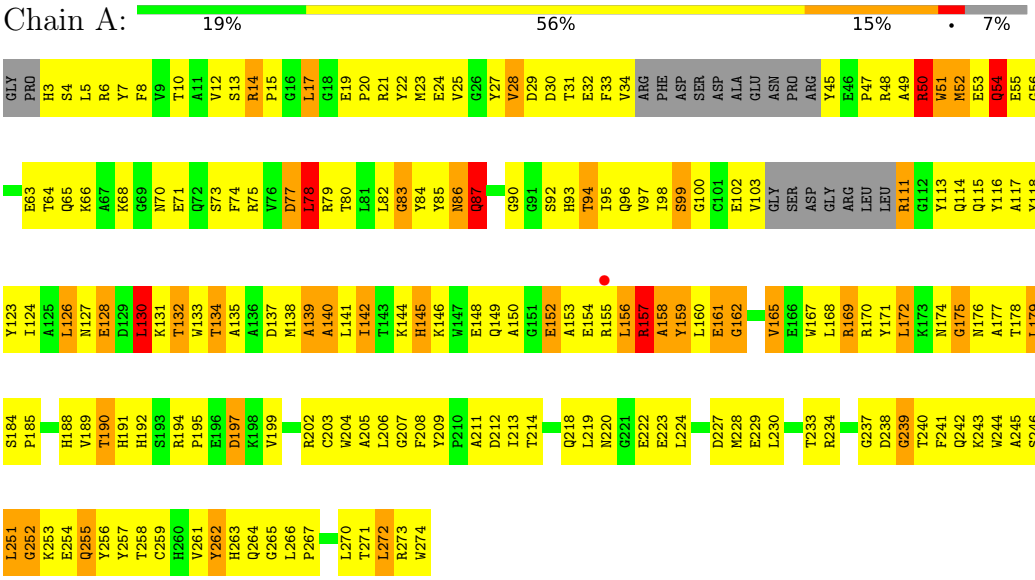
Chain	Residue	Modelled	Actual	Comment	Reference
D	144	VAL	LYS	CONFLICT	UNP Q64329

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.

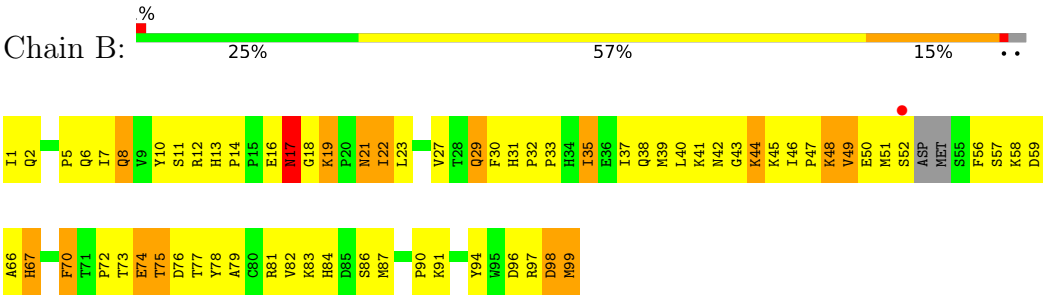
• Molecule 1: H-2 class I histocompatibility antigen, K-B alpha chain

Chain A:



• Molecule 2: Beta-2-microglobulin

Chain B:

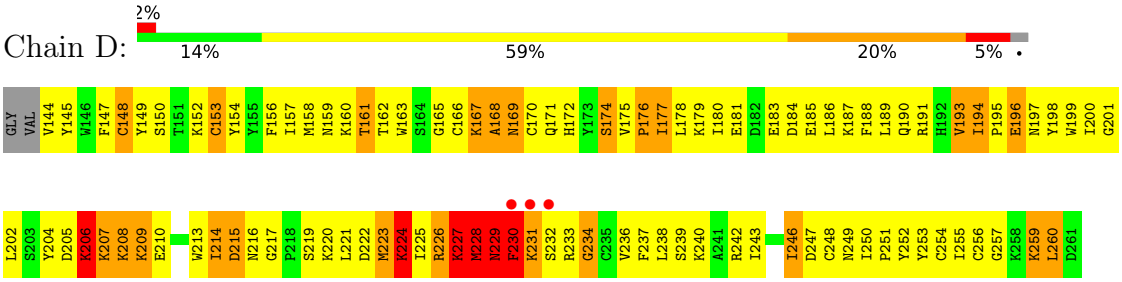


• Molecule 3: Ovalbumin peptide

Chain P:

• Molecule 4: LY49-C antigen

Chain D:


2%
14%
59%
20%
5%
GLY VAL V144 Y145 W146 F147 C148 Y149 S150 T151 K152 C153 Y154 Y155 F156 I157 M158 N159 K160 T161 T162 W163 S164 G165 C166 K167 A168 N169 C170 Q171 H172 Y173 S174 V175 P176 I177 L178 K179 I180 E181 D182 E183 D184 E185 L186 K187 F188 L189 Q190 R191 H192 V193 I194 P195 E196 N197 Y198 W199 I200 G201
L202 S203 Y204 D205 K206 K207 K208 K209 E210 W213 I214 D215 N216 G217 P218 S219 K220 L221 D222 M223 K224 I225 R226 K227 M228 N229 F230 K231 S232 R233 G234 C235 V236 F237 L238 S239 K240 A241 R242 I243 I246 D247 C248 N249 I250 P251 Y252 Y253 C254 I255 C256 G257 K258 K259 L260 D261

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	149.05Å 149.05Å 64.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.26 48.72 – 3.26	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-3.26) 99.5 (48.72-3.26)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.90 (at 3.25Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.263 , 0.316 0.260 , 0.280	Depositor DCC
R_{free} test set	558 reflections (4.75%)	wwPDB-VP
Wilson B-factor (Å^2)	79.2	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 89.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	3926	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.72% 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

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	0.54	0/2126	0.93	4/2885 (0.1%)
2	B	0.57	0/828	0.86	0/1122
3	P	0.63	0/68	0.90	0/88
4	D	0.67	1/1011 (0.1%)	1.09	5/1362 (0.4%)
All	All	0.58	1/4033 (0.0%)	0.96	9/5457 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	147	PHE	CB-CG	-5.15	1.42	1.51

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	59	TYR	N-CA-C	-8.61	87.75	111.00
1	A	28	VAL	N-CA-C	-7.01	92.07	111.00
4	D	234	GLY	N-CA-C	6.79	130.08	113.10
4	D	148	CYS	CA-CB-SG	6.48	125.66	114.00
4	D	230	PHE	N-CA-C	-6.17	94.35	111.00
4	D	224	LYS	N-CA-C	-5.97	94.88	111.00
1	A	57	PRO	N-CA-C	-5.74	97.19	112.10
1	A	58	GLU	N-CA-C	-5.37	96.51	111.00
4	D	226	ARG	N-CA-C	-5.18	97.01	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	262	TYR	Sidechain
1	A	59	TYR	Sidechain

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	2072	0	1968	330	0
2	B	803	0	776	118	0
3	P	68	0	74	26	0
4	D	983	0	949	180	0
All	All	3926	0	3767	610	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 79.

All (610) 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)
3:P:7:LYS:H	3:P:7:LYS:HD2	1.03	1.16
1:A:29:ASP:HA	4:D:230:PHE:CZ	1.81	1.13
4:D:157:ILE:HB	4:D:254:CYS:HB2	1.24	1.12
2:B:38:GLN:HB2	2:B:81:ARG:HB3	1.29	1.12
2:B:2:GLN:NE2	2:B:86:SER:HA	1.65	1.10
2:B:29:GLN:HA	2:B:61:SER:HB2	1.33	1.09
3:P:7:LYS:H	3:P:7:LYS:CD	1.63	1.08
2:B:83:LYS:HG3	2:B:90:PRO:HG3	1.27	1.08
4:D:224:LYS:O	4:D:227:LYS:HE3	1.53	1.07
2:B:38:GLN:HE22	2:B:45:LYS:HG3	1.20	1.06
4:D:227:LYS:HE2	4:D:227:LYS:HA	1.04	1.04
4:D:177:ILE:HD11	4:D:214:ILE:HG13	1.39	1.03
4:D:227:LYS:HA	4:D:227:LYS:CE	1.89	1.01
4:D:169:ASN:HD22	4:D:169:ASN:N	1.54	0.99
4:D:177:ILE:HD13	4:D:177:ILE:H	1.26	0.98
2:B:73:THR:HG22	2:B:74:GLU:H	1.26	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:LEU:H	1:A:172:LEU:HD22	1.30	0.97
4:D:148:CYS:CB	4:D:153:CYS:HA	1.95	0.97
4:D:227:LYS:HE2	4:D:227:LYS:CA	1.94	0.97
2:B:2:GLN:HE21	2:B:86:SER:HA	1.14	0.97
4:D:239:SER:HB2	4:D:242:ARG:HB2	1.46	0.96
4:D:169:ASN:H	4:D:169:ASN:ND2	1.55	0.95
4:D:148:CYS:HB3	4:D:153:CYS:HA	1.48	0.95
4:D:223:MET:HA	4:D:225:ILE:HG22	1.45	0.93
1:A:29:ASP:HA	4:D:230:PHE:HZ	1.23	0.93
4:D:226:ARG:O	4:D:228:MET:N	2.01	0.92
1:A:99:SER:OG	1:A:114:GLN:NE2	2.02	0.92
1:A:27:TYR:HA	1:A:31:THR:O	1.68	0.92
1:A:28:VAL:HG11	1:A:179:LEU:HD22	1.51	0.91
3:P:7:LYS:HD2	3:P:7:LYS:N	1.84	0.91
2:B:97:ARG:HG3	2:B:98:ASP:N	1.86	0.89
4:D:246:ILE:HG12	4:D:247:ASP:H	1.39	0.88
4:D:259:LYS:H	4:D:259:LYS:HD2	1.36	0.88
1:A:179:LEU:O	1:A:180:LEU:HD12	1.77	0.84
4:D:224:LYS:O	4:D:227:LYS:CE	2.24	0.84
1:A:93:HIS:HD2	1:A:118:TYR:OH	1.59	0.84
2:B:73:THR:HG22	2:B:74:GLU:N	1.92	0.83
2:B:31:HIS:ND1	2:B:32:PRO:HA	1.93	0.83
2:B:50:GLU:HB2	2:B:67:HIS:CD2	2.14	0.83
1:A:229:GLU:HB3	1:A:246:SER:OG	1.78	0.83
1:A:4:SER:OG	4:D:230:PHE:HE1	1.60	0.83
1:A:116:TYR:HB2	1:A:124:ILE:HG22	1.59	0.82
1:A:273:ARG:O	1:A:274:TRP:HB3	1.79	0.82
1:A:87:GLN:HG2	1:A:93:HIS:NE2	1.95	0.82
1:A:33:PHE:CD1	1:A:34:VAL:HG13	2.15	0.82
2:B:11:SER:HB2	2:B:21:ASN:HD22	1.45	0.82
2:B:83:LYS:CG	2:B:90:PRO:HG3	2.09	0.82
1:A:28:VAL:CG1	1:A:179:LEU:HD22	2.10	0.81
4:D:228:MET:O	4:D:229:ASN:HB2	1.77	0.81
1:A:128:GLU:HG3	4:D:223:MET:CE	2.11	0.81
1:A:4:SER:OG	4:D:230:PHE:CE1	2.34	0.81
1:A:5:LEU:HB2	1:A:168:LEU:HD13	1.63	0.80
2:B:32:PRO:HB2	2:B:33:PRO:HD2	1.63	0.80
2:B:73:THR:HG21	2:B:75:THR:HG23	1.62	0.80
4:D:224:LYS:O	4:D:224:LYS:HG2	1.78	0.80
4:D:223:MET:SD	4:D:225:ILE:HG21	2.22	0.80
2:B:73:THR:O	2:B:97:ARG:NH2	2.14	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:204:TYR:CD2	4:D:233:ARG:HD2	2.18	0.79
1:A:30:ASP:OD1	4:D:231:LYS:HE2	1.80	0.79
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.18	0.79
1:A:4:SER:HG	4:D:230:PHE:HE1	0.79	0.79
2:B:38:GLN:CB	2:B:81:ARG:HB3	2.10	0.78
2:B:21:ASN:N	2:B:70:PHE:O	2.16	0.78
4:D:178:LEU:HB2	4:D:255:ILE:HG22	1.65	0.77
4:D:259:LYS:HD2	4:D:259:LYS:N	1.99	0.77
1:A:51:TRP:HB2	1:A:174:ASN:O	1.85	0.77
1:A:15:PRO:C	1:A:17:LEU:H	1.88	0.76
1:A:47:PRO:HG3	1:A:60:TRP:HZ2	1.49	0.76
4:D:223:MET:SD	4:D:225:ILE:CG2	2.74	0.76
1:A:185:PRO:HB3	1:A:208:PHE:HB3	1.68	0.75
4:D:194:ILE:HG23	4:D:198:TYR:OH	1.85	0.75
3:P:7:LYS:CD	3:P:7:LYS:N	2.40	0.75
4:D:177:ILE:H	4:D:177:ILE:CD1	1.98	0.75
1:A:237:GLY:HA3	2:B:12:ARG:CZ	2.17	0.75
4:D:197:ASN:ND2	4:D:237:PHE:CE2	2.55	0.75
4:D:214:ILE:HD13	4:D:214:ILE:O	1.86	0.75
2:B:41:LYS:HG3	2:B:78:TYR:CE2	2.22	0.74
3:P:3:ILE:HD13	3:P:4:ASN:N	2.02	0.74
4:D:202:LEU:O	4:D:236:VAL:HG23	1.88	0.74
1:A:7:TYR:OH	3:P:1:SER:HB3	1.87	0.74
4:D:169:ASN:HD22	4:D:169:ASN:H	0.81	0.74
4:D:230:PHE:O	4:D:232:SER:N	2.19	0.74
4:D:193:VAL:HG13	4:D:198:TYR:CE2	2.23	0.74
1:A:79:ARG:HA	1:A:82:LEU:HD23	1.69	0.74
4:D:177:ILE:HD13	4:D:177:ILE:N	2.00	0.74
2:B:11:SER:HB2	2:B:21:ASN:ND2	2.03	0.73
4:D:223:MET:C	4:D:225:ILE:H	1.91	0.73
2:B:12:ARG:HD2	2:B:22:ILE:HD12	1.69	0.73
1:A:58:GLU:CD	1:A:58:GLU:O	2.27	0.73
4:D:229:ASN:HD21	4:D:233:ARG:NE	1.87	0.72
2:B:12:ARG:HD2	2:B:22:ILE:CD1	2.19	0.72
2:B:73:THR:HG22	2:B:75:THR:H	1.55	0.72
2:B:83:LYS:HE3	2:B:90:PRO:CG	2.20	0.72
1:A:272:LEU:HD12	1:A:272:LEU:N	2.04	0.72
1:A:47:PRO:HG3	1:A:60:TRP:CZ2	2.24	0.72
1:A:52:MET:HA	1:A:52:MET:CE	2.19	0.72
1:A:66:LYS:HB2	1:A:66:LYS:NZ	2.05	0.71
4:D:148:CYS:HB2	4:D:152:LYS:O	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:ASP:OD2	4:D:242:ARG:HD2	1.88	0.71
2:B:48:LYS:NZ	2:B:48:LYS:HA	2.03	0.71
1:A:24:GLU:CD	3:P:2:ILE:HD13	2.10	0.71
1:A:137:ASP:OD2	1:A:139:ALA:HB3	1.91	0.71
1:A:188:HIS:CD2	1:A:204:TRP:HB2	2.26	0.71
2:B:5:PRO:HA	2:B:30:PHE:HB3	1.72	0.71
1:A:73:SER:OG	3:P:7:LYS:HE3	1.90	0.71
2:B:38:GLN:NE2	2:B:45:LYS:HG3	2.01	0.71
1:A:66:LYS:HB2	1:A:66:LYS:HZ2	1.56	0.70
1:A:29:ASP:CA	4:D:230:PHE:HZ	2.01	0.70
1:A:126:LEU:HD13	1:A:130:LEU:HB3	1.73	0.70
1:A:159:TYR:CZ	3:P:3:ILE:HB	2.26	0.70
1:A:33:PHE:HA	1:A:49:ALA:HB2	1.74	0.70
1:A:168:LEU:O	1:A:172:LEU:HD22	1.92	0.70
1:A:169:ARG:HA	1:A:172:LEU:HD23	1.73	0.70
2:B:17:ASN:HA	2:B:72:PRO:HG2	1.72	0.70
1:A:3:HIS:O	1:A:103:VAL:HG22	1.91	0.70
1:A:82:LEU:HD12	1:A:87:GLN:HB3	1.73	0.70
4:D:194:ILE:HD12	4:D:195:PRO:HD2	1.74	0.70
1:A:7:TYR:CE2	3:P:2:ILE:HA	2.27	0.70
1:A:172:LEU:HD22	1:A:172:LEU:N	2.05	0.69
1:A:162:GLY:O	1:A:165:VAL:HG23	1.92	0.69
1:A:230:LEU:HD23	1:A:245:ALA:HB2	1.74	0.69
4:D:239:SER:CB	4:D:242:ARG:HB2	2.19	0.69
2:B:73:THR:CG2	2:B:75:THR:HG23	2.21	0.69
4:D:177:ILE:CD1	4:D:214:ILE:HG13	2.21	0.69
4:D:178:LEU:HG	4:D:179:LYS:N	2.05	0.69
4:D:144:VAL:HG22	4:D:158:MET:HG3	1.73	0.69
1:A:29:ASP:HA	4:D:230:PHE:CE1	2.27	0.69
2:B:39:MET:HG3	2:B:49:VAL:CG2	2.22	0.69
4:D:166:CYS:HB3	4:D:177:ILE:HG22	1.75	0.69
1:A:77:ASP:HA	1:A:80:THR:HG22	1.75	0.69
4:D:178:LEU:CD1	4:D:257:GLY:HA3	2.23	0.68
1:A:92:SER:O	1:A:93:HIS:ND1	2.26	0.68
4:D:170:CYS:SG	4:D:177:ILE:HA	2.32	0.68
1:A:29:ASP:HB3	4:D:231:LYS:CD	2.24	0.68
1:A:99:SER:HG	1:A:114:GLN:HE22	1.39	0.68
2:B:42:ASN:O	2:B:44:LYS:N	2.23	0.68
1:A:52:MET:HA	1:A:52:MET:HE3	1.76	0.68
1:A:59:TYR:CE1	1:A:63:GLU:OE1	2.47	0.68
2:B:96:ASP:O	2:B:99:MET:N	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:ASP:HB3	4:D:231:LYS:HD3	1.77	0.67
1:A:266:LEU:HD21	1:A:270:LEU:CD1	2.25	0.67
1:A:29:ASP:HB3	4:D:231:LYS:CG	2.24	0.67
1:A:167:TRP:O	1:A:171:TYR:HD2	1.78	0.67
2:B:73:THR:CG2	2:B:74:GLU:H	2.05	0.67
1:A:237:GLY:HA3	2:B:12:ARG:NH2	2.08	0.67
2:B:19:LYS:O	2:B:72:PRO:HD2	1.94	0.67
1:A:77:ASP:HA	1:A:80:THR:CG2	2.25	0.66
1:A:111:ARG:NH1	1:A:111:ARG:HB2	2.11	0.66
4:D:223:MET:CA	4:D:225:ILE:HG22	2.22	0.66
2:B:97:ARG:HG3	2:B:98:ASP:H	1.58	0.66
1:A:152:GLU:HG2	1:A:155:ARG:HD2	1.77	0.66
4:D:204:TYR:OH	4:D:209:LYS:HG3	1.94	0.66
1:A:12:VAL:HG12	1:A:12:VAL:O	1.96	0.66
1:A:27:TYR:CA	1:A:31:THR:O	2.44	0.66
1:A:12:VAL:HG22	1:A:94:THR:HB	1.78	0.66
3:P:5:PHE:CD1	3:P:5:PHE:N	2.63	0.66
1:A:204:TRP:HZ2	2:B:99:MET:O	1.79	0.66
4:D:198:TYR:O	4:D:237:PHE:HB2	1.96	0.65
2:B:39:MET:HG3	2:B:49:VAL:HG23	1.79	0.65
4:D:178:LEU:HD13	4:D:257:GLY:HA3	1.78	0.65
1:A:158:ALA:O	1:A:160:LEU:N	2.28	0.65
1:A:213:ILE:HG12	1:A:214:THR:N	2.11	0.65
1:A:168:LEU:O	1:A:172:LEU:CD2	2.44	0.65
1:A:175:GLY:C	1:A:177:ALA:H	1.98	0.65
1:A:233:THR:HB	1:A:243:LYS:NZ	2.11	0.65
1:A:169:ARG:C	1:A:171:TYR:H	2.00	0.65
4:D:204:TYR:CE2	4:D:233:ARG:HD2	2.32	0.65
1:A:63:GLU:O	1:A:66:LYS:HB2	1.97	0.64
4:D:157:ILE:CB	4:D:254:CYS:HB2	2.15	0.64
4:D:208:LYS:HD3	4:D:210:GLU:CD	2.18	0.64
4:D:166:CYS:CB	4:D:177:ILE:HG22	2.27	0.64
4:D:187:LYS:O	4:D:191:ARG:HG3	1.98	0.64
2:B:7:ILE:CG1	2:B:82:VAL:HG21	2.28	0.64
4:D:144:VAL:HG22	4:D:158:MET:CG	2.27	0.64
4:D:161:THR:O	4:D:251:PRO:HA	1.98	0.64
1:A:185:PRO:CB	1:A:208:PHE:HB3	2.28	0.64
2:B:38:GLN:HB2	2:B:81:ARG:CB	2.19	0.64
1:A:159:TYR:CE2	3:P:3:ILE:HB	2.33	0.64
4:D:225:ILE:C	4:D:227:LYS:N	2.50	0.63
1:A:99:SER:HA	1:A:113:TYR:O	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:THR:O	1:A:181:ARG:HG2	1.99	0.63
1:A:19:GLU:HB3	1:A:20:PRO:CD	2.29	0.63
1:A:111:ARG:CB	1:A:111:ARG:HH11	2.12	0.63
1:A:29:ASP:HB3	4:D:231:LYS:HG2	1.81	0.63
1:A:15:PRO:HG3	1:A:90:GLY:O	1.99	0.63
1:A:99:SER:HG	1:A:114:GLN:NE2	1.95	0.63
2:B:39:MET:CG	2:B:49:VAL:HG21	2.29	0.63
2:B:73:THR:HG22	2:B:75:THR:N	2.14	0.63
1:A:175:GLY:C	1:A:177:ALA:N	2.52	0.62
1:A:237:GLY:HA3	2:B:12:ARG:NE	2.14	0.62
2:B:60:TRP:NE1	4:D:242:ARG:NH1	2.48	0.62
1:A:128:GLU:HG3	4:D:223:MET:HE1	1.81	0.62
1:A:154:GLU:C	1:A:156:LEU:N	2.51	0.62
1:A:142:ILE:HG23	1:A:142:ILE:O	1.98	0.62
1:A:153:ALA:HB3	1:A:154:GLU:OE1	1.99	0.62
1:A:87:GLN:NE2	1:A:118:TYR:OH	2.32	0.62
1:A:117:ALA:HB2	2:B:60:TRP:CZ2	2.35	0.62
1:A:185:PRO:CA	1:A:208:PHE:HB3	2.30	0.62
1:A:224:LEU:O	1:A:228:MET:HG3	2.00	0.62
4:D:223:MET:C	4:D:225:ILE:N	2.50	0.62
1:A:169:ARG:HA	1:A:172:LEU:CD2	2.29	0.61
2:B:13:HIS:HB3	2:B:14:PRO:HD2	1.82	0.61
4:D:152:LYS:HE2	4:D:185:GLU:OE2	2.01	0.61
4:D:207:LYS:C	4:D:209:LYS:H	2.03	0.61
1:A:238:ASP:O	1:A:240:THR:N	2.31	0.61
1:A:7:TYR:CD2	3:P:2:ILE:HG13	2.36	0.61
1:A:172:LEU:O	1:A:175:GLY:N	2.34	0.61
4:D:180:ILE:O	4:D:219:SER:OG	2.14	0.61
1:A:169:ARG:O	1:A:171:TYR:N	2.34	0.61
4:D:224:LYS:HG2	4:D:227:LYS:HE3	1.83	0.60
1:A:197:ASP:OD2	1:A:197:ASP:N	2.30	0.60
2:B:16:GLU:O	2:B:17:ASN:O	2.19	0.60
4:D:157:ILE:HG22	4:D:159:ASN:H	1.66	0.60
3:P:3:ILE:HD13	3:P:4:ASN:H	1.66	0.60
1:A:10:THR:O	1:A:22:TYR:HA	2.02	0.60
1:A:190:THR:HB	1:A:192:HIS:NE2	2.16	0.60
4:D:190:GLN:O	4:D:240:LYS:HE3	2.02	0.59
2:B:17:ASN:CA	2:B:72:PRO:HG2	2.32	0.59
2:B:42:ASN:C	2:B:44:LYS:H	2.05	0.59
4:D:202:LEU:HD23	4:D:236:VAL:HG21	1.83	0.59
1:A:80:THR:OG1	1:A:84:TYR:CE2	2.55	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:TYR:C	1:A:87:GLN:H	2.05	0.59
1:A:219:LEU:O	1:A:220:ASN:HB2	2.02	0.59
2:B:41:LYS:HE2	2:B:78:TYR:OH	2.03	0.59
1:A:234:ARG:HD2	2:B:10:TYR:CD2	2.37	0.59
4:D:224:LYS:O	4:D:224:LYS:CG	2.49	0.59
1:A:78:LEU:HA	1:A:95:ILE:HD11	1.84	0.59
2:B:27:VAL:HG21	2:B:37:ILE:HD12	1.84	0.59
1:A:5:LEU:CB	1:A:168:LEU:HD13	2.31	0.59
1:A:207:GLY:HA2	1:A:240:THR:HB	1.84	0.58
1:A:251:LEU:HD23	1:A:252:GLY:H	1.68	0.58
4:D:144:VAL:N	4:D:156:PHE:O	2.35	0.58
1:A:244:TRP:CZ3	1:A:246:SER:HB3	2.38	0.58
2:B:48:LYS:HA	2:B:48:LYS:HZ3	1.66	0.58
3:P:5:PHE:H	3:P:5:PHE:HD1	1.50	0.58
2:B:7:ILE:HD12	2:B:7:ILE:H	1.68	0.58
4:D:259:LYS:O	4:D:260:LEU:HD22	2.03	0.58
1:A:29:ASP:CA	4:D:230:PHE:CZ	2.71	0.58
2:B:11:SER:CB	2:B:21:ASN:HD22	2.16	0.58
4:D:233:ARG:HG3	4:D:234:GLY:H	1.68	0.58
2:B:2:GLN:HE21	2:B:86:SER:CA	2.03	0.58
4:D:148:CYS:HB2	4:D:153:CYS:HA	1.82	0.58
4:D:178:LEU:CG	4:D:179:LYS:N	2.66	0.58
1:A:211:ALA:HB2	1:A:241:PHE:CE1	2.39	0.58
1:A:33:PHE:HA	1:A:49:ALA:CB	2.34	0.58
1:A:116:TYR:CB	1:A:124:ILE:HG22	2.30	0.58
4:D:175:VAL:O	4:D:256:CYS:HB3	2.03	0.58
2:B:29:GLN:HA	2:B:61:SER:CB	2.22	0.58
1:A:66:LYS:NZ	1:A:66:LYS:CB	2.66	0.57
2:B:32:PRO:HD2	2:B:84:HIS:NE2	2.19	0.57
1:A:243:LYS:HG2	1:A:244:TRP:N	2.19	0.57
4:D:229:ASN:ND2	4:D:233:ARG:NE	2.53	0.57
1:A:189:VAL:HG22	1:A:203:CYS:HA	1.86	0.57
2:B:73:THR:HG21	2:B:76:ASP:H	1.69	0.57
4:D:204:TYR:CD2	4:D:233:ARG:CD	2.87	0.57
1:A:128:GLU:HG3	4:D:223:MET:HE3	1.87	0.57
1:A:139:ALA:O	1:A:141:LEU:N	2.38	0.57
3:P:2:ILE:HG23	3:P:3:ILE:O	2.05	0.57
4:D:227:LYS:O	4:D:227:LYS:HD3	2.05	0.57
1:A:192:HIS:CD2	1:A:192:HIS:N	2.73	0.57
4:D:194:ILE:CD1	4:D:195:PRO:HD2	2.35	0.57
1:A:78:LEU:HD22	1:A:95:ILE:CD1	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:ARG:NH1	1:A:111:ARG:CB	2.68	0.56
1:A:152:GLU:HA	1:A:155:ARG:HB2	1.86	0.56
2:B:17:ASN:ND2	2:B:97:ARG:HH12	2.03	0.56
1:A:77:ASP:CA	1:A:80:THR:HG22	2.35	0.56
1:A:138:MET:O	1:A:141:LEU:HB3	2.05	0.56
1:A:168:LEU:O	1:A:171:TYR:HB2	2.05	0.56
1:A:233:THR:HB	1:A:243:LYS:HZ3	1.71	0.56
1:A:258:THR:HG22	1:A:273:ARG:HG2	1.86	0.56
2:B:96:ASP:O	2:B:97:ARG:C	2.43	0.56
1:A:135:ALA:HB1	1:A:140:ALA:HB3	1.88	0.56
2:B:46:ILE:HG22	2:B:48:LYS:O	2.06	0.56
1:A:118:TYR:O	1:A:119:ASP:HB2	2.06	0.56
1:A:273:ARG:O	1:A:274:TRP:CB	2.50	0.56
1:A:28:VAL:CG1	1:A:28:VAL:O	2.53	0.56
1:A:100:GLY:O	1:A:113:TYR:N	2.25	0.56
1:A:185:PRO:HB3	1:A:208:PHE:CB	2.34	0.55
1:A:97:VAL:HA	1:A:115:GLN:O	2.07	0.55
2:B:98:ASP:O	2:B:99:MET:C	2.44	0.55
4:D:225:ILE:O	4:D:227:LYS:N	2.34	0.55
4:D:178:LEU:HD12	4:D:179:LYS:H	1.72	0.55
1:A:111:ARG:HH11	1:A:111:ARG:HB3	1.72	0.55
4:D:227:LYS:CE	4:D:227:LYS:O	2.54	0.55
1:A:167:TRP:HB3	1:A:171:TYR:CE2	2.42	0.55
1:A:77:ASP:O	1:A:78:LEU:C	2.44	0.55
1:A:199:VAL:HG22	1:A:249:VAL:HG22	1.89	0.55
2:B:96:ASP:O	2:B:99:MET:HB2	2.06	0.55
1:A:158:ALA:O	1:A:159:TYR:C	2.45	0.55
1:A:211:ALA:HB2	1:A:241:PHE:CD1	2.42	0.55
4:D:196:GLU:HG3	4:D:253:TYR:CE2	2.41	0.55
1:A:123:TYR:HD2	1:A:124:ILE:HB	1.71	0.55
1:A:167:TRP:HB3	1:A:171:TYR:HE2	1.72	0.55
1:A:206:LEU:HD23	1:A:242:GLN:HB2	1.88	0.55
1:A:254:GLU:O	1:A:256:TYR:N	2.39	0.55
4:D:166:CYS:O	4:D:167:LYS:C	2.45	0.55
4:D:250:ILE:HG21	4:D:252:TYR:CZ	2.42	0.55
4:D:193:VAL:CG1	4:D:198:TYR:CE2	2.90	0.54
4:D:177:ILE:HD11	4:D:214:ILE:CG1	2.26	0.54
1:A:34:VAL:HA	1:A:47:PRO:HA	1.88	0.54
1:A:158:ALA:O	1:A:161:GLU:N	2.40	0.54
2:B:7:ILE:C	2:B:8:GLN:HG2	2.26	0.54
1:A:64:THR:O	1:A:65:GLN:C	2.44	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:ILE:CG1	1:A:214:THR:N	2.71	0.54
4:D:223:MET:SD	4:D:225:ILE:HG22	2.48	0.54
1:A:14:ARG:NE	1:A:19:GLU:O	2.39	0.54
1:A:127:ASN:HD21	1:A:133:TRP:C	2.11	0.54
1:A:31:THR:HG22	1:A:32:GLU:O	2.07	0.54
2:B:41:LYS:HE2	2:B:78:TYR:CE2	2.43	0.54
2:B:35:ILE:CD1	2:B:84:HIS:HB2	2.38	0.54
3:P:2:ILE:HG23	3:P:3:ILE:N	2.22	0.54
1:A:127:ASN:ND2	1:A:132:THR:O	2.40	0.54
1:A:128:GLU:CD	1:A:128:GLU:H	2.12	0.54
4:D:178:LEU:CD1	4:D:179:LYS:H	2.21	0.54
1:A:145:HIS:HA	1:A:148:GLU:OE2	2.08	0.53
1:A:14:ARG:H	1:A:14:ARG:HD3	1.73	0.53
1:A:28:VAL:O	1:A:29:ASP:HB2	2.09	0.53
4:D:197:ASN:O	4:D:252:TYR:HB3	2.08	0.53
1:A:56:GLY:O	1:A:59:TYR:HB3	2.08	0.53
4:D:205:ASP:O	4:D:206:LYS:C	2.46	0.53
4:D:229:ASN:HD21	4:D:233:ARG:CZ	2.21	0.53
1:A:51:TRP:CZ2	1:A:179:LEU:HD21	2.44	0.53
1:A:153:ALA:CB	1:A:154:GLU:OE1	2.57	0.53
1:A:211:ALA:HB2	1:A:241:PHE:CZ	2.44	0.53
1:A:63:GLU:OE2	1:A:66:LYS:HE3	2.09	0.53
1:A:139:ALA:C	1:A:141:LEU:N	2.61	0.53
2:B:31:HIS:ND1	2:B:32:PRO:CA	2.70	0.53
2:B:7:ILE:HD12	2:B:7:ILE:N	2.23	0.53
2:B:18:GLY:N	2:B:72:PRO:O	2.30	0.52
2:B:38:GLN:HB3	2:B:40:LEU:HD21	1.91	0.52
1:A:50:ARG:O	1:A:52:MET:N	2.42	0.52
2:B:5:PRO:CA	2:B:30:PHE:HB3	2.40	0.52
1:A:14:ARG:HG2	1:A:14:ARG:O	2.10	0.52
4:D:167:LYS:HA	4:D:177:ILE:HG23	1.92	0.52
1:A:154:GLU:O	1:A:156:LEU:N	2.43	0.52
2:B:73:THR:CG2	2:B:75:THR:CG2	2.88	0.52
1:A:171:TYR:O	1:A:172:LEU:C	2.48	0.52
4:D:178:LEU:CG	4:D:179:LYS:H	2.23	0.52
1:A:30:ASP:OD2	4:D:230:PHE:HE2	1.92	0.52
2:B:83:LYS:HE3	2:B:90:PRO:HG3	1.91	0.52
4:D:246:ILE:HG12	4:D:247:ASP:N	2.18	0.52
4:D:194:ILE:HG23	4:D:198:TYR:HH	1.75	0.52
4:D:227:LYS:O	4:D:227:LYS:CD	2.58	0.52
1:A:70:ASN:O	1:A:71:GLU:C	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:ASP:OD1	3:P:7:LYS:HA	2.10	0.51
4:D:190:GLN:HG2	4:D:239:SER:O	2.10	0.51
1:A:30:ASP:CG	4:D:231:LYS:HE2	2.31	0.51
4:D:190:GLN:O	4:D:240:LYS:CE	2.58	0.51
1:A:212:ASP:OD2	4:D:232:SER:HA	2.10	0.51
2:B:65:LEU:HD12	2:B:66:ALA:N	2.26	0.51
2:B:79:ALA:CB	2:B:94:TYR:HA	2.40	0.51
4:D:148:CYS:HB3	4:D:154:TYR:H	1.75	0.51
1:A:7:TYR:HD1	1:A:25:VAL:O	1.93	0.51
1:A:178:THR:C	1:A:180:LEU:H	2.14	0.51
1:A:258:THR:HG22	1:A:273:ARG:CG	2.41	0.51
2:B:79:ALA:HB2	2:B:94:TYR:HA	1.92	0.51
1:A:21:ARG:NH2	1:A:23:MET:HE1	2.26	0.51
1:A:144:LYS:O	1:A:146:LYS:N	2.43	0.51
1:A:126:LEU:HD22	1:A:130:LEU:HA	1.93	0.51
1:A:121:CYS:SG	2:B:1:ILE:HG12	2.51	0.51
1:A:271:THR:O	1:A:271:THR:CG2	2.59	0.51
2:B:40:LEU:HA	2:B:44:LYS:O	2.10	0.51
1:A:202:ARG:HD2	1:A:204:TRP:CE2	2.45	0.51
4:D:227:LYS:HE2	4:D:227:LYS:C	2.31	0.51
1:A:86:ASN:O	1:A:87:GLN:O	2.29	0.51
1:A:4:SER:HB2	1:A:102:GLU:HA	1.92	0.50
1:A:191:HIS:C	1:A:192:HIS:HD2	2.15	0.50
1:A:202:ARG:HD2	1:A:204:TRP:CZ2	2.46	0.50
4:D:148:CYS:HB3	4:D:153:CYS:CA	2.32	0.50
1:A:156:LEU:O	1:A:157:ARG:C	2.50	0.50
1:A:244:TRP:HZ3	1:A:246:SER:HB3	1.76	0.50
1:A:123:TYR:CD2	1:A:124:ILE:HB	2.47	0.50
1:A:63:GLU:O	1:A:66:LYS:N	2.45	0.50
4:D:163:TRP:C	4:D:165:GLY:N	2.62	0.50
1:A:266:LEU:HD21	1:A:270:LEU:HD13	1.93	0.50
1:A:205:ALA:O	1:A:242:GLN:HA	2.11	0.50
1:A:77:ASP:O	1:A:79:ARG:N	2.44	0.49
4:D:181:GLU:HA	4:D:219:SER:OG	2.12	0.49
1:A:230:LEU:CD2	1:A:245:ALA:HB2	2.42	0.49
4:D:160:LYS:HA	4:D:252:TYR:O	2.12	0.49
1:A:22:TYR:OH	1:A:24:GLU:HG3	2.11	0.49
1:A:127:ASN:OD1	1:A:134:THR:CG2	2.60	0.49
1:A:271:THR:O	1:A:271:THR:HG23	2.11	0.49
4:D:190:GLN:HB3	4:D:240:LYS:O	2.13	0.49
1:A:28:VAL:HG11	1:A:179:LEU:CD2	2.34	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:HIS:CD2	1:A:118:TYR:OH	2.51	0.49
1:A:52:MET:HA	1:A:52:MET:HE2	1.94	0.49
1:A:169:ARG:C	1:A:171:TYR:N	2.64	0.49
4:D:144:VAL:HG13	4:D:158:MET:HB2	1.93	0.49
1:A:251:LEU:O	1:A:252:GLY:C	2.50	0.49
1:A:29:ASP:OD1	4:D:230:PHE:CE1	2.65	0.49
1:A:33:PHE:HD1	1:A:34:VAL:HG13	1.73	0.49
1:A:167:TRP:C	1:A:171:TYR:HD2	2.16	0.49
1:A:213:ILE:HG12	1:A:214:THR:H	1.78	0.49
1:A:63:GLU:OE2	1:A:66:LYS:CE	2.61	0.48
2:B:49:VAL:HG13	2:B:49:VAL:O	2.13	0.48
2:B:57:SER:OG	2:B:59:ASP:OD2	2.21	0.48
3:P:6:GLU:O	3:P:7:LYS:C	2.52	0.48
4:D:144:VAL:CG2	4:D:158:MET:HG3	2.42	0.48
1:A:191:HIS:HB2	1:A:274:TRP:CE2	2.48	0.48
4:D:246:ILE:CG1	4:D:247:ASP:H	2.18	0.48
1:A:185:PRO:HD2	1:A:266:LEU:HD13	1.95	0.48
1:A:208:PHE:HB2	1:A:263:HIS:CD2	2.48	0.48
4:D:226:ARG:HB2	4:D:228:MET:CE	2.43	0.48
1:A:103:VAL:HG13	1:A:168:LEU:HD23	1.95	0.48
2:B:48:LYS:HA	2:B:48:LYS:HZ2	1.77	0.48
4:D:178:LEU:HD12	4:D:257:GLY:HA3	1.94	0.48
1:A:202:ARG:HD2	1:A:204:TRP:NE1	2.28	0.48
3:P:3:ILE:CD1	3:P:4:ASN:H	2.26	0.48
1:A:8:PHE:CE2	1:A:98:ILE:HG23	2.48	0.48
1:A:19:GLU:HB3	1:A:20:PRO:HD2	1.94	0.48
1:A:57:PRO:O	1:A:58:GLU:CB	2.62	0.48
4:D:145:TYR:CD1	4:D:145:TYR:C	2.87	0.48
4:D:169:ASN:N	4:D:169:ASN:ND2	2.28	0.48
1:A:77:ASP:O	1:A:80:THR:HG22	2.14	0.48
3:P:7:LYS:H	3:P:7:LYS:HD3	1.66	0.48
1:A:130:LEU:H	1:A:130:LEU:HG	1.32	0.48
1:A:171:TYR:O	1:A:174:ASN:N	2.35	0.48
2:B:97:ARG:CG	2:B:98:ASP:N	2.66	0.47
1:A:45:TYR:N	1:A:64:THR:HG1	2.11	0.47
4:D:180:ILE:HB	4:D:221:LEU:HD22	1.95	0.47
1:A:139:ALA:O	1:A:142:ILE:N	2.38	0.47
1:A:211:ALA:HB2	1:A:241:PHE:CG	2.49	0.47
2:B:73:THR:CG2	2:B:76:ASP:H	2.27	0.47
1:A:157:ARG:O	1:A:158:ALA:O	2.32	0.47
4:D:238:LEU:HD23	4:D:239:SER:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:222:ASP:OD1	4:D:222:ASP:O	2.32	0.47
1:A:21:ARG:NH2	1:A:23:MET:CE	2.77	0.47
1:A:30:ASP:H	4:D:231:LYS:HD3	1.79	0.47
4:D:168:ALA:O	4:D:169:ASN:C	2.51	0.47
4:D:169:ASN:HA	4:D:172:HIS:HB3	1.96	0.47
1:A:15:PRO:O	1:A:17:LEU:N	2.47	0.47
1:A:15:PRO:C	1:A:17:LEU:N	2.58	0.47
1:A:154:GLU:O	1:A:155:ARG:C	2.52	0.47
2:B:35:ILE:HD12	2:B:83:LYS:O	2.15	0.47
1:A:52:MET:CE	1:A:52:MET:CA	2.92	0.47
1:A:50:ARG:HD3	1:A:50:ARG:HA	1.42	0.46
1:A:73:SER:OG	3:P:7:LYS:CE	2.63	0.46
1:A:156:LEU:O	1:A:158:ALA:N	2.48	0.46
1:A:259:CYS:O	1:A:271:THR:HA	2.14	0.46
1:A:22:TYR:OH	1:A:24:GLU:CG	2.63	0.46
1:A:213:ILE:CG1	1:A:214:THR:H	2.28	0.46
2:B:21:ASN:O	2:B:70:PHE:N	2.37	0.46
4:D:178:LEU:HG	4:D:179:LYS:H	1.77	0.46
4:D:194:ILE:CG1	4:D:195:PRO:HD2	2.45	0.46
1:A:4:SER:O	1:A:29:ASP:N	2.48	0.46
1:A:74:PHE:HA	1:A:77:ASP:HB2	1.96	0.46
1:A:139:ALA:C	1:A:141:LEU:H	2.19	0.46
2:B:41:LYS:O	2:B:44:LYS:HB2	2.15	0.46
2:B:73:THR:CG2	2:B:75:THR:H	2.26	0.46
1:A:74:PHE:O	1:A:77:ASP:HB2	2.15	0.46
2:B:41:LYS:O	2:B:42:ASN:HB2	2.16	0.46
2:B:70:PHE:CD2	2:B:78:TYR:CE1	3.04	0.46
4:D:226:ARG:HB2	4:D:228:MET:HE2	1.97	0.46
1:A:85:TYR:O	1:A:87:GLN:N	2.49	0.46
1:A:130:LEU:HD12	1:A:157:ARG:HD3	1.98	0.46
1:A:53:GLU:C	1:A:55:GLU:H	2.19	0.46
2:B:16:GLU:HB2	2:B:19:LYS:HG2	1.97	0.46
4:D:179:LYS:HE2	4:D:217:GLY:O	2.16	0.46
4:D:198:TYR:O	4:D:237:PHE:CB	2.64	0.46
1:A:27:TYR:HB3	1:A:29:ASP:O	2.16	0.46
1:A:57:PRO:O	1:A:58:GLU:HB3	2.15	0.46
1:A:59:TYR:CD2	1:A:60:TRP:N	2.84	0.46
1:A:77:ASP:OD1	3:P:8:LEU:N	2.39	0.46
1:A:181:ARG:HH22	1:A:239:GLY:HA3	1.80	0.46
1:A:206:LEU:CD2	1:A:242:GLN:HB2	2.46	0.46
2:B:7:ILE:CG2	2:B:8:GLN:N	2.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:TYR:CD2	1:A:60:TRP:CD1	3.04	0.46
1:A:126:LEU:HD23	1:A:126:LEU:HA	1.64	0.46
1:A:243:LYS:HG2	1:A:244:TRP:H	1.80	0.46
4:D:230:PHE:CD2	4:D:231:LYS:N	2.84	0.46
1:A:211:ALA:HB2	1:A:241:PHE:CE2	2.50	0.46
2:B:51:MET:O	2:B:52:SER:O	2.34	0.46
3:P:2:ILE:HG12	3:P:3:ILE:H	1.81	0.46
4:D:227:LYS:O	4:D:228:MET:O	2.33	0.46
1:A:96:GLN:O	1:A:97:VAL:HG23	2.15	0.45
2:B:35:ILE:HG23	2:B:35:ILE:O	2.15	0.45
4:D:228:MET:O	4:D:229:ASN:CB	2.55	0.45
1:A:219:LEU:HD22	1:A:257:TYR:CE2	2.51	0.45
4:D:154:TYR:OH	4:D:185:GLU:OE2	2.32	0.45
1:A:70:ASN:O	1:A:73:SER:N	2.49	0.45
2:B:7:ILE:HG12	2:B:82:VAL:HG21	1.99	0.45
1:A:148:GLU:C	1:A:150:ALA:H	2.19	0.45
1:A:154:GLU:C	1:A:156:LEU:H	2.18	0.45
1:A:92:SER:C	1:A:93:HIS:HD1	2.17	0.45
1:A:161:GLU:O	1:A:165:VAL:HG21	2.16	0.45
1:A:52:MET:SD	1:A:55:GLU:HG3	2.56	0.45
1:A:97:VAL:HG22	1:A:116:TYR:CG	2.52	0.45
2:B:97:ARG:CG	2:B:98:ASP:H	2.28	0.45
4:D:207:LYS:O	4:D:209:LYS:N	2.48	0.44
1:A:194:ARG:HG3	1:A:195:PRO:HD2	1.99	0.44
1:A:63:GLU:O	1:A:64:THR:C	2.54	0.44
1:A:211:ALA:HB2	1:A:241:PHE:CD2	2.52	0.44
2:B:32:PRO:HB2	2:B:33:PRO:CD	2.40	0.44
2:B:76:ASP:C	2:B:77:THR:CG2	2.86	0.44
2:B:87:MET:SD	2:B:91:LYS:HE3	2.57	0.44
4:D:175:VAL:HG12	4:D:256:CYS:HB3	1.98	0.44
4:D:234:GLY:C	4:D:248:CYS:SG	2.96	0.44
1:A:28:VAL:O	1:A:28:VAL:HG13	2.18	0.44
2:B:59:ASP:O	2:B:60:TRP:HB2	2.17	0.44
3:P:3:ILE:CD1	3:P:4:ASN:N	2.79	0.44
1:A:13:SER:HB3	1:A:78:LEU:HG	1.99	0.44
1:A:51:TRP:HZ2	1:A:179:LEU:HD21	1.83	0.44
1:A:65:GLN:OE1	1:A:65:GLN:HA	2.18	0.44
2:B:76:ASP:C	2:B:77:THR:HG23	2.38	0.44
4:D:199:TRP:HE3	4:D:236:VAL:O	2.00	0.44
4:D:202:LEU:HD13	4:D:213:TRP:CD2	2.53	0.44
1:A:7:TYR:HA	1:A:25:VAL:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:ARG:NH1	1:A:244:TRP:CZ3	2.86	0.44
2:B:27:VAL:HG12	2:B:30:PHE:CD2	2.53	0.44
2:B:83:LYS:HE3	2:B:90:PRO:HG2	1.98	0.44
2:B:96:ASP:OD2	2:B:98:ASP:HB2	2.18	0.44
4:D:243:ILE:HD13	4:D:243:ILE:HA	1.68	0.44
1:A:59:TYR:CE2	1:A:60:TRP:CD1	3.05	0.43
1:A:116:TYR:CG	1:A:124:ILE:HG22	2.52	0.43
1:A:222:GLU:C	1:A:223:GLU:O	2.55	0.43
2:B:17:ASN:O	2:B:18:GLY:C	2.57	0.43
4:D:215:ASP:OD1	4:D:217:GLY:N	2.47	0.43
1:A:14:ARG:HG3	1:A:14:ARG:HH11	1.83	0.43
1:A:161:GLU:O	1:A:165:VAL:CG2	2.66	0.43
2:B:50:GLU:HB2	2:B:67:HIS:NE2	2.33	0.43
4:D:162:THR:O	4:D:165:GLY:HA3	2.18	0.43
4:D:179:LYS:HG3	4:D:181:GLU:HG2	2.00	0.43
1:A:263:HIS:ND1	1:A:264:GLN:N	2.66	0.43
4:D:229:ASN:ND2	4:D:233:ARG:HE	2.15	0.43
1:A:12:VAL:HG22	1:A:94:THR:CB	2.46	0.43
1:A:130:LEU:HD12	1:A:157:ARG:CD	2.49	0.43
1:A:233:THR:HB	1:A:243:LYS:HZ2	1.81	0.43
1:A:6:ARG:HA	1:A:100:GLY:HA3	1.99	0.43
2:B:23:LEU:HD13	2:B:70:PHE:CE1	2.54	0.43
2:B:42:ASN:C	2:B:44:LYS:N	2.67	0.43
4:D:200:ILE:O	4:D:200:ILE:HG13	2.17	0.43
4:D:225:ILE:C	4:D:227:LYS:H	2.09	0.43
4:D:161:THR:C	4:D:251:PRO:HA	2.39	0.43
1:A:266:LEU:HD21	1:A:270:LEU:HD12	1.97	0.43
4:D:166:CYS:HB2	4:D:177:ILE:HG22	1.99	0.43
1:A:263:HIS:O	1:A:266:LEU:HB2	2.19	0.43
2:B:60:TRP:HE1	4:D:242:ARG:NH1	2.17	0.43
1:A:74:PHE:O	1:A:78:LEU:N	2.47	0.42
1:A:142:ILE:O	1:A:142:ILE:CG2	2.66	0.42
1:A:202:ARG:HG3	1:A:202:ARG:HH11	1.84	0.42
4:D:204:TYR:CD1	4:D:204:TYR:C	2.93	0.42
1:A:78:LEU:HD22	1:A:95:ILE:HD12	2.01	0.42
1:A:213:ILE:HD11	1:A:261:VAL:HG13	2.01	0.42
3:P:3:ILE:HD13	3:P:4:ASN:C	2.38	0.42
1:A:183:ASP:O	1:A:208:PHE:HA	2.20	0.42
1:A:194:ARG:HD2	1:A:248:VAL:HG13	2.02	0.42
1:A:230:LEU:HD12	4:D:249:ASN:OD1	2.19	0.42
1:A:237:GLY:CA	2:B:12:ARG:NH2	2.79	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:GLU:CD	1:A:58:GLU:C	2.78	0.42
1:A:85:TYR:C	1:A:87:GLN:N	2.71	0.42
1:A:123:TYR:CE2	1:A:140:ALA:HA	2.55	0.42
1:A:127:ASN:OD1	1:A:134:THR:HG22	2.18	0.42
1:A:152:GLU:O	1:A:156:LEU:HB2	2.20	0.42
4:D:167:LYS:N	4:D:177:ILE:CG2	2.83	0.42
4:D:207:LYS:C	4:D:209:LYS:N	2.71	0.42
1:A:184:SER:HB3	1:A:266:LEU:CD1	2.50	0.42
1:A:65:GLN:O	1:A:68:LYS:HB2	2.20	0.42
1:A:146:LYS:O	1:A:149:GLN:N	2.53	0.42
1:A:255:GLN:O	1:A:256:TYR:HD1	2.01	0.42
4:D:152:LYS:HD3	4:D:154:TYR:OH	2.20	0.42
4:D:208:LYS:O	4:D:209:LYS:C	2.58	0.42
1:A:185:PRO:HB3	1:A:208:PHE:CG	2.55	0.42
4:D:227:LYS:O	4:D:228:MET:C	2.57	0.42
1:A:52:MET:CE	1:A:55:GLU:HG3	2.49	0.42
1:A:238:ASP:O	1:A:240:THR:HG23	2.19	0.42
4:D:206:LYS:NZ	4:D:206:LYS:CB	2.83	0.42
1:A:208:PHE:CD2	1:A:263:HIS:CD2	3.08	0.41
4:D:180:ILE:CG2	4:D:221:LEU:HD22	2.50	0.41
1:A:266:LEU:O	1:A:267:PRO:C	2.59	0.41
1:A:208:PHE:CD2	1:A:263:HIS:HD2	2.38	0.41
2:B:41:LYS:HE2	2:B:78:TYR:CZ	2.54	0.41
2:B:79:ALA:HB2	2:B:94:TYR:CD1	2.55	0.41
4:D:198:TYR:HB3	4:D:255:ILE:HG13	2.01	0.41
1:A:54:GLN:HB3	1:A:174:ASN:HD22	1.86	0.41
1:A:181:ARG:NH1	1:A:183:ASP:OD2	2.53	0.41
4:D:178:LEU:CB	4:D:255:ILE:HG22	2.43	0.41
1:A:4:SER:HA	1:A:168:LEU:HD21	2.02	0.41
1:A:21:ARG:HH21	1:A:23:MET:HE3	1.86	0.41
2:B:41:LYS:CG	2:B:78:TYR:CE2	2.99	0.41
1:A:19:GLU:HG3	1:A:75:ARG:NH1	2.34	0.41
1:A:74:PHE:HA	1:A:77:ASP:OD2	2.20	0.41
1:A:82:LEU:O	1:A:83:GLY:O	2.38	0.41
1:A:203:CYS:O	1:A:244:TRP:HB2	2.21	0.41
1:A:127:ASN:ND2	1:A:133:TRP:O	2.46	0.41
4:D:175:VAL:HA	4:D:176:PRO:HD2	1.76	0.41
1:A:205:ALA:O	1:A:208:PHE:HE1	2.04	0.41
2:B:12:ARG:HB3	2:B:22:ILE:HD12	2.02	0.41
4:D:169:ASN:O	4:D:170:CYS:C	2.57	0.41
1:A:22:TYR:CZ	1:A:24:GLU:HG3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:VAL:HG21	1:A:116:TYR:CE2	2.56	0.41
1:A:123:TYR:CZ	1:A:140:ALA:HA	2.56	0.41
1:A:137:ASP:O	1:A:138:MET:C	2.59	0.41
1:A:167:TRP:O	1:A:171:TYR:CD2	2.66	0.41
1:A:209:TYR:CD2	1:A:209:TYR:C	2.94	0.41
4:D:171:GLN:O	4:D:174:SER:N	2.50	0.41
4:D:226:ARG:O	4:D:227:LYS:C	2.50	0.41
1:A:172:LEU:O	1:A:176:ASN:N	2.54	0.41
1:A:218:GLN:HG2	1:A:222:GLU:O	2.20	0.41
2:B:56:PHE:HA	2:B:61:SER:O	2.22	0.40
4:D:144:VAL:CG1	4:D:158:MET:HB2	2.50	0.40
4:D:179:LYS:HA	4:D:213:TRP:CZ3	2.56	0.40
1:A:50:ARG:C	1:A:52:MET:N	2.75	0.40
2:B:83:LYS:HG3	2:B:90:PRO:CG	2.20	0.40
1:A:66:LYS:CB	1:A:66:LYS:HZ3	2.35	0.40
1:A:114:GLN:NE2	1:A:114:GLN:HA	2.37	0.40
1:A:152:GLU:HG2	1:A:155:ARG:HB2	2.02	0.40
1:A:265:GLY:O	1:A:266:LEU:HD12	2.21	0.40
4:D:193:VAL:HG12	4:D:194:ILE:O	2.21	0.40
4:D:260:LEU:HD22	4:D:260:LEU:HA	1.86	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	249/274 (91%)	167 (67%)	56 (22%)	26 (10%)	0 3
2	B	93/99 (94%)	77 (83%)	11 (12%)	5 (5%)	2 12
3	P	6/8 (75%)	3 (50%)	2 (33%)	1 (17%)	0 1
4	D	116/120 (97%)	75 (65%)	23 (20%)	18 (16%)	0 1
All	All	464/501 (93%)	322 (69%)	92 (20%)	50 (11%)	0 3

All (50) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	58	GLU
1	A	87	GLN
1	A	130	LEU
1	A	139	ALA
1	A	145	HIS
1	A	158	ALA
1	A	159	TYR
1	A	170	ARG
1	A	253	LYS
1	A	255	GLN
2	B	17	ASN
4	D	150	SER
4	D	168	ALA
4	D	174	SER
4	D	183	GLU
4	D	206	LYS
4	D	209	LYS
4	D	227	LYS
4	D	229	ASN
4	D	231	LYS
4	D	246	ILE
1	A	131	LYS
1	A	140	ALA
1	A	157	ARG
1	A	180	LEU
1	A	252	GLY
2	B	35	ILE
2	B	47	PRO
4	D	201	GLY
4	D	228	MET
1	A	50	ARG
1	A	51	TRP
1	A	54	GLN
1	A	83	GLY
1	A	175	GLY
1	A	182	THR
2	B	43	GLY
2	B	49	VAL
3	P	7	LYS
1	A	78	LEU
1	A	162	GLY
4	D	189	LEU

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Mol	Chain	Res	Type
4	D	196	GLU
4	D	208	LYS
1	A	77	ASP
1	A	179	LEU
4	D	167	LYS
1	A	239	GLY
4	D	193	VAL
4	D	176	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	214/232 (92%)	179 (84%)	35 (16%)	2 10
2	B	90/94 (96%)	74 (82%)	16 (18%)	2 7
3	P	8/8 (100%)	6 (75%)	2 (25%)	0 2
4	D	107/111 (96%)	84 (78%)	23 (22%)	1 4
All	All	419/445 (94%)	343 (82%)	76 (18%)	1 7

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ARG
1	A	17	LEU
1	A	48	ARG
1	A	50	ARG
1	A	52	MET
1	A	54	GLN
1	A	58	GLU
1	A	78	LEU
1	A	86	ASN
1	A	87	GLN
1	A	94	THR
1	A	99	SER
1	A	111	ARG

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Mol	Chain	Res	Type
1	A	122	ASP
1	A	126	LEU
1	A	128	GLU
1	A	130	LEU
1	A	132	THR
1	A	134	THR
1	A	142	ILE
1	A	152	GLU
1	A	156	LEU
1	A	157	ARG
1	A	161	GLU
1	A	165	VAL
1	A	169	ARG
1	A	172	LEU
1	A	180	LEU
1	A	183	ASP
1	A	190	THR
1	A	197	ASP
1	A	227	ASP
1	A	251	LEU
1	A	262	TYR
1	A	272	LEU
2	B	6	GLN
2	B	8	GLN
2	B	17	ASN
2	B	19	LYS
2	B	21	ASN
2	B	22	ILE
2	B	29	GLN
2	B	44	LYS
2	B	48	LYS
2	B	58	LYS
2	B	67	HIS
2	B	70	PHE
2	B	74	GLU
2	B	75	THR
2	B	98	ASP
2	B	99	MET
3	P	3	ILE
3	P	5	PHE
4	D	149	TYR
4	D	153	CYS

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Mol	Chain	Res	Type
4	D	161	THR
4	D	169	ASN
4	D	177	ILE
4	D	184	ASP
4	D	186	LEU
4	D	188	PHE
4	D	194	ILE
4	D	206	LYS
4	D	207	LYS
4	D	214	ILE
4	D	215	ASP
4	D	216	ASN
4	D	220	LYS
4	D	223	MET
4	D	224	LYS
4	D	227	LYS
4	D	228	MET
4	D	229	ASN
4	D	230	PHE
4	D	259	LYS
4	D	260	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	ASN
1	A	86	ASN
1	A	87	GLN
1	A	93	HIS
1	A	114	GLN
1	A	174	ASN
1	A	192	HIS
1	A	242	GLN
2	B	2	GLN
2	B	6	GLN
2	B	17	ASN
2	B	21	ASN
2	B	29	GLN
2	B	67	HIS
4	D	169	ASN
4	D	190	GLN
4	D	229	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	255/274 (93%)	-0.32	1 (0%)	92	92	18, 50, 84, 128	0
2	B	97/99 (97%)	-0.24	1 (1%)	82	82	16, 46, 81, 110	0
3	P	8/8 (100%)	-0.03	0	100	100	52, 54, 66, 74	0
4	D	118/120 (98%)	-0.23	3 (2%)	57	53	22, 48, 94, 142	0
All	All	478/501 (95%)	-0.28	5 (1%)	82	82	16, 49, 86, 142	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	230	PHE	4.0
4	D	231	LYS	2.8
2	B	52	SER	2.4
1	A	155	ARG	2.3
4	D	232	SER	2.1

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.