



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:12 AM GMT

PDB ID : 3DPR
Title : Human rhinovirus 2 bound to a concatamer of the VLDL receptor module V3
Authors : Querol-Audi, J.; Pous, J.; Fita, I.; Verdaguer, N.
Deposited on : 2008-07-09
Resolution : 3.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

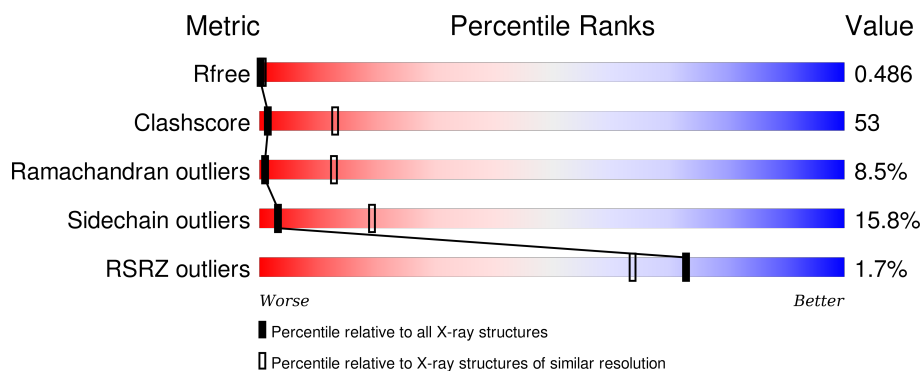
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	289	<div> <div>32%</div> <div>46%</div> <div>14%</div> <div>7%</div> </div>
2	B	261	<div> <div>30%</div> <div>50%</div> <div>16%</div> </div>
3	C	237	<div> <div>35%</div> <div>49%</div> <div>14%</div> </div>
4	D	68	<div> <div>3%</div> <div>10%</div> <div>21%</div> <div>63%</div> </div>
5	E	39	<div> <div>13%</div> <div>31%</div> <div>51%</div> <div>18%</div> </div>

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
6	DAO	A	290	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6450 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 Protein VP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	269	Total	C	N	O	S	0	0	0
			2155	1356	378	410	11			

- Molecule 2 is a protein called Protein VP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	250	Total	C	N	O	S	8	0	0
			1960	1245	339	368	8			

- Molecule 3 is a protein called Protein VP3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	237	Total	C	N	O	S	0	0	0
			1833	1172	304	345	12			

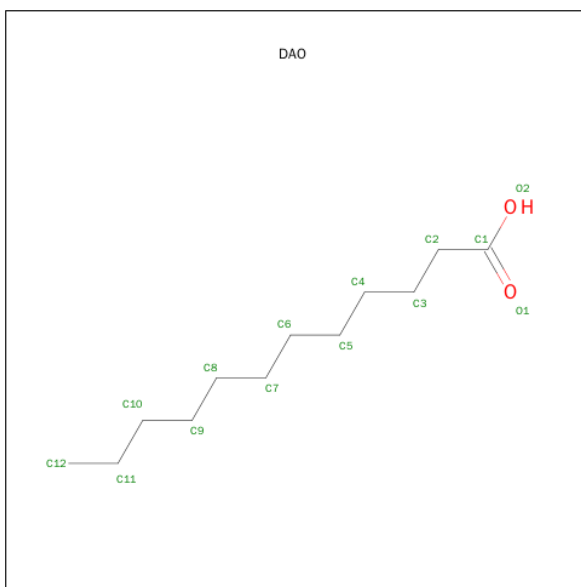
- Molecule 4 is a protein called Protein VP4.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	25	Total	C	N	O	0	0	0
			194	122	35	37			

- Molecule 5 is a protein called LDL-receptor class A 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	39	Total	C	N	O	S	0	0	0
			293	166	54	67	6			

- Molecule 6 is LAURIC ACID (three-letter code: DAO) (formula: C₁₂H₂₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			14	12	2		

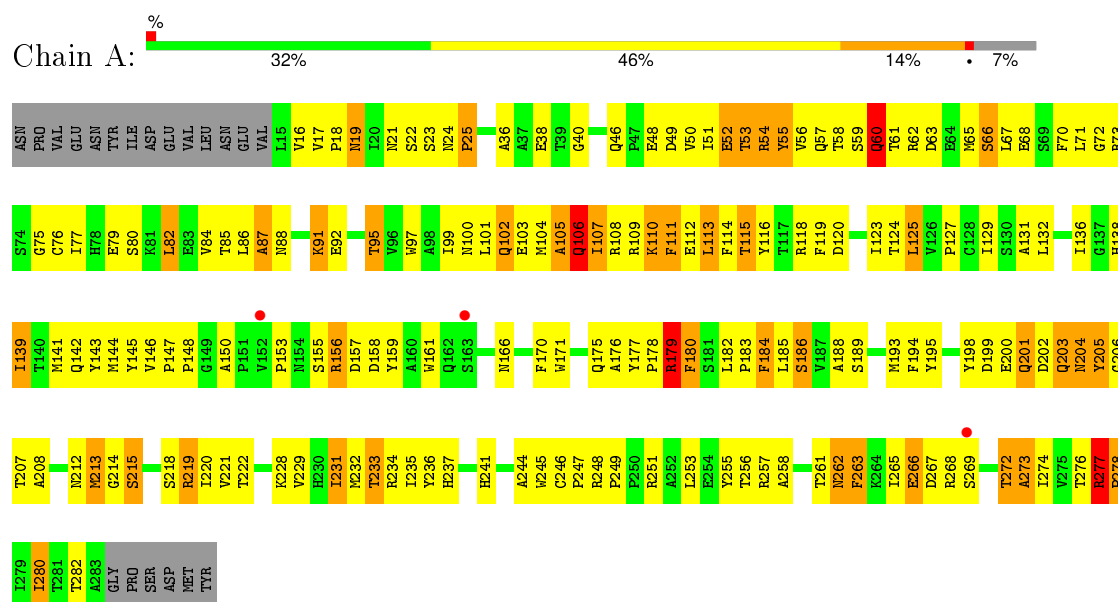
- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	E	1	Total	Ca	0	0
			1	1		

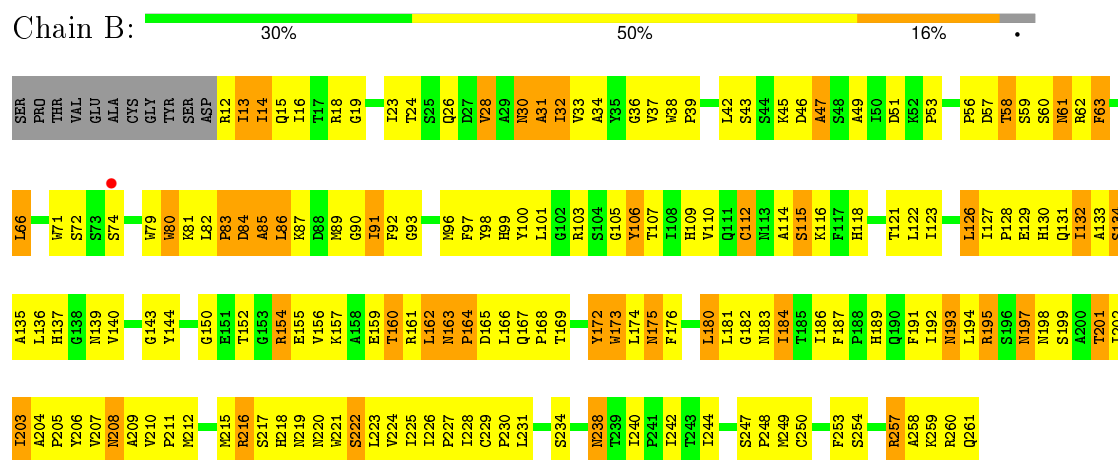
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Protein VP1

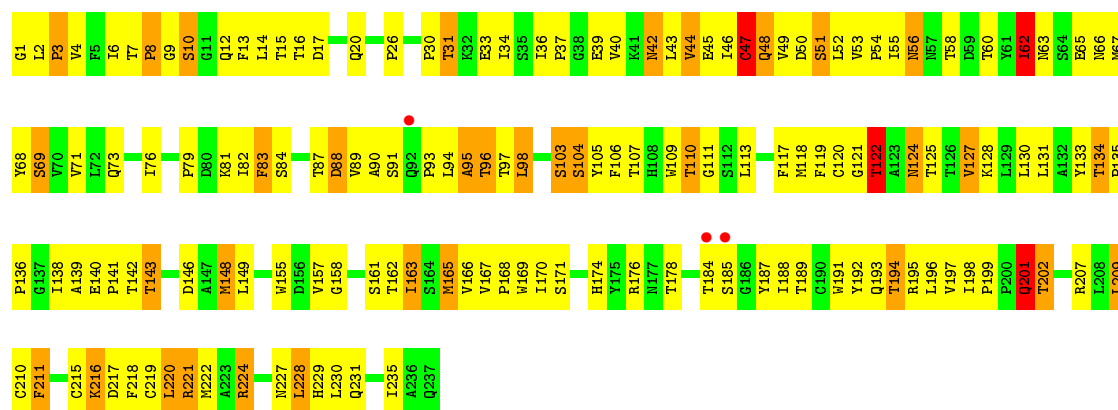


• Molecule 2: Protein VP2

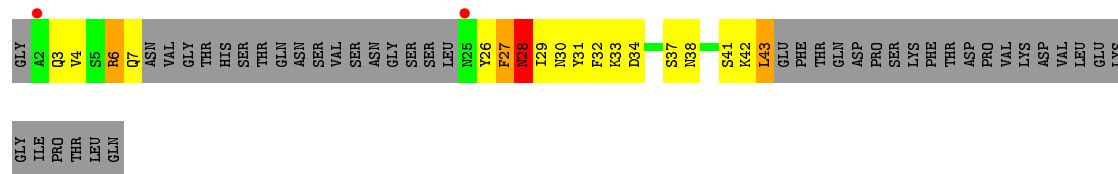


• Molecule 3: Protein VP3

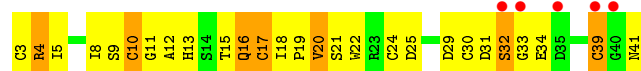




• Molecule 4: Protein VP4



• Molecule 5: LDL-receptor class A 3



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	498.12Å 498.12Å 658.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 3.50 15.00 – 3.50	Depositor EDS
% Data completeness (in resolution range)	61.6 (15.00-3.50) 61.6 (15.00-3.50)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.53 (at 3.48Å)	Xtriage
Refinement program	REFMAC5	Depositor
R, R_{free}	0.425 , 0.441 0.483 , 0.486	Depositor DCC
R_{free} test set	31034 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	41.0	Xtriage
Anisotropy	0.008	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 3.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 619760 reflections	Xtriage
F_o, F_c correlation	0.38	EDS
Total number of atoms	6450	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 20.26 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 9.0266e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	1.07	1/2211 (0.0%)	0.91	2/3011 (0.1%)
2	B	1.02	1/2015 (0.0%)	0.88	0/2752
3	C	1.05	0/1883	0.92	1/2579 (0.0%)
4	D	1.31	0/196	0.94	0/261
5	E	1.45	2/297 (0.7%)	1.07	0/399
All	All	1.07	4/6602 (0.1%)	0.91	3/9002 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	24	CYS	CB-SG	5.60	1.91	1.82
5	E	39	CYS	CB-SG	5.57	1.91	1.82
2	B	37	VAL	CA-CB	5.36	1.66	1.54
1	A	255	TYR	CE2-CZ	5.03	1.45	1.38

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	277	ARG	NE-CZ-NH1	5.91	123.26	120.30
3	C	221	ARG	NE-CZ-NH1	-5.76	117.42	120.30
1	A	179	ARG	NE-CZ-NH2	-5.17	117.72	120.30

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	2155	0	2080	222	0
2	B	1960	0	1902	250	0
3	C	1833	0	1817	193	0
4	D	194	0	180	26	0
5	E	293	0	238	23	0
6	A	14	0	23	0	0
7	E	1	0	0	0	0
All	All	6450	0	6240	671	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 53.

All (671) 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:110:LYS:O	1:A:113:LEU:HB2	1.39	1.20
3:C:122:THR:HG22	3:C:125:THR:OG1	1.38	1.19
3:C:39:GLU:HG2	3:C:40:VAL:H	1.09	1.09
2:B:38:TRP:CD1	2:B:39:PRO:HD2	1.88	1.08
2:B:203:ILE:HD12	2:B:203:ILE:N	1.66	1.08
2:B:172:TYR:HA	2:B:176:PHE:CE2	1.90	1.06
2:B:135:ALA:HB2	2:B:169:THR:HA	1.38	1.04
1:A:245:TRP:NE1	3:C:36:ILE:HG23	1.76	0.99
3:C:39:GLU:HG2	3:C:40:VAL:N	1.78	0.97
3:C:2:LEU:O	3:C:4:VAL:HG13	1.64	0.97
3:C:53:VAL:O	3:C:55:ILE:HD12	1.65	0.95
3:C:138:ILE:HG13	3:C:139:ALA:H	1.31	0.94
3:C:163:ILE:HG23	3:C:163:ILE:O	1.66	0.93
2:B:126:LEU:HD22	2:B:221:TRP:CE3	2.05	0.92
2:B:115:SER:HB3	2:B:118:HIS:CE1	2.05	0.91
2:B:34:ALA:HB3	2:B:205:PRO:CD	2.01	0.90
1:A:245:TRP:HE1	3:C:36:ILE:HG23	1.36	0.90
2:B:91:ILE:HD13	2:B:91:ILE:N	1.87	0.90
3:C:138:ILE:HG13	3:C:139:ALA:N	1.86	0.90
3:C:195:ARG:O	3:C:197:VAL:HG23	1.70	0.90
5:E:22:TRP:HD1	5:E:25:ASP:OD2	1.52	0.89
2:B:132:ILE:CG2	2:B:176:PHE:HB3	2.03	0.88
2:B:126:LEU:HD22	2:B:221:TRP:HE3	1.36	0.88
3:C:111:GLY:O	3:C:169:TRP:HB2	1.73	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:203:ILE:HD12	2:B:203:ILE:H	1.35	0.88
2:B:34:ALA:HB3	2:B:205:PRO:HD2	1.56	0.86
2:B:91:ILE:HD13	2:B:91:ILE:H	1.40	0.86
4:D:3:GLN:HB3	4:D:27:PHE:HA	1.58	0.86
1:A:65:MET:O	3:C:42:ASN:ND2	2.09	0.85
2:B:84:ASP:H	2:B:96:MET:HE1	1.41	0.85
1:A:25:PRO:HD3	1:A:52:GLU:OE2	1.76	0.85
2:B:80:TRP:CZ3	2:B:225:ILE:HD13	2.12	0.85
1:A:161:TRP:CD2	1:A:219:ARG:HG2	2.12	0.84
1:A:161:TRP:CE3	1:A:219:ARG:HG2	2.12	0.84
4:D:27:PHE:C	4:D:27:PHE:CD2	2.51	0.83
2:B:165:ASP:O	2:B:166:LEU:HD23	1.77	0.83
1:A:65:MET:O	3:C:42:ASN:CG	2.17	0.83
2:B:32:ILE:HD13	2:B:33:VAL:H	1.44	0.83
1:A:143:TYR:OH	1:A:233:THR:HG21	1.77	0.82
2:B:83:PRO:HB2	2:B:96:MET:HE1	1.59	0.82
3:C:55:ILE:HD11	3:C:210:CYS:HB3	1.61	0.82
1:A:75:GLY:HA3	1:A:107:ILE:HD11	1.62	0.81
1:A:198:TYR:CZ	2:B:144:TYR:HA	2.14	0.81
2:B:238:ASN:H	2:B:238:ASN:HD22	1.26	0.81
2:B:203:ILE:CD1	2:B:203:ILE:N	2.41	0.81
2:B:182:GLY:H	2:B:184:ILE:HG22	1.44	0.81
2:B:91:ILE:H	2:B:91:ILE:CD1	1.94	0.81
3:C:54:PRO:HG2	3:C:93:PRO:HB2	1.59	0.81
1:A:274:ILE:HD12	3:C:96:THR:HG21	1.62	0.81
1:A:23:SER:HB3	1:A:53:THR:HG22	1.61	0.81
4:D:43:LEU:N	4:D:43:LEU:HD12	1.96	0.80
3:C:169:TRP:CZ2	3:C:174:HIS:O	2.33	0.80
2:B:112:CYS:SG	2:B:242:ILE:CD1	2.69	0.80
2:B:23:ILE:HD13	2:B:63:PHE:CD1	2.17	0.80
2:B:260:ARG:HG3	2:B:261:GLN:N	1.95	0.79
1:A:50:VAL:HG12	1:A:51:ILE:HG23	1.62	0.79
1:A:156:ARG:NH2	1:A:221:VAL:O	2.15	0.79
2:B:128:PRO:HD2	2:B:187:PHE:CE2	2.18	0.79
1:A:115:THR:HG23	1:A:248:ARG:NH1	1.99	0.78
2:B:223:LEU:HD12	2:B:224:VAL:H	1.48	0.78
1:A:280:ILE:H	1:A:280:ILE:HD13	1.48	0.78
1:A:249:PRO:CD	2:B:187:PHE:HE1	1.96	0.78
4:D:27:PHE:HD2	4:D:27:PHE:O	1.67	0.78
2:B:38:TRP:CD1	2:B:39:PRO:CD	2.66	0.78
3:C:138:ILE:CG1	3:C:139:ALA:H	1.97	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:82:LEU:HA	2:B:83:PRO:O	1.84	0.78
3:C:128:LYS:HB2	3:C:194:THR:OG1	1.84	0.77
2:B:71:TRP:CE3	2:B:240:ILE:HD11	2.20	0.77
2:B:23:ILE:HD13	2:B:63:PHE:CE1	2.20	0.77
2:B:80:TRP:HZ3	2:B:225:ILE:HD13	1.50	0.77
1:A:199:ASP:HB2	1:A:203:GLN:O	1.83	0.77
2:B:34:ALA:CB	2:B:205:PRO:HD2	2.14	0.77
1:A:77:ILE:C	1:A:104:MET:HG3	2.06	0.76
2:B:161:ARG:O	2:B:164:PRO:HD3	1.84	0.76
1:A:115:THR:HG23	1:A:248:ARG:HH11	1.51	0.76
5:E:10:CYS:HB2	5:E:16:GLN:O	1.85	0.75
3:C:209:LEU:N	3:C:209:LEU:HD12	2.01	0.75
3:C:227:ASN:OD1	3:C:228:LEU:HD12	1.87	0.75
5:E:22:TRP:CD1	5:E:25:ASP:OD2	2.39	0.75
1:A:182:LEU:HD23	1:A:183:PRO:HD2	1.68	0.75
2:B:31:ALA:HB2	2:B:201:THR:HB	1.67	0.74
2:B:136:LEU:CD1	2:B:164:PRO:O	2.35	0.74
2:B:81:LYS:O	2:B:83:PRO:O	2.05	0.74
2:B:34:ALA:HB3	2:B:205:PRO:HD3	1.70	0.74
2:B:82:LEU:HB2	2:B:221:TRP:HB2	1.69	0.73
2:B:193:ASN:H	2:B:197:ASN:HD21	1.37	0.73
2:B:80:TRP:HZ3	2:B:225:ILE:CD1	2.01	0.73
3:C:42:ASN:C	3:C:42:ASN:HD22	1.92	0.73
5:E:11:GLY:O	5:E:34:GLU:HB3	1.89	0.72
1:A:153:PRO:HA	1:A:158:ASP:OD2	1.89	0.72
1:A:249:PRO:HD3	2:B:187:PHE:HE1	1.52	0.72
4:D:3:GLN:HB2	4:D:26:TYR:O	1.89	0.72
1:A:161:TRP:HB2	1:A:219:ARG:HH21	1.54	0.72
3:C:39:GLU:CG	3:C:40:VAL:H	1.97	0.71
2:B:159:GLU:HG3	2:B:159:GLU:O	1.90	0.71
2:B:13:ILE:O	2:B:14:ILE:HB	1.88	0.71
2:B:80:TRP:N	2:B:80:TRP:CE3	2.58	0.71
2:B:112:CYS:HB2	2:B:242:ILE:HD12	1.72	0.71
3:C:201:GLN:HA	3:C:201:GLN:HE21	1.55	0.71
2:B:127:ILE:HG13	2:B:187:PHE:CD2	2.25	0.71
3:C:131:LEU:HB3	3:C:165:MET:CE	2.21	0.71
3:C:130:LEU:C	3:C:130:LEU:HD23	2.11	0.71
1:A:185:LEU:O	1:A:186:SER:O	2.08	0.71
2:B:123:ILE:HG12	2:B:191:PHE:HE1	1.55	0.71
2:B:83:PRO:HB2	2:B:96:MET:CE	2.21	0.70
3:C:111:GLY:HA3	3:C:218:PHE:HA	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:60:SER:O	2:B:62:ARG:N	2.23	0.70
1:A:145:TYR:HE1	1:A:147:PRO:HG3	1.55	0.70
3:C:189:THR:HG1	3:C:191:TRP:HE1	1.38	0.70
2:B:13:ILE:HG22	2:B:14:ILE:H	1.54	0.70
1:A:65:MET:HB3	3:C:42:ASN:HD21	1.56	0.69
1:A:23:SER:CB	1:A:53:THR:HG22	2.21	0.69
3:C:103:SER:HA	3:C:220:LEU:HD21	1.73	0.69
2:B:234:SER:HB2	3:C:201:GLN:O	1.93	0.69
1:A:142:GLN:HG3	1:A:170:PHE:CE1	2.28	0.69
1:A:76:CYS:HB2	1:A:236:TYR:CE2	2.28	0.69
1:A:79:GLU:HG2	1:A:234:ARG:HG2	1.74	0.69
3:C:52:LEU:HD23	3:C:210:CYS:O	1.93	0.69
3:C:163:ILE:CG2	3:C:163:ILE:O	2.40	0.69
1:A:203:GLN:O	1:A:204:ASN:HB2	1.92	0.69
5:E:15:THR:HG22	5:E:16:GLN:H	1.56	0.68
3:C:111:GLY:C	3:C:169:TRP:HB2	2.12	0.68
2:B:180:LEU:H	2:B:180:LEU:HD12	1.58	0.68
2:B:122:LEU:HD23	2:B:227:PRO:HA	1.75	0.68
2:B:154:ARG:NH2	2:B:168:PRO:HG2	2.08	0.68
2:B:193:ASN:H	2:B:197:ASN:ND2	1.92	0.68
1:A:244:ALA:HA	1:A:245:TRP:CE3	2.29	0.68
1:A:161:TRP:CE2	1:A:219:ARG:HG2	2.28	0.68
1:A:19:ASN:OD1	1:A:57:GLN:HA	1.92	0.68
2:B:83:PRO:HD2	2:B:219:ASN:HA	1.74	0.68
3:C:120:CYS:SG	3:C:209:LEU:CD1	2.82	0.68
1:A:111:PHE:C	1:A:113:LEU:H	1.96	0.67
3:C:168:PRO:O	3:C:170:ILE:HG12	1.94	0.67
2:B:115:SER:HB3	2:B:118:HIS:HE1	1.56	0.67
5:E:4:ARG:HA	5:E:8:ILE:O	1.95	0.67
2:B:128:PRO:HD2	2:B:187:PHE:CD2	2.30	0.67
2:B:86:LEU:HB3	2:B:89:MET:HG3	1.78	0.66
2:B:106:TYR:HA	2:B:249:MET:HE2	1.76	0.66
2:B:80:TRP:CZ3	2:B:225:ILE:CD1	2.77	0.66
1:A:124:THR:HG23	1:A:179:ARG:HB2	1.75	0.66
2:B:31:ALA:CB	2:B:201:THR:HB	2.25	0.66
1:A:55:TYR:C	1:A:55:TYR:CD2	2.68	0.66
3:C:51:SER:HB3	3:C:98:LEU:HG	1.77	0.66
2:B:12:ARG:N	2:B:13:ILE:HD12	2.10	0.66
2:B:165:ASP:C	2:B:166:LEU:HD23	2.15	0.66
3:C:138:ILE:CG1	3:C:139:ALA:N	2.57	0.66
2:B:59:SER:O	2:B:62:ARG:HD2	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:ARG:NH2	3:C:17:ASP:OD1	2.27	0.65
3:C:122:THR:HG22	3:C:125:THR:HG1	1.58	0.65
1:A:48:GLU:HG3	1:A:53:THR:HG21	1.78	0.65
1:A:265:ILE:HD12	1:A:266:GLU:H	1.61	0.65
1:A:125:LEU:HB2	1:A:178:PRO:HG2	1.79	0.65
2:B:98:TYR:CE1	2:B:259:LYS:HB2	2.31	0.65
1:A:161:TRP:CZ3	1:A:219:ARG:HG2	2.30	0.65
1:A:183:PRO:O	1:A:185:LEU:HD23	1.96	0.65
2:B:203:ILE:CD1	2:B:203:ILE:H	2.06	0.65
5:E:8:ILE:HG23	5:E:17:CYS:HB2	1.78	0.65
1:A:19:ASN:HB3	1:A:56:VAL:O	1.96	0.65
3:C:42:ASN:O	3:C:45:GLU:HG3	1.95	0.65
3:C:184:THR:HG21	3:C:187:TYR:CE1	2.31	0.65
3:C:122:THR:HG23	3:C:124:ASN:H	1.61	0.65
1:A:144:MET:HE3	1:A:146:VAL:HG22	1.76	0.65
3:C:33:GLU:HG2	3:C:34:ILE:N	2.12	0.65
3:C:55:ILE:H	3:C:55:ILE:HD12	1.62	0.65
2:B:127:ILE:HG22	2:B:130:HIS:HB2	1.78	0.65
3:C:162:THR:HG22	3:C:163:ILE:N	2.11	0.64
2:B:106:TYR:CA	2:B:249:MET:HE2	2.26	0.64
3:C:104:SER:HB3	3:C:228:LEU:HD13	1.77	0.64
4:D:27:PHE:O	4:D:27:PHE:CD2	2.50	0.64
3:C:42:ASN:ND2	3:C:44:VAL:HG12	2.11	0.64
4:D:3:GLN:CB	4:D:26:TYR:O	2.45	0.64
3:C:215:CYS:C	3:C:217:ASP:N	2.47	0.64
1:A:277:ARG:HB2	1:A:278:PRO:CD	2.28	0.64
2:B:32:ILE:HD13	2:B:33:VAL:N	2.12	0.64
2:B:84:ASP:O	2:B:87:LYS:N	2.30	0.64
1:A:145:TYR:CE1	1:A:147:PRO:HG3	2.32	0.64
2:B:126:LEU:C	2:B:127:ILE:HD12	2.18	0.64
3:C:125:THR:CG2	3:C:196:LEU:HD11	2.27	0.64
1:A:86:LEU:O	1:A:87:ALA:HB3	1.97	0.64
2:B:106:TYR:C	2:B:249:MET:CE	2.66	0.63
1:A:55:TYR:HD2	1:A:55:TYR:C	2.02	0.63
2:B:223:LEU:HD12	2:B:224:VAL:N	2.11	0.63
2:B:112:CYS:CB	2:B:242:ILE:HD12	2.27	0.63
2:B:136:LEU:HD11	2:B:164:PRO:O	1.99	0.63
3:C:120:CYS:SG	3:C:209:LEU:HD11	2.38	0.63
1:A:17:VAL:HG21	1:A:60:GLN:HB2	1.79	0.63
2:B:132:ILE:HG23	2:B:176:PHE:HB3	1.78	0.63
2:B:112:CYS:HB2	2:B:242:ILE:CD1	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:136:LEU:HD12	2:B:164:PRO:O	1.98	0.63
1:A:143:TYR:CZ	1:A:233:THR:HG21	2.33	0.63
2:B:172:TYR:O	2:B:175:ASN:N	2.32	0.63
2:B:132:ILE:HG22	2:B:176:PHE:HB3	1.81	0.62
1:A:245:TRP:NE1	3:C:36:ILE:CG2	2.59	0.62
1:A:198:TYR:CE1	1:A:205:TYR:HB2	2.34	0.62
3:C:211:PHE:CD1	3:C:211:PHE:N	2.65	0.62
2:B:110:VAL:HG22	2:B:244:ILE:HG12	1.81	0.62
3:C:155:TRP:CD2	3:C:163:ILE:HG21	2.35	0.61
1:A:88:ASN:O	1:A:91:LYS:HB3	2.00	0.61
2:B:15:GLN:C	2:B:16:ILE:HD13	2.20	0.61
3:C:65:GLU:HG2	3:C:66:ASN:N	2.14	0.61
3:C:127:VAL:HG22	3:C:128:LYS:N	2.14	0.61
1:A:156:ARG:O	1:A:156:ARG:HG2	1.99	0.61
3:C:44:VAL:HA	3:C:47:CYS:SG	2.40	0.61
3:C:107:THR:OG1	3:C:222:MET:HG2	2.01	0.61
1:A:23:SER:HB3	1:A:53:THR:H	1.65	0.61
2:B:84:ASP:O	2:B:85:ALA:C	2.38	0.61
2:B:13:ILE:N	2:B:13:ILE:HD12	2.15	0.61
3:C:82:ILE:HG12	3:C:192:TYR:CE1	2.36	0.61
3:C:127:VAL:CG2	3:C:128:LYS:N	2.63	0.61
1:A:272:THR:OG1	1:A:273:ALA:N	2.33	0.61
1:A:97:TRP:HH2	1:A:100:ASN:O	1.82	0.60
1:A:276:THR:HG22	3:C:62:ILE:HG13	1.83	0.60
2:B:18:ARG:NH1	2:B:107:THR:OG1	2.34	0.60
2:B:128:PRO:HD2	2:B:187:PHE:HE2	1.65	0.60
2:B:57:ASP:HA	2:B:61:ASN:HD22	1.66	0.60
3:C:46:ILE:O	3:C:49:VAL:HG23	2.00	0.60
3:C:88:ASP:HB2	3:C:91:SER:HB3	1.83	0.60
2:B:193:ASN:O	2:B:195:ARG:N	2.34	0.60
2:B:172:TYR:HA	2:B:176:PHE:HE2	1.61	0.60
2:B:123:ILE:HG12	2:B:191:PHE:CE1	2.36	0.60
1:A:46:GLN:O	1:A:49:ASP:HB2	2.01	0.59
1:A:73:ARG:HG2	3:C:16:THR:HG22	1.84	0.59
2:B:197:ASN:HD22	2:B:197:ASN:H	1.49	0.59
1:A:111:PHE:HD1	1:A:111:PHE:H	1.48	0.59
3:C:224:ARG:HH12	3:C:227:ASN:HD22	1.49	0.59
1:A:16:VAL:HG12	1:A:17:VAL:N	2.17	0.59
2:B:208:ASN:OD1	2:B:209:ALA:N	2.36	0.59
3:C:148:MET:SD	3:C:149:LEU:HD23	2.43	0.59
1:A:68:GLU:O	1:A:72:GLY:HA3	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:PRO:HD2	2:B:187:PHE:HE1	1.66	0.59
3:C:169:TRP:CZ2	3:C:171:SER:HB3	2.38	0.59
1:A:77:ILE:HD11	1:A:235:ILE:CG2	2.33	0.59
1:A:82:LEU:HB2	1:A:95:THR:CG2	2.33	0.59
1:A:109:ARG:NH1	1:A:251:ARG:O	2.36	0.59
2:B:260:ARG:HG3	2:B:261:GLN:H	1.68	0.58
1:A:110:LYS:O	1:A:113:LEU:CB	2.32	0.58
2:B:86:LEU:HA	2:B:89:MET:HG2	1.85	0.58
3:C:224:ARG:HH12	3:C:227:ASN:ND2	2.00	0.58
1:A:36:ALA:HB1	1:A:38:GLU:OE2	2.02	0.58
4:D:6:ARG:HG2	4:D:7:GLN:H	1.68	0.58
3:C:43:LEU:O	3:C:45:GLU:N	2.36	0.58
2:B:175:ASN:HD21	2:B:180:LEU:C	2.07	0.58
3:C:128:LYS:O	3:C:193:GLN:HB3	2.03	0.58
1:A:86:LEU:O	1:A:87:ALA:CB	2.52	0.58
2:B:105:GLY:HA3	2:B:204:ALA:O	2.03	0.58
1:A:63:ASP:O	1:A:66:SER:HB3	2.03	0.58
1:A:111:PHE:C	1:A:113:LEU:N	2.57	0.58
5:E:3:CYS:O	5:E:4:ARG:HB2	2.04	0.58
2:B:66:LEU:HD12	2:B:244:ILE:HB	1.86	0.58
1:A:131:ALA:O	1:A:132:LEU:HD23	2.03	0.58
1:A:182:LEU:CD2	1:A:183:PRO:HD2	2.34	0.57
1:A:19:ASN:ND2	1:A:58:THR:OG1	2.37	0.57
1:A:132:LEU:HB2	1:A:228:LYS:O	2.03	0.57
3:C:130:LEU:HD12	3:C:193:GLN:HE22	1.69	0.57
1:A:97:TRP:CH2	1:A:100:ASN:O	2.56	0.57
2:B:207:VAL:HG22	3:C:37:PRO:HG2	1.86	0.57
3:C:215:CYS:C	3:C:217:ASP:H	2.07	0.57
5:E:10:CYS:N	5:E:17:CYS:HB3	2.19	0.57
2:B:127:ILE:CG2	2:B:130:HIS:HB2	2.35	0.57
5:E:31:ASP:C	5:E:33:GLY:H	2.08	0.57
1:A:102:GLN:HA	1:A:108:ARG:HD2	1.87	0.56
1:A:54:ARG:HD3	1:A:55:TYR:H	1.70	0.56
2:B:128:PRO:O	2:B:129:GLU:C	2.43	0.56
1:A:87:ALA:O	1:A:88:ASN:HB2	2.05	0.56
1:A:232:MET:HE2	1:A:232:MET:C	2.24	0.56
3:C:2:LEU:O	3:C:4:VAL:CG1	2.47	0.56
2:B:106:TYR:C	2:B:249:MET:HE1	2.26	0.56
2:B:98:TYR:CZ	2:B:259:LYS:HB2	2.40	0.56
1:A:99:ILE:O	1:A:100:ASN:HB3	2.04	0.56
1:A:195:TYR:H	2:B:131:GLN:HE21	1.54	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:69:SER:OG	3:C:207:ARG:NH1	2.39	0.56
2:B:96:MET:CG	2:B:215:MET:HB3	2.35	0.56
2:B:175:ASN:O	2:B:176:PHE:HB2	2.06	0.56
2:B:105:GLY:O	2:B:249:MET:N	2.31	0.56
2:B:106:TYR:C	2:B:249:MET:HE2	2.26	0.56
5:E:20:VAL:O	5:E:22:TRP:N	2.38	0.56
3:C:131:LEU:HB3	3:C:165:MET:HE3	1.88	0.56
3:C:109:TRP:CB	3:C:220:LEU:HD12	2.36	0.56
2:B:167:GLN:OE1	2:B:168:PRO:HD2	2.05	0.56
1:A:16:VAL:HG12	1:A:17:VAL:O	2.06	0.56
1:A:193:MET:HA	1:A:193:MET:CE	2.36	0.56
1:A:148:PRO:HD3	1:A:214:GLY:CA	2.36	0.56
4:D:30:ASN:ND2	4:D:30:ASN:N	2.50	0.56
2:B:32:ILE:HG22	2:B:202:ILE:HG12	1.87	0.55
2:B:184:ILE:O	2:B:184:ILE:HG13	2.07	0.55
2:B:71:TRP:HE3	2:B:240:ILE:HD11	1.69	0.55
1:A:16:VAL:CG1	1:A:17:VAL:N	2.69	0.55
3:C:106:PHE:O	3:C:178:THR:HG21	2.07	0.55
2:B:32:ILE:CD1	2:B:33:VAL:N	2.69	0.55
1:A:124:THR:HG21	3:C:13:PHE:CE1	2.42	0.55
1:A:171:TRP:HA	1:A:175:GLN:OE1	2.06	0.55
3:C:107:THR:CB	3:C:222:MET:HG2	2.36	0.55
1:A:204:ASN:O	1:A:205:TYR:C	2.44	0.55
1:A:277:ARG:HB2	1:A:278:PRO:HD2	1.86	0.55
2:B:173:TRP:CH2	3:C:63:ASN:CG	2.80	0.55
2:B:238:ASN:N	2:B:238:ASN:HD22	1.99	0.55
3:C:141:PRO:CG	3:C:189:THR:HG21	2.36	0.55
3:C:109:TRP:CB	3:C:220:LEU:CD1	2.85	0.55
1:A:146:VAL:HG13	1:A:150:ALA:HB3	1.88	0.55
3:C:82:ILE:O	3:C:83:PHE:HB3	2.07	0.55
2:B:57:ASP:HA	2:B:61:ASN:ND2	2.20	0.55
2:B:91:ILE:O	2:B:92:PHE:C	2.43	0.55
2:B:112:CYS:CB	2:B:242:ILE:CD1	2.85	0.55
3:C:20:GLN:HE21	4:D:32:PHE:HD2	1.55	0.55
2:B:100:TYR:CD2	2:B:101:LEU:HG	2.42	0.55
5:E:4:ARG:O	5:E:8:ILE:HB	2.07	0.55
3:C:110:THR:HA	3:C:169:TRP:CZ3	2.42	0.55
1:A:228:LYS:O	1:A:229:VAL:HG13	2.07	0.55
4:D:30:ASN:HD22	4:D:30:ASN:N	2.04	0.55
1:A:183:PRO:O	1:A:184:PHE:C	2.44	0.55
1:A:265:ILE:HG23	1:A:268:ARG:HB2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:9:GLY:O	3:C:12:GLN:HG2	2.07	0.55
2:B:215:MET:HA	2:B:215:MET:CE	2.38	0.54
1:A:237:HIS:ND1	1:A:237:HIS:C	2.61	0.54
2:B:84:ASP:O	2:B:87:LYS:HG2	2.06	0.54
1:A:161:TRP:CZ2	1:A:219:ARG:HB3	2.42	0.54
3:C:104:SER:CB	3:C:228:LEU:HD13	2.37	0.54
2:B:86:LEU:HB3	2:B:89:MET:CG	2.37	0.54
1:A:161:TRP:HB2	1:A:219:ARG:NH2	2.22	0.54
2:B:99:HIS:CG	2:B:253:PHE:HB3	2.41	0.54
3:C:55:ILE:CD1	3:C:210:CYS:HB3	2.33	0.54
2:B:93:GLY:O	2:B:96:MET:HB3	2.08	0.54
3:C:46:ILE:C	3:C:48:GLN:N	2.61	0.54
1:A:38:GLU:HA	2:B:191:PHE:HB2	1.90	0.54
3:C:81:LYS:HZ1	3:C:140:GLU:HG2	1.73	0.54
3:C:168:PRO:HB2	3:C:170:ILE:HD11	1.90	0.54
3:C:120:CYS:SG	3:C:209:LEU:HD13	2.47	0.54
3:C:88:ASP:O	3:C:91:SER:N	2.33	0.54
2:B:208:ASN:OD1	2:B:208:ASN:C	2.44	0.54
1:A:142:GLN:O	1:A:218:SER:HA	2.08	0.54
3:C:42:ASN:ND2	3:C:42:ASN:C	2.61	0.54
4:D:42:LYS:C	4:D:43:LEU:HD12	2.27	0.54
3:C:2:LEU:HD23	3:C:2:LEU:C	2.28	0.54
2:B:23:ILE:CD1	2:B:63:PHE:CD1	2.91	0.54
3:C:46:ILE:O	3:C:48:GLN:N	2.41	0.54
1:A:262:ASN:HA	2:B:133:ALA:HB1	1.90	0.54
2:B:56:PRO:HG2	2:B:60:SER:HB3	1.89	0.54
3:C:43:LEU:O	3:C:44:VAL:C	2.46	0.53
2:B:62:ARG:O	2:B:248:PRO:HD2	2.08	0.53
1:A:129:ILE:HG12	1:A:139:ILE:HD13	1.89	0.53
2:B:96:MET:HG2	2:B:215:MET:HB3	1.90	0.53
2:B:13:ILE:HD12	2:B:13:ILE:H	1.72	0.53
3:C:97:THR:O	3:C:98:LEU:C	2.47	0.53
3:C:167:VAL:O	3:C:167:VAL:HG12	2.09	0.53
3:C:125:THR:HG23	3:C:198:ILE:HG22	1.91	0.53
2:B:210:VAL:HB	2:B:211:PRO:HD2	1.91	0.53
4:D:27:PHE:C	4:D:27:PHE:HD2	1.99	0.53
4:D:30:ASN:HB3	4:D:38:ASN:OD1	2.08	0.53
1:A:125:LEU:CB	1:A:178:PRO:HG2	2.38	0.53
3:C:130:LEU:HD23	3:C:131:LEU:N	2.23	0.53
1:A:201:GLN:O	1:A:203:GLN:HB2	2.07	0.53
2:B:172:TYR:O	2:B:174:LEU:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:209:LEU:CD1	3:C:209:LEU:N	2.70	0.53
2:B:186:ILE:HG23	2:B:187:PHE:CD1	2.44	0.53
2:B:143:GLY:O	2:B:144:TYR:C	2.46	0.53
3:C:106:PHE:HB3	3:C:221:ARG:O	2.08	0.53
3:C:130:LEU:CD2	3:C:130:LEU:C	2.77	0.53
3:C:46:ILE:C	3:C:48:GLN:H	2.10	0.53
1:A:23:SER:HB2	1:A:48:GLU:HB3	1.90	0.53
2:B:34:ALA:CB	2:B:204:ALA:HA	2.39	0.52
3:C:46:ILE:O	3:C:49:VAL:N	2.41	0.52
1:A:256:THR:O	3:C:235:ILE:HG23	2.10	0.52
2:B:84:ASP:OD2	2:B:87:LYS:HD3	2.10	0.52
3:C:52:LEU:O	3:C:97:THR:HG22	2.09	0.52
3:C:109:TRP:HB2	3:C:220:LEU:CD1	2.40	0.52
2:B:66:LEU:HD12	2:B:244:ILE:CG2	2.39	0.52
1:A:80:SER:N	1:A:232:MET:HE1	2.24	0.52
3:C:56:ASN:HB3	3:C:67:MET:HA	1.90	0.52
5:E:8:ILE:CG2	5:E:17:CYS:SG	2.98	0.52
3:C:122:THR:HG23	3:C:124:ASN:N	2.25	0.52
2:B:172:TYR:CG	2:B:173:TRP:N	2.77	0.52
1:A:19:ASN:N	1:A:19:ASN:HD22	2.06	0.52
1:A:249:PRO:HB3	2:B:183:ASN:O	2.11	0.51
2:B:127:ILE:HG23	2:B:187:PHE:CE2	2.46	0.51
3:C:198:ILE:HB	3:C:199:PRO:HD2	1.91	0.51
2:B:202:ILE:C	2:B:203:ILE:HD12	2.29	0.51
1:A:108:ARG:HH12	1:A:258:ALA:HA	1.76	0.51
3:C:215:CYS:O	3:C:217:ASP:N	2.43	0.51
1:A:119:PHE:HD1	1:A:120:ASP:O	1.92	0.51
2:B:103:ARG:HB2	2:B:212:MET:HG2	1.92	0.51
4:D:6:ARG:CG	4:D:7:GLN:N	2.72	0.51
1:A:228:LYS:O	1:A:229:VAL:CG1	2.59	0.51
1:A:249:PRO:HD3	2:B:187:PHE:CE1	2.38	0.51
1:A:85:THR:HG21	1:A:92:GLU:OE1	2.10	0.51
1:A:171:TRP:CD1	1:A:178:PRO:HD3	2.46	0.51
2:B:42:LEU:HD12	2:B:43:SER:H	1.76	0.51
1:A:213:MET:HE2	1:A:213:MET:HA	1.93	0.51
2:B:97:PHE:O	2:B:257:ARG:NH1	2.43	0.51
3:C:131:LEU:HB3	3:C:165:MET:HE2	1.91	0.51
3:C:103:SER:C	3:C:105:TYR:H	2.14	0.51
3:C:143:THR:HG23	3:C:146:ASP:HB2	1.92	0.50
1:A:99:ILE:HG13	1:A:215:SER:HA	1.93	0.50
2:B:134:SER:HA	2:B:168:PRO:HA	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:10:CYS:C	5:E:12:ALA:H	2.15	0.50
1:A:111:PHE:O	1:A:113:LEU:N	2.44	0.50
2:B:86:LEU:CA	2:B:89:MET:HG2	2.42	0.50
3:C:42:ASN:HD22	3:C:43:LEU:N	2.10	0.50
2:B:216:ARG:HG2	2:B:217:SER:N	2.26	0.50
2:B:51:ASP:O	2:B:53:PRO:HD3	2.12	0.50
1:A:161:TRP:CH2	1:A:219:ARG:HB3	2.47	0.50
1:A:143:TYR:OH	1:A:233:THR:CG2	2.55	0.50
2:B:175:ASN:ND2	2:B:180:LEU:C	2.66	0.50
2:B:80:TRP:N	2:B:80:TRP:CD2	2.80	0.50
3:C:107:THR:HB	3:C:222:MET:HG2	1.94	0.50
1:A:232:MET:HE3	1:A:232:MET:HA	1.94	0.50
2:B:79:TRP:C	2:B:80:TRP:CE3	2.85	0.50
1:A:138:HIS:O	1:A:222:THR:HG21	2.11	0.50
2:B:87:LYS:HE2	2:B:150:GLY:CA	2.41	0.49
1:A:23:SER:CB	1:A:53:THR:CG2	2.89	0.49
3:C:141:PRO:HG2	3:C:189:THR:HG21	1.94	0.49
2:B:42:LEU:HD21	2:B:211:PRO:HB3	1.94	0.49
1:A:204:ASN:O	1:A:206:GLY:N	2.45	0.49
1:A:105:ALA:O	1:A:106:GLN:C	2.49	0.49
1:A:51:ILE:O	1:A:51:ILE:HG13	2.11	0.49
1:A:179:ARG:HH22	3:C:17:ASP:CG	2.12	0.49
3:C:162:THR:HG22	3:C:163:ILE:H	1.77	0.49
1:A:17:VAL:HG22	1:A:60:GLN:O	2.13	0.49
1:A:123:ILE:HB	1:A:180:PHE:CE1	2.47	0.49
1:A:142:GLN:HG3	1:A:170:PHE:HE1	1.74	0.49
1:A:107:ILE:O	1:A:108:ARG:C	2.50	0.49
1:A:232:MET:CE	1:A:232:MET:HA	2.42	0.49
2:B:16:ILE:N	2:B:16:ILE:HD13	2.27	0.49
1:A:110:LYS:O	1:A:113:LEU:N	2.44	0.49
2:B:221:TRP:O	2:B:222:SER:HB2	2.13	0.49
1:A:206:GLY:C	1:A:208:ALA:N	2.66	0.49
2:B:30:ASN:O	2:B:31:ALA:O	2.31	0.49
4:D:6:ARG:HG2	4:D:7:GLN:N	2.28	0.48
4:D:30:ASN:OD1	4:D:38:ASN:ND2	2.46	0.48
2:B:132:ILE:HG22	2:B:176:PHE:O	2.12	0.48
2:B:186:ILE:O	2:B:186:ILE:HG13	2.13	0.48
1:A:161:TRP:CE3	1:A:219:ARG:CG	2.94	0.48
2:B:23:ILE:HG21	2:B:109:HIS:CD2	2.49	0.48
2:B:161:ARG:HB2	2:B:167:GLN:HG3	1.93	0.48
2:B:136:LEU:HB2	2:B:140:VAL:HG21	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:ALA:HB2	5:E:25:ASP:HB2	1.94	0.48
2:B:182:GLY:HA2	3:C:52:LEU:HB2	1.96	0.48
1:A:114:PHE:O	1:A:193:MET:HG3	2.13	0.48
1:A:54:ARG:HD3	1:A:55:TYR:N	2.28	0.48
2:B:206:TYR:CE1	2:B:208:ASN:HB3	2.48	0.48
1:A:101:LEU:C	1:A:103:GLU:H	2.17	0.48
2:B:174:LEU:C	2:B:176:PHE:H	2.15	0.48
2:B:80:TRP:CH2	2:B:225:ILE:HD13	2.48	0.48
2:B:115:SER:HB3	2:B:118:HIS:ND1	2.28	0.48
1:A:245:TRP:CD1	3:C:36:ILE:O	2.67	0.48
1:A:24:ASN:CB	1:A:25:PRO:HD2	2.43	0.48
1:A:161:TRP:CZ3	1:A:219:ARG:CG	2.96	0.48
2:B:112:CYS:SG	2:B:242:ILE:HD13	2.52	0.48
1:A:77:ILE:CA	1:A:104:MET:HG3	2.44	0.48
2:B:106:TYR:O	2:B:249:MET:HE1	2.14	0.48
2:B:112:CYS:SG	2:B:242:ILE:HD11	2.51	0.48
3:C:58:THR:C	3:C:60:THR:H	2.15	0.47
1:A:161:TRP:CH2	1:A:219:ARG:HG2	2.49	0.47
2:B:159:GLU:O	2:B:160:THR:O	2.31	0.47
2:B:34:ALA:C	2:B:36:GLY:H	2.18	0.47
3:C:76:ILE:O	3:C:195:ARG:HG3	2.15	0.47
3:C:194:THR:HB	3:C:195:ARG:H	1.49	0.47
3:C:49:VAL:HG12	3:C:50:ASP:N	2.29	0.47
3:C:81:LYS:NZ	3:C:140:GLU:HG2	2.28	0.47
1:A:148:PRO:HD3	1:A:214:GLY:HA3	1.96	0.47
1:A:142:GLN:CG	1:A:170:PHE:CE1	2.98	0.47
3:C:58:THR:C	3:C:60:THR:N	2.68	0.47
4:D:32:PHE:HB3	4:D:37:SER:CB	2.44	0.47
3:C:6:ILE:N	3:C:6:ILE:HD12	2.29	0.47
3:C:94:LEU:O	3:C:95:ALA:C	2.53	0.47
1:A:62:ARG:O	1:A:65:MET:N	2.48	0.47
2:B:107:THR:N	2:B:247:SER:O	2.31	0.47
1:A:202:ASP:N	1:A:202:ASP:OD2	2.46	0.47
3:C:119:PHE:HB2	3:C:157:VAL:HG21	1.97	0.47
2:B:218:HIS:CD2	2:B:219:ASN:N	2.82	0.47
3:C:43:LEU:O	3:C:46:ILE:N	2.27	0.47
3:C:162:THR:CG2	3:C:163:ILE:N	2.78	0.47
3:C:124:ASN:N	3:C:124:ASN:HD22	2.13	0.46
2:B:87:LYS:HE2	2:B:150:GLY:HA2	1.96	0.46
2:B:14:ILE:HG12	2:B:16:ILE:HD11	1.98	0.46
3:C:62:ILE:HD13	3:C:62:ILE:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:134:THR:HA	3:C:135:PRO:HD2	1.73	0.46
2:B:223:LEU:HD21	2:B:225:ILE:HD11	1.96	0.46
2:B:225:ILE:HD12	2:B:225:ILE:N	2.30	0.46
3:C:69:SER:CB	3:C:207:ARG:HH11	2.28	0.46
3:C:227:ASN:C	3:C:229:HIS:H	2.19	0.46
1:A:161:TRP:CZ2	1:A:219:ARG:HG2	2.50	0.46
2:B:156:VAL:HG12	2:B:156:VAL:O	2.16	0.46
3:C:169:TRP:O	3:C:170:ILE:HD13	2.15	0.46
2:B:105:GLY:CA	2:B:204:ALA:O	2.63	0.46
1:A:17:VAL:HG23	1:A:17:VAL:O	2.15	0.46
1:A:180:PHE:C	1:A:180:PHE:CD1	2.89	0.46
2:B:155:GLU:HB3	2:B:157:LYS:CE	2.46	0.45
3:C:117:PHE:O	3:C:162:THR:HA	2.16	0.45
2:B:93:GLY:O	2:B:96:MET:CB	2.64	0.45
3:C:140:GLU:N	3:C:187:TYR:HE2	2.14	0.45
2:B:198:ASN:OD1	2:B:198:ASN:C	2.54	0.45
2:B:34:ALA:O	2:B:36:GLY:N	2.49	0.45
3:C:65:GLU:OE2	3:C:65:GLU:N	2.49	0.45
1:A:155:SER:C	1:A:157:ASP:H	2.20	0.45
2:B:14:ILE:CG1	2:B:16:ILE:HD11	2.46	0.45
1:A:146:VAL:CG1	1:A:150:ALA:HB3	2.46	0.45
1:A:84:VAL:HG23	1:A:229:VAL:O	2.17	0.45
4:D:32:PHE:CB	4:D:37:SER:HB3	2.46	0.45
2:B:118:HIS:O	3:C:122:THR:HA	2.16	0.45
3:C:36:ILE:HD12	3:C:37:PRO:HD2	1.99	0.45
1:A:161:TRP:CB	1:A:219:ARG:HH21	2.26	0.45
1:A:141:MET:HB3	1:A:143:TYR:CE2	2.51	0.45
1:A:267:ASP:O	1:A:268:ARG:HG3	2.16	0.45
3:C:9:GLY:O	3:C:10:SER:O	2.35	0.45
1:A:212:ASN:O	1:A:213:MET:HE3	2.16	0.45
2:B:19:GLY:HA2	2:B:58:THR:HG22	1.98	0.45
1:A:263:PHE:CD2	1:A:263:PHE:N	2.84	0.45
1:A:244:ALA:CA	1:A:245:TRP:CE3	3.00	0.45
2:B:80:TRP:N	2:B:80:TRP:HE3	2.12	0.45
1:A:75:GLY:CA	1:A:107:ILE:HD11	2.42	0.45
1:A:67:LEU:HA	1:A:67:LEU:HD23	1.80	0.45
3:C:12:GLN:O	3:C:12:GLN:HG3	2.16	0.45
2:B:182:GLY:N	2:B:184:ILE:HG22	2.23	0.45
4:D:43:LEU:N	4:D:43:LEU:CD1	2.67	0.45
5:E:10:CYS:SG	5:E:17:CYS:HA	2.57	0.45
3:C:118:MET:HG3	3:C:161:SER:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:80:TRP:H	2:B:80:TRP:HE3	1.66	0.44
1:A:50:VAL:O	1:A:50:VAL:CG1	2.65	0.44
2:B:172:TYR:N	2:B:172:TYR:CD2	2.85	0.44
2:B:72:SER:C	2:B:74:SER:H	2.20	0.44
2:B:83:PRO:O	2:B:84:ASP:HB3	2.17	0.44
3:C:169:TRP:CZ2	3:C:171:SER:CB	3.01	0.44
4:D:42:LYS:HA	4:D:43:LEU:HD12	1.99	0.44
3:C:69:SER:HB2	3:C:207:ARG:HH11	1.81	0.44
1:A:70:PHE:CD2	1:A:71:LEU:CD2	3.00	0.44
1:A:249:PRO:HD3	2:B:186:ILE:CG2	2.47	0.44
1:A:182:LEU:HD23	1:A:182:LEU:HA	1.81	0.44
3:C:109:TRP:HB3	3:C:220:LEU:CD1	2.47	0.44
3:C:184:THR:HG21	3:C:187:TYR:HE1	1.76	0.44
2:B:81:LYS:HA	2:B:222:SER:HA	1.99	0.44
4:D:6:ARG:CG	4:D:7:GLN:H	2.30	0.44
2:B:229:CYS:HA	2:B:230:PRO:HD2	1.72	0.44
2:B:23:ILE:CG2	2:B:24:THR:N	2.81	0.44
3:C:82:ILE:HG12	3:C:192:TYR:HE1	1.81	0.44
2:B:28:VAL:HG12	2:B:199:SER:OG	2.18	0.44
1:A:176:ALA:O	1:A:177:TYR:C	2.56	0.44
1:A:206:GLY:C	1:A:208:ALA:H	2.19	0.43
1:A:119:PHE:O	1:A:184:PHE:HB2	2.18	0.43
2:B:43:SER:C	2:B:45:LYS:N	2.70	0.43
1:A:18:PRO:C	1:A:19:ASN:HD22	2.22	0.43
2:B:155:GLU:HB3	2:B:157:LYS:HE2	2.00	0.43
2:B:72:SER:C	2:B:74:SER:N	2.71	0.43
2:B:192:ILE:HD13	2:B:199:SER:HA	1.99	0.43
2:B:13:ILE:N	2:B:13:ILE:CD1	2.78	0.43
1:A:194:PHE:N	1:A:194:PHE:CD1	2.86	0.43
2:B:34:ALA:HB2	2:B:204:ALA:HA	2.01	0.43
1:A:54:ARG:HD3	1:A:55:TYR:O	2.18	0.43
3:C:88:ASP:O	3:C:91:SER:CB	2.66	0.43
5:E:10:CYS:C	5:E:12:ALA:N	2.72	0.43
3:C:215:CYS:O	3:C:216:LYS:C	2.57	0.43
3:C:165:MET:HG2	3:C:166:VAL:N	2.34	0.43
1:A:148:PRO:HD3	1:A:214:GLY:N	2.34	0.43
2:B:127:ILE:HD12	2:B:127:ILE:N	2.33	0.43
2:B:66:LEU:HD12	2:B:244:ILE:CB	2.48	0.43
2:B:121:THR:O	2:B:228:ILE:HG22	2.19	0.43
2:B:181:LEU:HD12	2:B:184:ILE:HG21	2.00	0.43
3:C:113:LEU:HB2	3:C:167:VAL:HB	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:112:CYS:SG	2:B:242:ILE:HD12	2.58	0.43
5:E:12:ALA:HB3	5:E:30:CYS:SG	2.58	0.43
3:C:109:TRP:HB3	3:C:220:LEU:HD12	2.01	0.43
2:B:103:ARG:HG3	2:B:206:TYR:CD2	2.54	0.43
5:E:19:PRO:O	5:E:20:VAL:C	2.57	0.43
1:A:115:THR:HG1	1:A:246:CYS:HB2	1.84	0.43
3:C:56:ASN:O	3:C:67:MET:HA	2.18	0.43
2:B:28:VAL:CG1	2:B:199:SER:OG	2.67	0.43
1:A:53:THR:OG1	1:A:54:ARG:N	2.52	0.42
1:A:21:ASN:O	1:A:22:SER:C	2.56	0.42
2:B:56:PRO:HG2	2:B:60:SER:CB	2.49	0.42
1:A:124:THR:HG21	3:C:13:PHE:CD1	2.54	0.42
1:A:59:SER:OG	1:A:60:GLN:N	2.52	0.42
3:C:199:PRO:HD2	3:C:202:THR:OG1	2.19	0.42
3:C:166:VAL:HG12	3:C:167:VAL:N	2.34	0.42
2:B:61:ASN:OD1	2:B:250:CYS:N	2.52	0.42
1:A:111:PHE:CD1	1:A:111:PHE:N	2.87	0.42
2:B:174:LEU:C	2:B:176:PHE:N	2.72	0.42
2:B:34:ALA:HB3	2:B:204:ALA:HA	2.01	0.42
3:C:42:ASN:ND2	3:C:44:VAL:H	2.18	0.42
1:A:143:TYR:CD1	1:A:218:SER:HB3	2.55	0.42
1:A:118:ARG:O	1:A:119:PHE:HB3	2.19	0.42
3:C:84:SER:HA	3:C:188:ILE:O	2.19	0.42
3:C:34:ILE:O	3:C:36:ILE:HG22	2.20	0.42
3:C:51:SER:HB3	3:C:98:LEU:CG	2.47	0.42
1:A:85:THR:O	1:A:85:THR:HG23	2.18	0.42
4:D:29:ILE:C	4:D:30:ASN:HD22	2.22	0.42
2:B:257:ARG:HG2	2:B:258:ALA:H	1.84	0.42
3:C:125:THR:HG22	3:C:196:LEU:HD11	2.00	0.42
2:B:84:ASP:O	2:B:86:LEU:N	2.52	0.42
1:A:129:ILE:HD11	1:A:171:TRP:HH2	1.84	0.42
3:C:184:THR:HG22	3:C:185:SER:N	2.34	0.42
3:C:7:THR:HA	3:C:8:PRO:HD2	1.85	0.42
1:A:19:ASN:CG	1:A:58:THR:H	2.23	0.42
1:A:232:MET:CE	1:A:232:MET:CA	2.98	0.42
1:A:232:MET:CE	1:A:232:MET:C	2.87	0.42
4:D:34:ASP:O	4:D:37:SER:HB2	2.19	0.42
3:C:30:PRO:O	3:C:31:THR:C	2.58	0.42
2:B:13:ILE:HG22	2:B:14:ILE:N	2.27	0.42
3:C:26:PRO:HA	4:D:34:ASP:OD1	2.20	0.42
2:B:46:ASP:O	2:B:47:ALA:C	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:162:LEU:HG	2:B:162:LEU:H	1.57	0.42
1:A:68:GLU:OE1	1:A:241:HIS:N	2.37	0.42
1:A:228:LYS:C	1:A:229:VAL:HG13	2.40	0.42
1:A:40:GLY:HA3	2:B:189:HIS:O	2.20	0.42
2:B:175:ASN:C	2:B:176:PHE:HD2	2.24	0.41
3:C:53:VAL:O	3:C:55:ILE:CD1	2.52	0.41
1:A:237:HIS:HD1	1:A:237:HIS:C	2.23	0.41
1:A:23:SER:HB3	1:A:53:THR:CG2	2.41	0.41
5:E:4:ARG:HB3	5:E:5:ILE:H	1.58	0.41
1:A:265:ILE:HD12	1:A:266:GLU:N	2.30	0.41
1:A:144:MET:CE	1:A:166:ASN:HD22	2.33	0.41
3:C:121:GLY:O	3:C:122:THR:C	2.59	0.41
1:A:116:TYR:OH	2:B:208:ASN:HA	2.20	0.41
3:C:90:ALA:HB3	3:C:178:THR:O	2.20	0.41
1:A:188:ALA:HB1	2:B:210:VAL:HG12	2.02	0.41
3:C:231:GLN:HG3	3:C:235:ILE:HD11	2.02	0.41
1:A:180:PHE:C	1:A:180:PHE:HD1	2.24	0.41
1:A:77:ILE:HD11	1:A:235:ILE:HG21	2.00	0.41
1:A:245:TRP:N	1:A:245:TRP:CE3	2.88	0.41
1:A:144:MET:HE3	1:A:166:ASN:HD22	1.86	0.41
1:A:101:LEU:O	1:A:103:GLU:N	2.54	0.41
3:C:1:GLY:O	3:C:3:PRO:HD3	2.20	0.41
3:C:110:THR:O	3:C:219:CYS:N	2.54	0.41
1:A:48:GLU:CG	1:A:53:THR:HG21	2.47	0.41
1:A:16:VAL:CG1	1:A:17:VAL:H	2.33	0.41
2:B:121:THR:HB	2:B:228:ILE:HG23	2.01	0.41
1:A:249:PRO:HD3	2:B:186:ILE:HG21	2.03	0.41
3:C:169:TRP:HH2	3:C:176:ARG:HB2	1.85	0.41
4:D:27:PHE:O	4:D:28:ASN:HB3	2.20	0.41
3:C:44:VAL:HG22	3:C:48:GLN:NE2	2.36	0.41
3:C:87:THR:O	3:C:88:ASP:C	2.59	0.41
1:A:132:LEU:H	1:A:229:VAL:HG12	1.86	0.41
2:B:38:TRP:HA	2:B:39:PRO:HD3	1.86	0.41
2:B:126:LEU:HD21	2:B:221:TRP:HB3	2.03	0.41
5:E:18:ILE:HG13	5:E:30:CYS:H	1.85	0.41
1:A:278:PRO:O	3:C:58:THR:HG22	2.21	0.41
1:A:70:PHE:CD2	1:A:71:LEU:HD21	2.56	0.41
1:A:245:TRP:CE2	3:C:36:ILE:CG2	3.03	0.41
1:A:249:PRO:HD2	2:B:187:PHE:CE1	2.50	0.41
2:B:34:ALA:C	2:B:36:GLY:N	2.74	0.41
1:A:23:SER:HB2	1:A:53:THR:HG22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:VAL:O	1:A:222:THR:C	2.59	0.41
1:A:193:MET:HA	1:A:193:MET:HE2	2.02	0.41
3:C:14:LEU:HD12	3:C:15:THR:N	2.36	0.41
1:A:231:ILE:O	1:A:231:ILE:HG22	2.20	0.41
3:C:166:VAL:CG1	3:C:167:VAL:N	2.84	0.41
3:C:83:PHE:CD2	3:C:84:SER:N	2.89	0.41
1:A:220:ILE:O	1:A:220:ILE:HG23	2.21	0.41
3:C:169:TRP:HZ2	3:C:174:HIS:O	1.95	0.40
1:A:92:GLU:O	1:A:156:ARG:HB2	2.21	0.40
3:C:103:SER:HA	3:C:220:LEU:CD2	2.48	0.40
5:E:31:ASP:O	5:E:33:GLY:N	2.52	0.40
2:B:132:ILE:HG13	2:B:132:ILE:H	1.58	0.40
3:C:2:LEU:C	3:C:2:LEU:CD2	2.90	0.40
1:A:185:LEU:HB2	1:A:186:SER:H	1.67	0.40
2:B:103:ARG:HG3	2:B:206:TYR:CG	2.56	0.40
3:C:89:VAL:HG23	3:C:90:ALA:N	2.36	0.40
2:B:42:LEU:HD12	2:B:43:SER:N	2.36	0.40
2:B:257:ARG:HG2	2:B:258:ALA:N	2.36	0.40
2:B:181:LEU:O	3:C:68:TYR:CE1	2.74	0.40
5:E:22:TRP:HA	5:E:25:ASP:CG	2.42	0.40
3:C:169:TRP:CE2	3:C:171:SER:HB3	2.57	0.40
2:B:225:ILE:O	2:B:226:ILE:HG13	2.21	0.40
1:A:247:PRO:HG2	2:B:186:ILE:HD11	2.03	0.40
2:B:106:TYR:CA	2:B:249:MET:CE	2.95	0.40
2:B:71:TRP:CE2	2:B:231:LEU:HB2	2.57	0.40
1:A:262:ASN:ND2	2:B:134:SER:OG	2.54	0.40
2:B:167:GLN:HA	2:B:167:GLN:OE1	2.21	0.40
1:A:282:THR:HG22	1:A:282:THR:O	2.22	0.40
2:B:112:CYS:O	2:B:112:CYS:SG	2.79	0.40
2:B:240:ILE:O	2:B:240:ILE:HD12	2.22	0.40
1:A:127:PRO:HG2	1:A:171:TRP:CD2	2.56	0.40
2:B:99:HIS:HB3	2:B:254:SER:O	2.22	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	267/289 (92%)	203 (76%)	42 (16%)	22 (8%)	1	13
2	B	248/261 (95%)	187 (75%)	39 (16%)	22 (9%)	1	11
3	C	235/237 (99%)	173 (74%)	43 (18%)	19 (8%)	1	13
4	D	21/68 (31%)	16 (76%)	4 (19%)	1 (5%)	3	28
5	E	37/39 (95%)	15 (40%)	17 (46%)	5 (14%)	0	4
All	All	808/894 (90%)	594 (74%)	145 (18%)	69 (8%)	1	13

All (69) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	60	GLN
1	A	102	GLN
1	A	105	ALA
1	A	106	GLN
1	A	186	SER
2	B	14	ILE
2	B	31	ALA
2	B	47	ALA
2	B	83	PRO
2	B	160	THR
2	B	163	ASN
2	B	194	LEU
2	B	222	SER
3	C	10	SER
5	E	4	ARG
5	E	21	SER
5	E	32	SER
1	A	87	ALA
1	A	91	LYS
1	A	205	TYR
1	A	263	PHE
1	A	273	ALA
2	B	61	ASN
2	B	85	ALA
2	B	90	GLY
2	B	139	ASN
2	B	173	TRP

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Mol	Chain	Res	Type
2	B	208	ASN
3	C	44	VAL
3	C	201	GLN
3	C	216	LYS
5	E	20	VAL
1	A	52	GLU
1	A	112	GLU
1	A	272	THR
2	B	49	ALA
2	B	164	PRO
2	B	175	ASN
3	C	47	CYS
3	C	62	ILE
3	C	95	ALA
3	C	228	LEU
5	E	9	SER
1	A	25	PRO
1	A	110	LYS
1	A	204	ASN
1	A	262	ASN
2	B	30	ASN
2	B	66	LEU
2	B	84	ASP
2	B	114	ALA
3	C	79	PRO
3	C	83	PHE
3	C	104	SER
3	C	158	GLY
4	D	28	ASN
1	A	156	ARG
1	A	266	GLU
2	B	172	TYR
3	C	98	LEU
3	C	122	THR
1	A	107	ILE
1	A	184	PHE
3	C	127	VAL
3	C	136	PRO
3	C	163	ILE
3	C	8	PRO
1	A	278	PRO
3	C	3	PRO

5.3.2 Protein sidechains ⓘ

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	238/257 (93%)	203 (85%)	35 (15%)	4	22
2	B	216/226 (96%)	184 (85%)	32 (15%)	4	22
3	C	210/210 (100%)	180 (86%)	30 (14%)	4	24
4	D	19/59 (32%)	11 (58%)	8 (42%)	0	1
5	E	34/34 (100%)	26 (76%)	8 (24%)	1	5
All	All	717/786 (91%)	604 (84%)	113 (16%)	3	19

All (113) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	ASN
1	A	53	THR
1	A	54	ARG
1	A	55	TYR
1	A	60	GLN
1	A	61	THR
1	A	66	SER
1	A	82	LEU
1	A	95	THR
1	A	106	GLN
1	A	111	PHE
1	A	113	LEU
1	A	115	THR
1	A	125	LEU
1	A	136	ILE
1	A	139	ILE
1	A	159	TYR
1	A	179	ARG
1	A	180	PHE
1	A	189	SER
1	A	200	GLU
1	A	201	GLN
1	A	203	GLN

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Mol	Chain	Res	Type
1	A	207	THR
1	A	213	MET
1	A	215	SER
1	A	219	ARG
1	A	231	ILE
1	A	233	THR
1	A	253	LEU
1	A	257	ARG
1	A	261	THR
1	A	269	SER
1	A	277	ARG
1	A	280	ILE
2	B	13	ILE
2	B	26	GLN
2	B	28	VAL
2	B	32	ILE
2	B	58	THR
2	B	63	PHE
2	B	80	TRP
2	B	86	LEU
2	B	91	ILE
2	B	106	TYR
2	B	112	CYS
2	B	115	SER
2	B	116	LYS
2	B	126	LEU
2	B	132	ILE
2	B	134	SER
2	B	137	HIS
2	B	152	THR
2	B	154	ARG
2	B	162	LEU
2	B	163	ASN
2	B	180	LEU
2	B	184	ILE
2	B	193	ASN
2	B	195	ARG
2	B	197	ASN
2	B	201	THR
2	B	203	ILE
2	B	216	ARG
2	B	220	ASN

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Mol	Chain	Res	Type
2	B	238	ASN
2	B	257	ARG
3	C	31	THR
3	C	42	ASN
3	C	47	CYS
3	C	48	GLN
3	C	51	SER
3	C	56	ASN
3	C	62	ILE
3	C	69	SER
3	C	71	VAL
3	C	73	GLN
3	C	88	ASP
3	C	96	THR
3	C	103	SER
3	C	110	THR
3	C	122	THR
3	C	124	ASN
3	C	133	TYR
3	C	134	THR
3	C	142	THR
3	C	143	THR
3	C	148	MET
3	C	165	MET
3	C	194	THR
3	C	201	GLN
3	C	202	THR
3	C	209	LEU
3	C	211	PHE
3	C	220	LEU
3	C	224	ARG
3	C	230	LEU
4	D	4	VAL
4	D	6	ARG
4	D	27	PHE
4	D	28	ASN
4	D	31	TYR
4	D	33	LYS
4	D	41	SER
4	D	43	LEU
5	E	10	CYS
5	E	13	HIS

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Mol	Chain	Res	Type
5	E	16	GLN
5	E	17	CYS
5	E	29	ASP
5	E	32	SER
5	E	39	CYS
5	E	41	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	ASN
1	A	138	HIS
1	A	166	ASN
1	A	201	GLN
1	A	262	ASN
2	B	15	GLN
2	B	26	GLN
2	B	109	HIS
2	B	131	GLN
2	B	137	HIS
2	B	193	ASN
2	B	197	ASN
2	B	219	ASN
2	B	238	ASN
3	C	20	GLN
3	C	42	ASN
3	C	48	GLN
3	C	56	ASN
3	C	73	GLN
3	C	124	ASN
3	C	193	GLN
3	C	201	GLN
3	C	227	ASN
4	D	30	ASN
4	D	38	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	DAO	A	290	-	10,13,13	0.55	0	10,13,13	0.68	0

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
6	DAO	A	290	-	-	0/9/11/11	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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, 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	269/289 (93%)	0.26	3 (1%) 82 73	23, 23, 23, 23	0
2	B	249/261 (95%)	0.18	1 (0%) 93 90	20, 23, 23, 23	0
3	C	237/237 (100%)	0.28	3 (1%) 79 70	20, 23, 23, 23	0
4	D	25/68 (36%)	0.58	2 (8%) 15 12	23, 23, 23, 23	0
5	E	39/39 (100%)	1.04	5 (12%) 5 5	23, 23, 23, 23	0
All	All	819/894 (91%)	0.29	14 (1%) 73 64	20, 23, 23, 23	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	269	SER	3.6
5	E	40	GLY	2.8
4	D	25	ASN	2.8
5	E	35	ASP	2.7
1	A	152	VAL	2.4
2	B	74	SER	2.4
4	D	2	ALA	2.4
3	C	184	THR	2.1
5	E	33	GLY	2.1
1	A	163	SER	2.1
3	C	185	SER	2.1
5	E	39	CYS	2.1
3	C	92	GLN	2.0
5	E	32	SER	2.0

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 [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(\AA^2)	Q<0.9
6	DAO	A	290	14/14	0.69	0.44	2.75	22,22,22,22	0
7	CA	E	50	1/1	0.71	0.20	-2.33	22,22,22,22	0

6.5 Other polymers [i](#)

There are no such residues in this entry.