



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 27, 2026 – 05:07 PM EDT

PDB ID : 3DPR / pdb\_00003dpr  
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](mailto: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>.

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

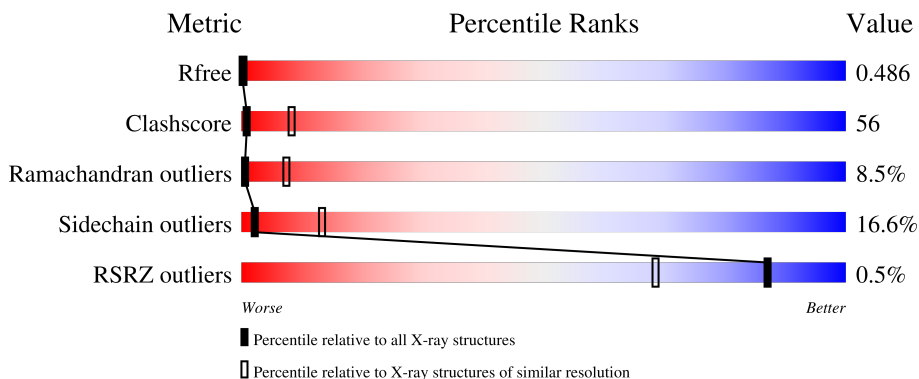
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.50 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))
$R_{free}$	180053	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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  $\geq 3$ , 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	289	
2	B	261	
3	C	237	
4	D	68	
5	E	39	

## 2 Entry composition [i](#)

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
			Total	C	N	O	S			
1	A	269	2155	1356	378	410	11	0	0	0

- Molecule 2 is a protein called Protein VP2.

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

- Molecule 3 is a protein called Protein VP3.

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

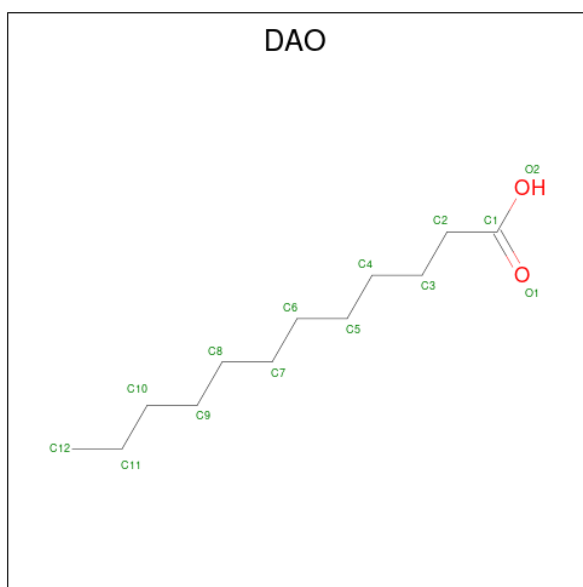
- Molecule 4 is a protein called Protein VP4.

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

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

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

- Molecule 6 is LAURIC ACID (CCD ID: DAO) (formula: C<sub>12</sub>H<sub>24</sub>O<sub>2</sub>).



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

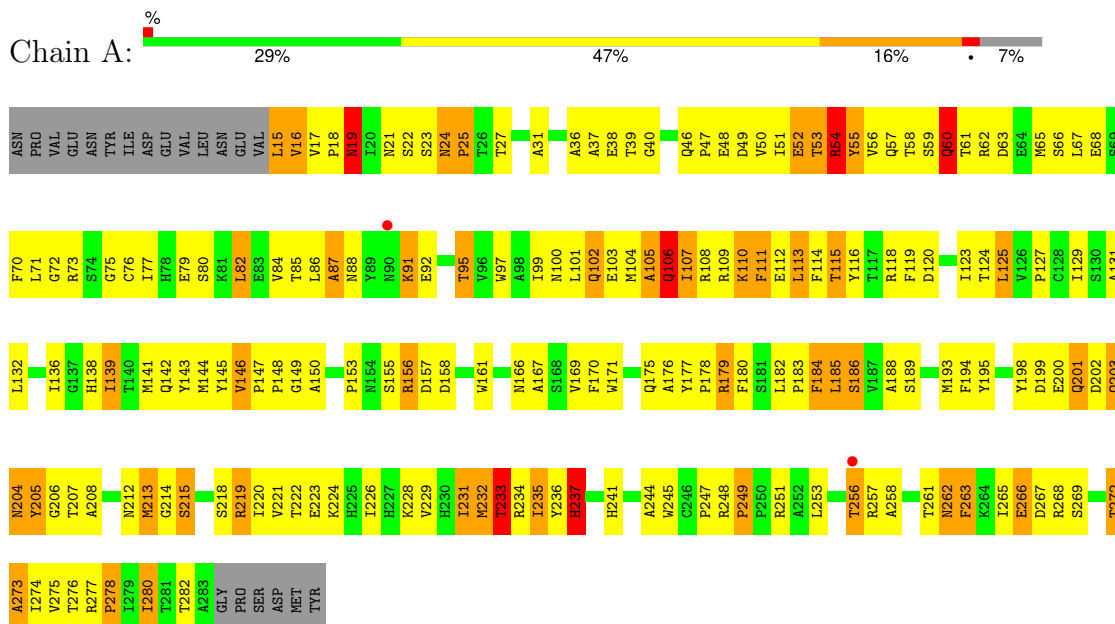
- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

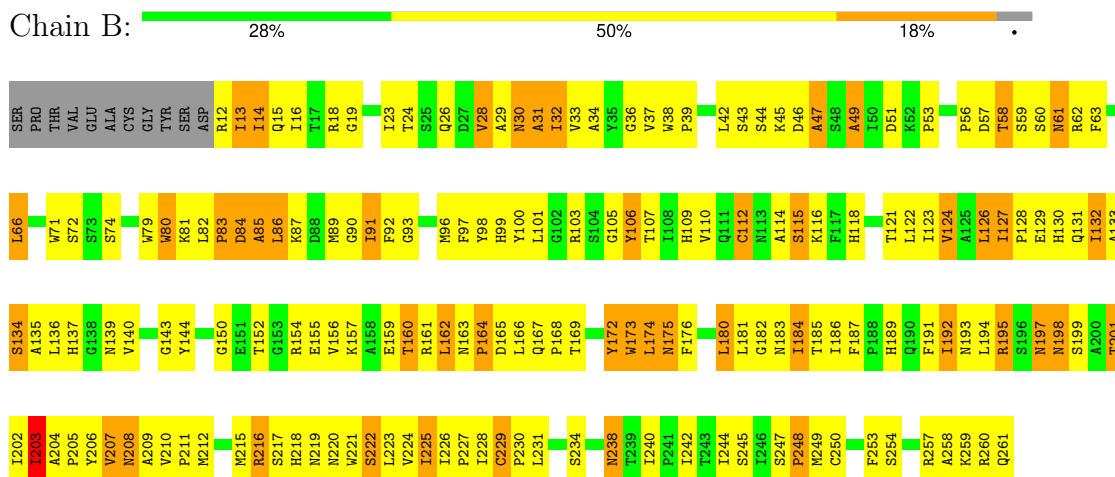
### 3 Residue-property plots [i](#)

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.

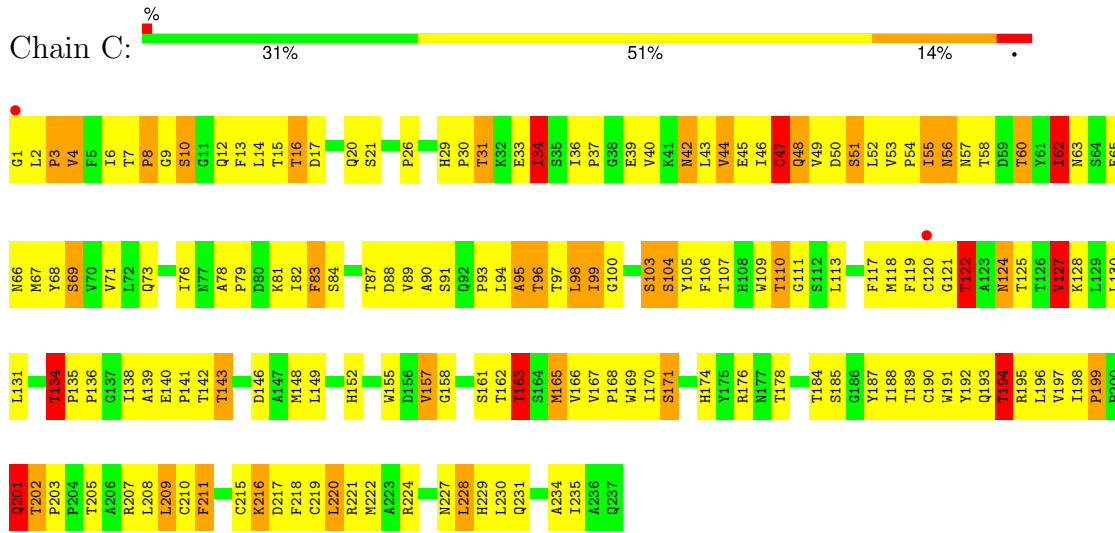
- Molecule 1: Protein VP1



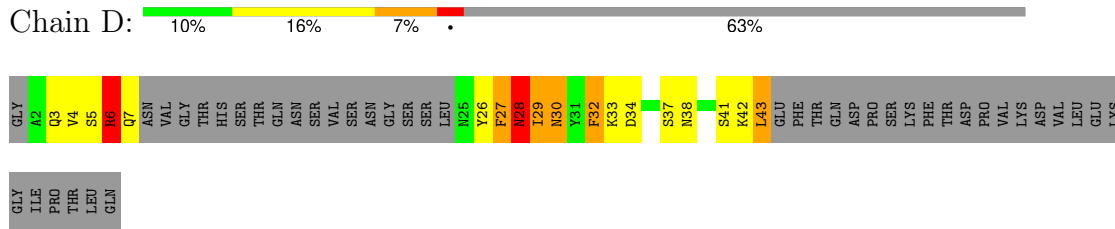
- Molecule 2: Protein VP2



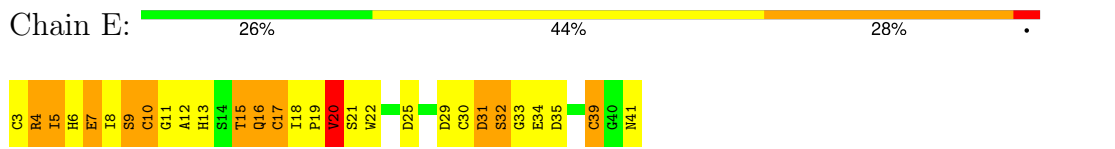
- Molecule 3: Protein VP3



• 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, $\alpha$ , $\beta$ , $\gamma$	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) 60.8 (15.00-3.50)	Depositor EDS
$R_{merge}$	0.20	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.53 (at 3.48Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.425 , 0.441 0.483 , 0.486	Depositor DCC
$R_{free}$ test set	31034 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	41.0	Xtrriage
Anisotropy	0.008	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 76.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.05	EDS
Total number of atoms	6450	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtrriage'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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: 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	1.35	8/2211 (0.4%)	1.23	10/3011 (0.3%)
2	B	1.35	6/2015 (0.3%)	1.18	7/2752 (0.3%)
3	C	1.39	10/1883 (0.5%)	1.26	11/2579 (0.4%)
4	D	1.52	2/196 (1.0%)	1.34	1/261 (0.4%)
5	E	1.88	7/297 (2.4%)	1.38	2/399 (0.5%)
All	All	1.40	33/6602 (0.5%)	1.23	31/9002 (0.3%)

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	256	THR	CA-CB	9.27	1.65	1.53
2	B	37	VAL	CA-CB	8.83	1.66	1.54
3	C	16	THR	CA-CB	8.19	1.64	1.53
2	B	207	VAL	CA-CB	-7.30	1.45	1.54
1	A	233	THR	CA-CB	6.82	1.61	1.53
1	A	235	ILE	CA-CB	-6.76	1.46	1.54
2	B	124	VAL	CA-CB	-6.76	1.46	1.54
3	C	55	ILE	CA-CB	6.46	1.61	1.54
3	C	60	THR	CA-CB	6.41	1.63	1.53
4	D	6	ARG	CA-C	6.37	1.61	1.52
5	E	29	ASP	CA-C	6.12	1.60	1.52
5	E	35	ASP	CA-C	6.12	1.61	1.52
5	E	15	THR	CA-CB	6.05	1.64	1.52
3	C	55	ILE	N-CA	6.04	1.53	1.46
3	C	57	ASN	N-CA	6.04	1.52	1.46
5	E	5	ILE	CA-CB	6.00	1.62	1.54
1	A	31	ALA	CA-C	5.69	1.59	1.52
5	E	9	SER	CA-C	5.60	1.60	1.52
3	C	4	VAL	CA-CB	-5.59	1.46	1.54
1	A	19	ASN	CA-C	-5.49	1.46	1.52
3	C	199	PRO	CA-C	5.42	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	203	PRO	CA-C	5.41	1.57	1.52
2	B	248	PRO	N-CA	-5.41	1.40	1.47
4	D	5	SER	CA-C	5.38	1.58	1.52
5	E	39	CYS	CA-C	5.36	1.59	1.53
2	B	245	SER	CA-C	-5.32	1.46	1.52
1	A	249	PRO	CA-C	5.25	1.54	1.51
2	B	198	ASN	CA-C	5.25	1.59	1.52
3	C	171	SER	CA-C	-5.24	1.46	1.52
5	E	6	HIS	N-CA	5.22	1.52	1.46
3	C	163	ILE	CA-CB	-5.13	1.47	1.54
1	A	167	ALA	CA-CB	-5.03	1.46	1.53
1	A	54	ARG	C-O	-5.02	1.18	1.23

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	78	ALA	N-CA-C	10.14	117.25	108.13
2	B	229	CYS	CA-C-N	8.68	128.70	119.76
2	B	229	CYS	C-N-CA	8.68	128.70	119.76
1	A	24	ASN	CA-C-N	7.85	129.65	119.84
1	A	24	ASN	C-N-CA	7.85	129.65	119.84
3	C	194	THR	CA-C-O	7.56	122.32	117.94
1	A	249	PRO	O-C-N	7.19	124.62	121.31
1	A	146	VAL	CA-C-N	7.18	124.90	119.66
1	A	146	VAL	C-N-CA	7.18	124.90	119.66
5	E	31	ASP	N-CA-C	7.07	118.99	111.28
1	A	16	VAL	N-CA-C	6.53	119.22	109.17
3	C	134	THR	CA-C-N	6.52	127.10	120.38
3	C	134	THR	C-N-CA	6.52	127.10	120.38
2	B	127	ILE	CA-C-N	6.51	127.04	120.14
2	B	127	ILE	C-N-CA	6.51	127.04	120.14
4	D	32	PHE	N-CA-C	6.38	120.23	109.76
1	A	27	THR	N-CA-C	-6.29	102.99	110.41
3	C	34	ILE	N-CA-C	6.24	117.69	108.65
2	B	29	ALA	N-CA-C	-6.17	99.22	109.46
2	B	44	SER	N-CA-C	-6.06	104.99	112.38
5	E	7	GLU	N-CA-C	-5.71	104.47	112.12
1	A	149	GLY	N-CA-C	-5.71	107.47	113.58
3	C	152	HIS	N-CA-C	5.61	115.51	108.45
2	B	203	ILE	CB-CA-C	-5.38	102.67	110.63
3	C	62	ILE	N-CA-C	5.32	120.41	109.34
3	C	234	ALA	N-CA-C	5.27	122.03	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	194	THR	CB-CA-C	-5.24	109.53	117.07
1	A	235	ILE	N-CA-C	5.14	115.37	108.17
1	A	237	HIS	N-CA-C	5.09	116.72	108.26
3	C	29	HIS	CA-C-N	5.03	125.03	119.90
3	C	29	HIS	C-N-CA	5.03	125.03	119.90

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	2155	0	2080	235	0
2	B	1960	0	1902	260	0
3	C	1833	0	1817	204	0
4	D	194	0	180	27	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	706	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 56.

All (706) 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:N	2:B:203:ILE:HD12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:N	2:B:91:ILE:HD13	1.87	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:126:LEU:HD22	2:B:221:TRP:HE3	1.36	0.88
2:B:132:ILE:CG2	2:B:176:PHE:HB3	2.03	0.88
3:C:111:GLY:O	3:C:169:TRP:HB2	1.73	0.88
4:D:27:PHE:C	4:D:27:PHE:CD2	2.51	0.88
2:B:203:ILE:HD12	2:B:203:ILE:H	1.35	0.88
1:A:65:MET:O	3:C:42:ASN:CG	2.17	0.88
1:A:193:MET:HE2	1:A:193:MET:HA	1.56	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
1:A:25:PRO:HD3	1:A:52:GLU:OE2	1.76	0.85
2:B:84:ASP:H	2:B:96:MET:HE1	1.40	0.85
3:C:138:ILE:HG13	3:C:139:ALA:N	1.86	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
2:B:106:TYR:C	2:B:249:MET:HE2	2.02	0.84
2:B:165:ASP:O	2:B:166:LEU:HD23	1.77	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
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:91:ILE:H	2:B:91:ILE:CD1	1.94	0.81
2:B:182:GLY:H	2:B:184:ILE:HG22	1.44	0.81
2:B:203:ILE:N	2:B:203:ILE:CD1	2.41	0.81
3:C:54:PRO:HG2	3:C:93:PRO:HB2	1.59	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD12	4:D:43:LEU:N	1.96	0.80
1:A:77:ILE:C	1:A:104:MET:HG3	2.06	0.80
2:B:112:CYS:SG	2:B:242:ILE:CD1	2.69	0.80
3:C:169:TRP:CZ2	3:C:174:HIS:O	2.33	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
1:A:280:ILE:HD13	1:A:280:ILE:H	1.48	0.78
2:B:223:LEU:HD12	2:B:224:VAL:H	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
2:B:82:LEU:HA	2:B:83:PRO:O	1.84	0.78
3:C:138:ILE:CG1	3:C:139:ALA:H	1.97	0.78
3:C:42:ASN:C	3:C:42:ASN:HD22	1.92	0.77
2:B:71:TRP:CE3	2:B:240:ILE:HD11	2.20	0.77
3:C:128:LYS:HB2	3:C:194:THR:OG1	1.84	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
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
3:C:130:LEU:HD23	3:C:130:LEU:C	2.11	0.76
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:10:CYS:HB2	5:E:16:GLN:O	1.85	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
1:A:232:MET:HA	1:A:232:MET:HE3	1.67	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
1:A:144:MET:HE3	1:A:166:ASN:HD22	1.52	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:PHE:C	1:A:113:LEU:H	1.96	0.73
2:B:193:ASN:H	2:B:197:ASN:HD21	1.37	0.73
3:C:111:GLY:C	3:C:169:TRP:HB2	2.12	0.73
2:B:80:TRP:HZ3	2:B:225:ILE:CD1	2.01	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:13:ILE:O	2:B:14:ILE:HB	1.88	0.71
2:B:80:TRP:CE3	2:B:80:TRP:N	2.58	0.71
2:B:112:CYS:HB2	2:B:242:ILE:HD12	1.72	0.71
3:C:201:GLN:HE21	3:C:201:GLN:HA	1.55	0.71
2:B:127:ILE:HG13	2:B:187:PHE:CD2	2.25	0.71
1:A:55:TYR:C	1:A:55:TYR:CD2	2.68	0.71
3:C:131:LEU:HB3	3:C:165:MET:CE	2.21	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:159:GLU:HG3	2:B:159:GLU:O	1.90	0.71
2:B:165:ASP:C	2:B:166:LEU:HD23	2.15	0.70
2:B:83:PRO:HB2	2:B:96:MET:CE	2.21	0.70
2:B:60:SER:O	2:B:62:ARG:N	2.23	0.70
3:C:111:GLY:HA3	3:C:218:PHE:HA	1.72	0.70
1:A:145:TYR:HE1	1:A:147:PRO:HG3	1.55	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
2:B:215:MET:HA	2:B:215:MET:HE2	1.72	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: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
1:A:142:GLN:HG3	1:A:170:PHE:CE1	2.28	0.69
3:C:52:LEU:HD23	3:C:210:CYS:O	1.93	0.69
3:C:163:ILE:O	3:C:163:ILE:CG2	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
2:B:106:TYR:C	2:B:249:MET:CE	2.66	0.68
2:B:122:LEU:HD23	2:B:227:PRO:HA	1.75	0.68
2:B:180:LEU:H	2:B:180:LEU:HD12	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:19:ASN:OD1	1:A:57:GLN:HA	1.92	0.68
1:A:161:TRP:CE2	1:A:219:ARG:HG2	2.28	0.68
1:A:244:ALA:HA	1:A:245:TRP:CE3	2.29	0.68
2:B:126:LEU:C	2:B:127:ILE:HD12	2.18	0.68
1:A:55:TYR:C	1:A:55:TYR:HD2	2.02	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:161:TRP:CG	1:A:219:ARG:HE	2.12	0.67
3:C:168:PRO:O	3:C:170:ILE:HG12	1.94	0.67
3:C:215:CYS:C	3:C:217:ASP:N	2.47	0.67
2:B:15:GLN:C	2:B:16:ILE:HD13	2.20	0.67
2:B:106:TYR:CA	2:B:249:MET:HE2	2.25	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
1:A:124:THR:HG23	1:A:179:ARG:HB2	1.75	0.66
2:B:80:TRP:CZ3	2:B:225:ILE:CD1	2.77	0.66
2:B:86:LEU:HB3	2:B:89:MET:HG3	1.78	0.66
2:B:31:ALA:CB	2:B:201:THR:HB	2.25	0.66
2:B:12:ARG:N	2:B:13:ILE:HD12	2.10	0.66
2:B:83:PRO:HB2	2:B:96:MET:HE1	1.77	0.66
3:C:51:SER:HB3	3:C:98:LEU:HG	1.77	0.66
2:B:84:ASP:O	2:B:85:ALA:C	2.38	0.66
3:C:138:ILE:CG1	3:C:139:ALA:N	2.57	0.66
1:A:179:ARG:NH2	3:C:17:ASP:OD1	2.27	0.65
2:B:59:SER:O	2:B:62:ARG:HD2	1.96	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
3:C:122:THR:HG22	3:C:125:THR:HG1	1.58	0.65
1:A:125:LEU:HB2	1:A:178:PRO:HG2	1.79	0.65
1:A:232:MET:HE3	1:A:232:MET:C	2.21	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
3:C:131:LEU:HB3	3:C:165:MET:HE3	1.78	0.65
1:A:19:ASN:HB3	1:A:56:VAL:O	1.96	0.65
2:B:203:ILE:H	2:B:203:ILE:CD1	2.06	0.65
5:E:8:ILE:HG23	5:E:17:CYS:HB2	1.78	0.65
3:C:42:ASN:O	3:C:45:GLU:HG3	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:C:33:GLU:HG2	3:C:34:ILE:N	2.12	0.65
3:C:55:ILE:HD12	3:C:55:ILE:H	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
3:C:104:SER:HB3	3:C:228:LEU:HD13	1.77	0.64
3:C:42:ASN:ND2	3:C:44:VAL:HG12	2.11	0.64
4:D:27:PHE:CD2	4:D:27:PHE:O	2.50	0.64
4:D:3:GLN:CB	4:D:26:TYR:O	2.45	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
1:A:145:TYR:CE1	1:A:147:PRO:HG3	2.32	0.64
2:B:84:ASP:O	2:B:87:LYS:N	2.30	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
1:A:232:MET:HE3	1:A:232:MET:CA	2.27	0.63
2:B:112:CYS:CB	2:B:242:ILE:HD12	2.27	0.63
2:B:223:LEU:HD12	2:B:224:VAL:N	2.11	0.63
1:A:17:VAL:HG21	1:A:60:GLN:HB2	1.79	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
2:B:112:CYS:HB2	2:B:242:ILE:CD1	2.29	0.63
2:B:132:ILE:HG23	2:B:176:PHE:HB3	1.78	0.63
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:175:ASN:HD21	2:B:180:LEU:C	2.07	0.63
2:B:132:ILE:HG22	2:B:176:PHE:HB3	1.81	0.62
4:D:27:PHE:C	4:D:27:PHE:HD2	1.99	0.62
1:A:245:TRP:NE1	3:C:36:ILE:CG2	2.59	0.62
2:B:49:ALA:HB3	2:B:212:MET:HE1	1.79	0.62
1:A:198:TYR:CE1	1:A:205:TYR:HB2	2.34	0.62
2:B:110:VAL:HG22	2:B:244:ILE:HG12	1.81	0.62
3:C:211:PHE:N	3:C:211:PHE:CD1	2.65	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
3:C:215:CYS:C	3:C:217:ASP:H	2.07	0.61
1:A:156:ARG:O	1:A:156:ARG:HG2	1.99	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:128:PRO:O	2:B:129:GLU:C	2.43	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
3:C:189:THR:HG1	3:C:191:TRP:NE1	1.99	0.61
5:E:31:ASP:C	5:E:33:GLY:H	2.08	0.61
2:B:13:ILE:HD12	2:B:13:ILE:N	2.15	0.61
3:C:82:ILE:HG12	3:C:192:TYR:CE1	2.36	0.61
1:A:232:MET:HE3	1:A:233:THR:N	2.16	0.61
3:C:127:VAL:CG2	3:C:128:LYS:N	2.63	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
1:A:204:ASN:O	1:A:205:TYR:C	2.44	0.60
2:B:193:ASN:O	2:B:195:ARG:N	2.34	0.60
2:B:123:ILE:HG12	2:B:191:PHE:CE1	2.36	0.60
2:B:172:TYR:HA	2:B:176:PHE:HE2	1.61	0.60
2:B:173:TRP:CH2	3:C:63:ASN:CG	2.80	0.60
2:B:91:ILE:O	2:B:92:PHE:C	2.43	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
1:A:183:PRO:O	1:A:184:PHE:C	2.44	0.59
3:C:224:ARG:HH12	3:C:227:ASN:HD22	1.49	0.59
1:A:237:HIS:C	1:A:237:HIS:ND1	2.61	0.59
3:C:46:ILE:C	3:C:48:GLN:H	2.10	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
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
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
2:B:208:ASN:OD1	2:B:208:ASN:C	2.44	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:260:ARG:HG3	2:B:261:GLN:H	1.68	0.58
4:D:42:LYS:C	4:D:43:LEU:HD12	2.27	0.58
1:A:36:ALA:HB1	1:A:38:GLU:OE2	2.02	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:2:LEU:HD23	3:C:2:LEU:C	2.28	0.58
3:C:224:ARG:HH12	3:C:227:ASN:ND2	2.00	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
3:C:43:LEU:O	3:C:44:VAL:C	2.46	0.58
3:C:46:ILE:C	3:C:48:GLN:N	2.61	0.58
1:A:86:LEU:O	1:A:87:ALA:CB	2.52	0.58
3:C:128:LYS:O	3:C:193:GLN:HB3	2.03	0.58
2:B:106:TYR:HA	2:B:249:MET:HE2	1.84	0.58
3:C:97:THR:O	3:C:98:LEU:C	2.47	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:131:ALA:O	1:A:132:LEU:HD23	2.03	0.58
2:B:66:LEU:HD12	2:B:244:ILE:HB	1.86	0.58
5:E:3:CYS:O	5:E:4:ARG:HB2	2.04	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
1:A:97:TRP:CH2	1:A:100:ASN:O	2.56	0.57
1:A:179:ARG:HH22	3:C:17:ASP:CG	2.12	0.57
2:B:49:ALA:CB	2:B:212:MET:HE1	2.34	0.57
3:C:130:LEU:HD12	3:C:193:GLN:HE22	1.69	0.57
2:B:143:GLY:O	2:B:144:TYR:C	2.46	0.57
2:B:207:VAL:HG22	3:C:37:PRO:HG2	1.86	0.57
1:A:144:MET:HE3	1:A:166:ASN:ND2	2.19	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
3:C:189:THR:OG1	3:C:191:TRP:NE1	2.34	0.57
1:A:54:ARG:HD3	1:A:55:TYR:H	1.70	0.56
1:A:102:GLN:HA	1:A:108:ARG:HD2	1.87	0.56
1:A:111:PHE:C	1:A:113:LEU:N	2.57	0.56
1:A:87:ALA:O	1:A:88:ASN:HB2	2.05	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
2:B:98:TYR:CZ	2:B:259:LYS:HB2	2.40	0.56
3:C:2:LEU:O	3:C:4:VAL:CG1	2.47	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:202:ILE:C	2:B:203:ILE:HD12	2.29	0.56
3:C:189:THR:HG1	3:C:191:TRP:CD1	2.23	0.56
2:B:105:GLY:O	2:B:249:MET:N	2.31	0.56
2:B:175:ASN:O	2:B:176:PHE:HB2	2.06	0.56
5:E:20:VAL:O	5:E:22:TRP:N	2.38	0.56
3:C:109:TRP:CB	3:C:220:LEU:HD12	2.36	0.56
3:C:130:LEU:C	3:C:130:LEU:CD2	2.77	0.56
1:A:16:VAL:HG12	1:A:17:VAL:O	2.06	0.56
1:A:148:PRO:HD3	1:A:214:GLY:CA	2.36	0.56
2:B:167:GLN:OE1	2:B:168:PRO:HD2	2.05	0.56
4:D:30:ASN:N	4:D:30:ASN:ND2	2.50	0.56
1:A:16:VAL:CG1	1:A:17:VAL:N	2.69	0.55
2:B:32:ILE:HG22	2:B:202:ILE:HG12	1.87	0.55
2:B:71:TRP:HE3	2:B:240:ILE:HD11	1.69	0.55
2:B:184:ILE:HG13	2:B:184:ILE:O	2.07	0.55
3:C:106:PHE:O	3:C:178:THR:HG21	2.07	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
2:B:32:ILE:CD1	2:B:33:VAL:N	2.69	0.55
3:C:107:THR:CB	3:C:222:MET:HG2	2.36	0.55
1:A:277:ARG:HB2	1:A:278:PRO:HD2	1.86	0.55
3:C:103:SER:C	3:C:105:TYR:H	2.14	0.55
1:A:146:VAL:HG13	1:A:150:ALA:HB3	1.88	0.55
2:B:57:ASP:HA	2:B:61:ASN:ND2	2.20	0.55
2:B:238:ASN:HD22	2:B:238:ASN:N	1.99	0.55
3:C:82:ILE:O	3:C:83:PHE:HB3	2.07	0.55
3:C:109:TRP:CB	3:C:220:LEU:CD1	2.85	0.55
3:C:141:PRO:CG	3:C:189:THR:HG21	2.36	0.55
2:B:100:TYR:CD2	2:B:101:LEU:HG	2.42	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
5:E:4:ARG:O	5:E:8:ILE:HB	2.07	0.55
5:E:10:CYS:C	5:E:12:ALA:H	2.15	0.55
1:A:228:LYS:O	1:A:229:VAL:HG13	2.07	0.55
3:C:110:THR:HA	3:C:169:TRP:CZ3	2.42	0.55
4:D:30:ASN:N	4:D:30:ASN:HD22	2.04	0.55
1:A:265:ILE:HG23	1:A:268:ARG:HB2	1.89	0.55
3:C:9:GLY:O	3:C:12:GLN:HG2	2.07	0.55
2:B:79:TRP:C	2:B:80:TRP:CE3	2.85	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:175:ASN:ND2	2:B:180:LEU:C	2.66	0.54
2:B:215:MET:HA	2:B:215:MET:CE	2.38	0.54
1:A:161:TRP:CZ2	1:A:219:ARG:HB3	2.42	0.54
2:B:84:ASP:O	2:B:87:LYS:HG2	2.06	0.54
3:C:104:SER:CB	3:C:228:LEU:HD13	2.37	0.54
1:A:105:ALA:O	1:A:106:GLN:C	2.49	0.54
1:A:161:TRP:HB2	1:A:219:ARG:NH2	2.22	0.54
1:A:272:THR:OG1	1:A:273:ALA:N	2.33	0.54
2:B:86:LEU:HB3	2:B:89:MET:CG	2.37	0.54
2:B:99:HIS:CG	2:B:253:PHE:HB3	2.41	0.54
1:A:38:GLU:HA	2:B:191:PHE:HB2	1.90	0.54
1:A:80:SER:N	1:A:232:MET:HE1	2.22	0.54
2:B:93:GLY:O	2:B:96:MET:HB3	2.08	0.54
3:C:55:ILE:CD1	3:C:210:CYS:HB3	2.33	0.54
1:A:107:ILE:O	1:A:108:ARG:C	2.50	0.54
3:C:88:ASP:O	3:C:91:SER:N	2.33	0.54
3:C:120:CYS:SG	3:C:209:LEU:HD13	2.47	0.54
3:C:168:PRO:HB2	3:C:170:ILE:HD11	1.90	0.54
1:A:142:GLN:O	1:A:218:SER:HA	2.08	0.54
2:B:23:ILE:CD1	2:B:63:PHE:CD1	2.91	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:46:ILE:O	3:C:48:GLN:N	2.41	0.54
1:A:129:ILE:HG12	1:A:139:ILE:HD13	1.89	0.53
2:B:62:ARG:O	2:B:248:PRO:HD2	2.08	0.53
2:B:13:ILE:HD12	2:B:13:ILE:H	1.72	0.53
2:B:96:MET:HG2	2:B:215:MET:HB3	1.90	0.53
3:C:167:VAL:HG12	3:C:167:VAL:O	2.09	0.53
2:B:210:VAL:HB	2:B:211:PRO:HD2	1.91	0.53
3:C:58:THR:C	3:C:60:THR:H	2.15	0.53
3:C:125:THR:HG23	3:C:198:ILE:HG22	1.91	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
2:B:83:PRO:HB2	2:B:96:MET:HE3	1.89	0.53
1:A:201:GLN:O	1:A:203:GLN:HB2	2.07	0.53
3:C:130:LEU:HD23	3:C:131:LEU:N	2.23	0.53
2:B:172:TYR:O	2:B:174:LEU:N	2.41	0.53
3:C:209:LEU:N	3:C:209:LEU:CD1	2.70	0.53
1:A:101:LEU:C	1:A:103:GLU:H	2.17	0.53
2:B:186:ILE:HG23	2:B:187:PHE:CD1	2.44	0.53
3:C:106:PHE:HB3	3:C:221:ARG:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:SER:HB2	1:A:48:GLU:HB3	1.90	0.53
1:A:206:GLY:C	1:A:208:ALA:N	2.66	0.52
2:B:174:LEU:C	2:B:176:PHE:H	2.15	0.52
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
2:B:66:LEU:HD12	2:B:244:ILE:CG2	2.39	0.52
3:C:52:LEU:O	3:C:97:THR:HG22	2.09	0.52
3:C:56:ASN:HB3	3:C:67:MET:HA	1.90	0.52
3:C:109:TRP:HB2	3:C:220:LEU:CD1	2.40	0.52
2:B:34:ALA:C	2:B:36:GLY:H	2.18	0.52
5:E:8:ILE:CG2	5:E:17:CYS:SG	2.98	0.52
1:A:19:ASN:N	1:A:19:ASN:HD22	2.06	0.52
2:B:172:TYR:CG	2:B:173:TRP:N	2.77	0.52
3:C:122:THR:HG23	3:C:124:ASN:N	2.25	0.52
3:C:94:LEU:O	3:C:95:ALA:C	2.53	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
1:A:108:ARG:HH12	1:A:258:ALA:HA	1.76	0.51
3:C:198:ILE:HB	3:C:199:PRO:HD2	1.91	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
1:A:228:LYS:O	1:A:229:VAL:CG1	2.59	0.51
4:D:6:ARG:CG	4:D:7:GLN:N	2.72	0.51
1:A:85:THR:HG21	1:A:92:GLU:OE1	2.10	0.51
1:A:249:PRO:HD3	2:B:187:PHE:CE1	2.38	0.51
1:A:171:TRP:CD1	1:A:178:PRO:HD3	2.46	0.51
3:C:42:ASN:ND2	3:C:42:ASN:C	2.61	0.51
2:B:42:LEU:HD12	2:B:43:SER:H	1.76	0.51
3:C:227:ASN:C	3:C:229:HIS:H	2.19	0.51
2:B:97:PHE:O	2:B:257:ARG:NH1	2.43	0.51
3:C:143:THR:HG23	3:C:146:ASP:HB2	1.92	0.50
1:A:193:MET:HA	1:A:193:MET:CE	2.36	0.50
1:A:99:ILE:HG13	1:A:215:SER:HA	1.93	0.50
1:A:180:PHE:CD1	1:A:180:PHE:C	2.89	0.50
2:B:134:SER:HA	2:B:168:PRO:HA	1.94	0.50
1:A:111:PHE:O	1:A:113:LEU:N	2.44	0.50
1:A:212:ASN:O	1:A:213:MET:HE3	2.12	0.50
2:B:86:LEU:CA	2:B:89:MET:HG2	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:216:ARG:HG2	2:B:217:SER:N	2.26	0.50
3:C:42:ASN:HD22	3:C:43:LEU:N	2.10	0.50
1:A:155:SER:C	1:A:157:ASP:H	2.20	0.50
2:B:51:ASP:O	2:B:53:PRO:HD3	2.12	0.50
1:A:143:TYR:OH	1:A:233:THR:CG2	2.55	0.50
1:A:161:TRP:CH2	1:A:219:ARG:HB3	2.47	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:138:HIS:O	1:A:222:THR:HG21	2.11	0.50
1:A:206:GLY:C	1:A:208:ALA:H	2.19	0.50
1:A:23:SER:CB	1:A:53:THR:CG2	2.89	0.49
2:B:42:LEU:HD21	2:B:211:PRO:HB3	1.94	0.49
2:B:87:LYS:HE2	2:B:150:GLY:CA	2.41	0.49
3:C:141:PRO:HG2	3:C:189:THR:HG21	1.94	0.49
1:A:204:ASN:O	1:A:206:GLY:N	2.45	0.49
2:B:198:ASN:C	2:B:198:ASN:OD1	2.54	0.49
1:A:51:ILE:O	1:A:51:ILE:HG13	2.11	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
3:C:162:THR:HG22	3:C:163:ILE:H	1.77	0.49
1:A:142:GLN:HG3	1:A:170:PHE:HE1	1.74	0.49
2:B:16:ILE:HD13	2:B:16:ILE:N	2.27	0.49
1:A:110:LYS:O	1:A:113:LEU:N	2.44	0.49
2:B:72:SER:C	2:B:74:SER:H	2.20	0.49
2:B:221:TRP:O	2:B:222:SER:HB2	2.13	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
1:A:161:TRP:CE3	1:A:219:ARG:CG	2.94	0.48
1:A:176:ALA:O	1:A:177:TYR:C	2.56	0.48
2:B:23:ILE:HG21	2:B:109:HIS:CD2	2.49	0.48
2:B:132:ILE:HG22	2:B:176:PHE:O	2.12	0.48
2:B:161:ARG:HB2	2:B:167:GLN:HG3	1.93	0.48
2:B:186:ILE:HG13	2:B:186:ILE:O	2.13	0.48
1:A:18:PRO:C	1:A:19:ASN:HD22	2.22	0.48
2:B:136:LEU:HB2	2:B:140:VAL:HG21	1.95	0.48
1:A:87:ALA:HB2	5:E:25:ASP:HB2	1.94	0.48
1:A:114:PHE:O	1:A:193:MET:HG3	2.13	0.48
2:B:182:GLY:HA2	3:C:52:LEU:HB2	1.96	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:10:CYS:C	5:E:12:ALA:N	2.72	0.48
2:B:80:TRP:CH2	2:B:225:ILE:HD13	2.48	0.48
3:C:215:CYS:O	3:C:216:LYS:C	2.57	0.48
1:A:24:ASN:CB	1:A:25:PRO:HD2	2.43	0.48
1:A:77:ILE:CA	1:A:104:MET:HG3	2.44	0.48
1:A:161:TRP:CZ3	1:A:219:ARG:CG	2.96	0.48
1:A:245:TRP:CD1	3:C:36:ILE:O	2.67	0.48
2:B:112:CYS:SG	2:B:242:ILE:HD13	2.52	0.48
2:B:115:SER:HB3	2:B:118:HIS:ND1	2.28	0.48
2:B:112:CYS:SG	2:B:242:ILE:HD11	2.51	0.48
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
4:D:29:ILE:C	4:D:30:ASN:HD22	2.22	0.47
5:E:19:PRO:O	5:E:20:VAL:C	2.57	0.47
1:A:21:ASN:O	1:A:22:SER:C	2.56	0.47
1:A:232:MET:C	1:A:232:MET:CE	2.87	0.47
3:C:76:ILE:O	3:C:195:ARG:HG3	2.15	0.47
1:A:148:PRO:HD3	1:A:214:GLY:HA3	1.96	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
3:C:194:THR:HB	3:C:195:ARG:H	1.49	0.47
1:A:142:GLN:CG	1:A:170:PHE:CE1	2.98	0.47
3:C:6:ILE:N	3:C:6:ILE:HD12	2.29	0.47
4:D:32:PHE:HB3	4:D:37:SER:CB	2.44	0.47
1:A:62:ARG:O	1:A:65:MET:N	2.48	0.47
1:A:202:ASP:N	1:A:202:ASP:OD2	2.46	0.47
2:B:107:THR:N	2:B:247:SER:O	2.31	0.47
3:C:58:THR:C	3:C:60:THR:N	2.68	0.47
3:C:119:PHE:HB2	3:C:157:VAL:HG21	1.97	0.47
1:A:19:ASN:CG	1:A:58:THR:H	2.23	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:30:PRO:O	3:C:31:THR:C	2.58	0.47
3:C:162:THR:CG2	3:C:163:ILE:N	2.78	0.47
2:B:46:ASP:O	2:B:47:ALA:C	2.58	0.46
2:B:87:LYS:HE2	2:B:150:GLY:HA2	1.96	0.46
3:C:124:ASN:N	3:C:124:ASN:HD22	2.13	0.46
2:B:175:ASN:C	2:B:176:PHE:HD2	2.24	0.46
1:A:228:LYS:C	1:A:229:VAL:HG13	2.40	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
1:A:237:HIS:C	1:A:237:HIS:HD1	2.23	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
1:A:180:PHE:C	1:A:180:PHE:HD1	2.24	0.46
2:B:72:SER:C	2:B:74:SER:N	2.71	0.46
2:B:174:LEU:C	2:B:176:PHE:N	2.72	0.46
3:C:121:GLY:O	3:C:122:THR:C	2.59	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
3:C:87:THR:O	3:C:88:ASP:C	2.59	0.46
1:A:17:VAL:O	1:A:17:VAL:HG23	2.15	0.46
2:B:105:GLY:CA	2:B:204:ALA:O	2.63	0.46
1:A:80:SER:C	1:A:232:MET:HE1	2.41	0.45
1:A:221:VAL:O	1:A:222:THR:C	2.59	0.45
2:B:155:GLU:HB3	2:B:157:LYS:CE	2.46	0.45
2:B:43:SER:C	2:B:45:LYS:N	2.70	0.45
2:B:93:GLY:O	2:B:96:MET:CB	2.64	0.45
3:C:117:PHE:O	3:C:162:THR:HA	2.16	0.45
3:C:140:GLU:N	3:C:187:TYR:HE2	2.14	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:84:VAL:HG23	1:A:229:VAL:O	2.17	0.45
1:A:146:VAL:CG1	1:A:150:ALA:HB3	2.46	0.45
2:B:14:ILE:CG1	2:B:16:ILE:HD11	2.46	0.45
4:D:32:PHE:CB	4:D:37:SER:HB3	2.46	0.45
1:A:141:MET:HB3	1:A:143:TYR:CE2	2.51	0.45
1:A:161:TRP:CB	1:A:219:ARG:HH21	2.26	0.45
1:A:263:PHE:N	1:A:263:PHE:CD2	2.84	0.45
1:A:267:ASP:O	1:A:268:ARG:HG3	2.16	0.45
2:B:19:GLY:HA2	2:B:58:THR:HG22	1.98	0.45
2:B:118:HIS:O	3:C:122:THR:HA	2.16	0.45
3:C:9:GLY:O	3:C:10:SER:O	2.35	0.45
3:C:36:ILE:HD12	3:C:37:PRO:HD2	1.99	0.45
5:E:22:TRP:HA	5:E:25:ASP:CG	2.42	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:67:LEU:HD23	1:A:67:LEU:HA	1.80	0.45
1:A:75:GLY:CA	1:A:107:ILE:HD11	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:2:LEU:C	3:C:2:LEU:CD2	2.90	0.45
3:C:12:GLN:O	3:C:12:GLN:HG3	2.16	0.45
1:A:145:TYR:CD1	1:A:145:TYR:C	2.95	0.45
2:B:182:GLY:N	2:B:184:ILE:HG22	2.23	0.45
3:C:118:MET:HG3	3:C:161:SER:HB2	1.98	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
1:A:50:VAL:O	1:A:50:VAL:CG1	2.65	0.44
2:B:80:TRP:HE3	2:B:80:TRP:H	1.66	0.44
2:B:172:TYR:CD2	2:B:172:TYR:N	2.85	0.44
3:C:155:TRP:CD1	3:C:155:TRP:C	2.93	0.44
1:A:70:PHE:CD2	1:A:71:LEU:CD2	3.00	0.44
2:B:83:PRO:O	2:B:84:ASP:HB3	2.17	0.44
3:C:69:SER:HB2	3:C:207:ARG:HH11	1.81	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
1:A:249:PRO:HD3	2:B:186:ILE:CG2	2.47	0.44
3:C:39:GLU:C	3:C:40:VAL:HG23	2.42	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
2:B:229:CYS:HA	2:B:230:PRO:HD2	1.72	0.44
4:D:6:ARG:CG	4:D:7:GLN:H	2.30	0.44
2:B:23:ILE:CG2	2:B:24:THR:N	2.81	0.44
2:B:28:VAL:HG12	2:B:199:SER:OG	2.18	0.44
3:C:82:ILE:HG12	3:C:192:TYR:HE1	1.81	0.44
1:A:119:PHE:O	1:A:184:PHE:HB2	2.18	0.43
1:A:213:MET:HE2	1:A:213:MET:HA	2.00	0.43
2:B:155:GLU:HB3	2:B:157:LYS:HE2	2.00	0.43
4:D:6:ARG:HD2	4:D:7:GLN:C	2.43	0.43
2:B:192:ILE:HD13	2:B:199:SER:HA	1.99	0.43
3:C:99:ILE:O	3:C:100:GLY:C	2.60	0.43
1:A:194:PHE:N	1:A:194:PHE:CD1	2.86	0.43
2:B:13:ILE:N	2:B:13:ILE:CD1	2.78	0.43
2:B:34:ALA:C	2:B:36:GLY:N	2.74	0.43
1:A:54:ARG:HD3	1:A:55:TYR:O	2.18	0.43
2:B:34:ALA:HB2	2:B:204:ALA:HA	2.01	0.43
3:C:88:ASP:O	3:C:91:SER:CB	2.66	0.43
1:A:148:PRO:HD3	1:A:214:GLY:N	2.34	0.43
3:C:165:MET:HG2	3:C:166:VAL:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:127:ILE:HD12	2:B:127:ILE:N	2.33	0.43
2:B:103:ARG:HG3	2:B:206:TYR:CD2	2.54	0.43
2:B:112:CYS:SG	2:B:242:ILE:HD12	2.58	0.43
2:B:181:LEU:HD12	2:B:184:ILE:HG21	2.00	0.43
2:B:249:MET:HE3	2:B:249:MET:HB2	1.90	0.43
3:C:109:TRP:HB3	3:C:220:LEU:HD12	2.01	0.43
3:C:113:LEU:HB2	3:C:167:VAL:HB	2.01	0.43
5:E:12:ALA:HB3	5:E:30:CYS:SG	2.58	0.43
2:B:28:VAL:CG1	2:B:199:SER:OG	2.67	0.43
3:C:56:ASN:O	3:C:67:MET:HA	2.18	0.43
1:A:38:GLU:C	1:A:40:GLY:N	2.76	0.42
1:A:53:THR:OG1	1:A:54:ARG:N	2.52	0.42
2:B:92:PHE:O	2:B:93:GLY:C	2.61	0.42
1:A:59:SER:OG	1:A:60:GLN:N	2.52	0.42
1:A:124:THR:HG21	3:C:13:PHE:CD1	2.54	0.42
2:B:56:PRO:HG2	2:B:60:SER:CB	2.49	0.42
2:B:61:ASN:OD1	2:B:250:CYS:N	2.52	0.42
3:C:106:PHE:O	3:C:178:THR:OG1	2.33	0.42
3:C:166:VAL:HG12	3:C:167:VAL:N	2.34	0.42
3:C:199:PRO:HD2	3:C:202:THR:OG1	2.19	0.42
1:A:111:PHE:CD1	1:A:111:PHE:N	2.87	0.42
1:A:118:ARG:O	1:A:119:PHE:HB3	2.19	0.42
1:A:143:TYR:CD1	1:A:218:SER:HB3	2.55	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
3:C:84:SER:HA	3:C:188:ILE:O	2.19	0.42
1:A:85:THR:HG23	1:A:85:THR:O	2.18	0.42
2:B:30:ASN:O	2:B:31:ALA:C	2.63	0.42
2:B:257:ARG:HG2	2:B:258:ALA:H	1.84	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:129:ILE:HD11	1:A:171:TRP:HH2	1.84	0.42
2:B:83:PRO:CB	2:B:96:MET:HE3	2.49	0.42
2:B:84:ASP:O	2:B:86:LEU:N	2.52	0.42
3:C:7:THR:HA	3:C:8:PRO:HD2	1.85	0.42
3:C:125:THR:HG22	3:C:196:LEU:HD11	2.00	0.42
3:C:184:THR:HG22	3:C:185:SER:N	2.34	0.42
2:B:107:THR:N	2:B:249:MET:HE2	2.32	0.42
3:C:208:LEU:C	3:C:209:LEU:HD12	2.43	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:34:ASP:O	4:D:37:SER:HB2	2.19	0.42
1:A:15:LEU:C	1:A:15:LEU:CD2	2.93	0.42
2:B:13:ILE:HG22	2:B:14:ILE:N	2.27	0.42
2:B:162:LEU:H	2:B:162:LEU:HG	1.57	0.42
3:C:26:PRO:HA	4:D:34:ASP:OD1	2.20	0.42
1:A:40:GLY:HA3	2:B:189:HIS:O	2.20	0.42
1:A:68:GLU:OE1	1:A:241:HIS:N	2.37	0.42
1:A:71:LEU:C	1:A:73:ARG:H	2.28	0.41
3:C:53:VAL:O	3:C:55:ILE:CD1	2.52	0.41
3:C:187:TYR:C	3:C:188:ILE:HG13	2.45	0.41
1:A:23:SER:HB3	1:A:53:THR:CG2	2.41	0.41
1:A:265:ILE:HD12	1:A:266:GLU:N	2.30	0.41
5:E:4:ARG:HB3	5:E:5:ILE:H	1.58	0.41
1:A:116:TYR:OH	2:B:208:ASN:HA	2.20	0.41
1:A:188:ALA:HB1	2:B:210:VAL:HG12	2.02	0.41
1:A:280:ILE:C	1:A:282:THR:H	2.27	0.41
3:C:81:LYS:HZ1	3:C:140:GLU:HG2	1.85	0.41
3:C:90:ALA:HB3	3:C:178:THR:O	2.20	0.41
3:C:231:GLN:HG3	3:C:235:ILE:HD11	2.02	0.41
1:A:77:ILE:HD11	1:A:235:ILE:HG21	2.00	0.41
1:A:148:PRO:HD3	1:A:213:MET:C	2.45	0.41
1:A:101:LEU:O	1:A:103:GLU:N	2.54	0.41
1:A:245:TRP:CE3	1:A:245:TRP:N	2.88	0.41
3:C:1:GLY:O	3:C:3:PRO:HD3	2.20	0.41
1:A:16:VAL:CG1	1:A:17:VAL:H	2.33	0.41
1:A:48:GLU:CG	1:A:53:THR:HG21	2.47	0.41
2:B:121:THR:HB	2:B:228:ILE:HG23	2.01	0.41
3:C:82:ILE:HD12	3:C:190:CYS:C	2.45	0.41
3:C:103:SER:C	3:C:105:TYR:N	2.79	0.41
3:C:110:THR:O	3:C:219:CYS:N	2.54	0.41
1:A:38:GLU:O	1:A:39:THR:C	2.63	0.41
1:A:119:PHE:CD1	1:A:119:PHE:C	2.98	0.41
1:A:132:LEU:H	1:A:229:VAL:HG12	1.86	0.41
1:A:223:GLU:O	1:A:224:LYS:C	2.64	0.41
1:A:249:PRO:HD3	2:B:186:ILE:HG21	2.03	0.41
3:C:44:VAL:HG22	3:C:48:GLN:NE2	2.36	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
1:A:37:ALA:O	1:A:38:GLU:C	2.63	0.41
1:A:70:PHE:CD2	1:A:71:LEU:HD21	2.56	0.41
1:A:278:PRO:O	3:C:58:THR:HG22	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:185:THR:C	2:B:187:PHE:N	2.79	0.41
5:E:18:ILE:HG13	5:E:30:CYS:H	1.85	0.41
1:A:23:SER:HB2	1:A:53:THR:HG22	2.03	0.41
1:A:193:MET:C	1:A:194:PHE:CD1	2.99	0.41
1:A:231:ILE:O	1:A:231:ILE:HG22	2.20	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
3:C:14:LEU:HD12	3:C:15:THR:N	2.36	0.41
1:A:220:ILE:O	1:A:220:ILE:HG23	2.21	0.41
2:B:185:THR:C	2:B:187:PHE:H	2.28	0.41
3:C:83:PHE:CD2	3:C:84:SER:N	2.89	0.41
3:C:166:VAL:CG1	3:C:167:VAL:N	2.84	0.41
1:A:92:GLU:O	1:A:156:ARG:HB2	2.21	0.40
2:B:60:SER:C	2:B:62:ARG:N	2.79	0.40
3:C:103:SER:HA	3:C:220:LEU:CD2	2.48	0.40
3:C:169:TRP:HZ2	3:C:174:HIS:O	1.95	0.40
5:E:31:ASP:O	5:E:33:GLY:N	2.52	0.40
1:A:185:LEU:HB2	1:A:186:SER:H	1.67	0.40
2:B:42:LEU:HD12	2:B:43:SER:N	2.36	0.40
2:B:103:ARG:HG3	2:B:206:TYR:CG	2.56	0.40
2:B:132:ILE:H	2:B:132:ILE:HG13	1.58	0.40
2:B:257:ARG:HG2	2:B:258:ALA:N	2.36	0.40
3:C:89:VAL:HG23	3:C:90:ALA:N	2.36	0.40
2:B:181:LEU:O	3:C:68:TYR:CE1	2.74	0.40
2:B:218:HIS:CD2	2:B:218:HIS:C	3.00	0.40
2:B:225:ILE:O	2:B:226:ILE:HG13	2.21	0.40
3:C:131:LEU:HB3	3:C:165:MET:HE2	2.02	0.40
3:C:169:TRP:CE2	3:C:171:SER:HB3	2.57	0.40
1:A:247:PRO:HG2	2:B:186:ILE:HD11	2.03	0.40
1:A:262:ASN:ND2	2:B:134:SER:OG	2.54	0.40
1:A:282:THR:O	1:A:282:THR:HG22	2.22	0.40
2:B:71:TRP:CE2	2:B:231:LEU:HB2	2.57	0.40
2:B:106:TYR:CA	2:B:249:MET:CE	2.95	0.40
2:B:167:GLN:OE1	2:B:167:GLN:HA	2.21	0.40
3:C:83:PHE:CD2	3:C:83:PHE:C	2.99	0.40
1:A:46:GLN:O	1:A:47:PRO:C	2.65	0.40
1:A:59:SER:O	1:A:60:GLN:C	2.65	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:240:ILE:HD12	2:B:240:ILE:O	2.22	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	267/289 (92%)	203 (76%)	42 (16%)	22 (8%)	0	8
2	B	248/261 (95%)	187 (75%)	39 (16%)	22 (9%)	0	7
3	C	235/237 (99%)	173 (74%)	43 (18%)	19 (8%)	1	8
4	D	21/68 (31%)	16 (76%)	4 (19%)	1 (5%)	2	16
5	E	37/39 (95%)	15 (40%)	17 (46%)	5 (14%)	0	3
All	All	808/894 (90%)	594 (74%)	145 (18%)	69 (8%)	0	7

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

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
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
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

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Mol	Chain	Res	Type
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 [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	238/257 (93%)	200 (84%)	38 (16%)	<b>2</b> <b>14</b>
2	B	216/226 (96%)	185 (86%)	31 (14%)	<b>3</b> <b>18</b>
3	C	210/210 (100%)	178 (85%)	32 (15%)	<b>3</b> <b>16</b>
4	D	19/59 (32%)	10 (53%)	9 (47%)	<b>0</b> <b>0</b>
5	E	34/34 (100%)	25 (74%)	9 (26%)	<b>0</b> <b>3</b>
All	All	717/786 (91%)	598 (83%)	119 (17%)	<b>2</b> <b>13</b>

All (119) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	LEU
1	A	19	ASN
1	A	53	THR
1	A	54	ARG
1	A	55	TYR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	60	GLN
1	A	61	THR
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	169	VAL
1	A	179	ARG
1	A	185	LEU
1	A	189	SER
1	A	200	GLU
1	A	201	GLN
1	A	203	GLN
1	A	207	THR
1	A	213	MET
1	A	215	SER
1	A	219	ARG
1	A	226	ILE
1	A	231	ILE
1	A	232	MET
1	A	233	THR
1	A	237	HIS
1	A	253	LEU
1	A	257	ARG
1	A	261	THR
1	A	269	SER
1	A	275	VAL
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	80	TRP
2	B	86	LEU
2	B	91	ILE
2	B	106	TYR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	B	112	CYS
2	B	115	SER
2	B	116	LYS
2	B	124	VAL
2	B	126	LEU
2	B	132	ILE
2	B	134	SER
2	B	137	HIS
2	B	152	THR
2	B	162	LEU
2	B	174	LEU
2	B	180	LEU
2	B	184	ILE
2	B	192	ILE
2	B	195	ARG
2	B	197	ASN
2	B	201	THR
2	B	203	ILE
2	B	216	ARG
2	B	220	ASN
2	B	225	ILE
2	B	238	ASN
3	C	21	SER
3	C	31	THR
3	C	34	ILE
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	96	THR
3	C	99	ILE
3	C	103	SER
3	C	110	THR
3	C	122	THR
3	C	124	ASN
3	C	127	VAL
3	C	134	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	C	142	THR
3	C	143	THR
3	C	157	VAL
3	C	165	MET
3	C	194	THR
3	C	201	GLN
3	C	202	THR
3	C	205	THR
3	C	209	LEU
3	C	211	PHE
3	C	220	LEU
3	C	230	LEU
4	D	4	VAL
4	D	6	ARG
4	D	27	PHE
4	D	28	ASN
4	D	29	ILE
4	D	30	ASN
4	D	33	LYS
4	D	41	SER
4	D	43	LEU
5	E	7	GLU
5	E	10	CYS
5	E	13	HIS
5	E	16	GLN
5	E	17	CYS
5	E	20	VAL
5	E	32	SER
5	E	39	CYS
5	E	41	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	19	ASN
1	A	60	GLN
1	A	138	HIS
1	A	162	GLN
1	A	201	GLN
2	B	15	GLN
2	B	26	GLN
2	B	131	GLN

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Mol	Chain	Res	Type
2	B	193	ASN
2	B	197	ASN
2	B	219	ASN
2	B	238	ASN
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
3	C	231	GLN
4	D	30	ASN
4	D	38	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	-	13,13,13	0.81	1 (7%)	13,13,13	1.21	2 (15%)

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	-	-	6/11/11/11	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	290	DAO	O2-C1	-2.11	1.23	1.30

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	290	DAO	O2-C1-C2	2.63	122.30	114.00
6	A	290	DAO	O1-C1-C2	-2.33	115.71	123.09

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	290	DAO	C1-C2-C3-C4
6	A	290	DAO	C5-C6-C7-C8
6	A	290	DAO	C2-C3-C4-C5
6	A	290	DAO	C11-C10-C9-C8
6	A	290	DAO	O2-C1-C2-C3
6	A	290	DAO	O1-C1-C2-C3

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

There are no chain breaks in this entry.

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

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	269/289 (93%)	-0.10	2 (0%) 84 63	23, 23, 23, 23	0
2	B	249/261 (95%)	-0.08	0 100 100	20, 23, 23, 23	0
3	C	237/237 (100%)	-0.14	2 (0%) 82 60	20, 23, 23, 23	0
4	D	25/68 (36%)	0.04	0 100 100	23, 23, 23, 23	0
5	E	39/39 (100%)	-0.15	0 100 100	23, 23, 23, 23	0
All	All	819/894 (91%)	-0.10	4 (0%) 87 68	20, 23, 23, 23	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	1	GLY	2.4
1	A	256	THR	2.1
3	C	120	CYS	2.1
1	A	90	ASN	2.0

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

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

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
6	DAO	A	290	14/14	0.97	0.11	22,22,22,22	0
7	CA	E	50	1/1	0.98	0.07	22,22,22,22	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.