



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 02:28 AM UTC

PDB ID : 1V9U / pdb_00001v9u
Title : Human Rhinovirus 2 bound to a fragment of its cellular receptor protein
Authors : Verdaguer, N.; Fita, I.; Reithmayer, M.; Moser, R.; Blaas, D.
Deposited on : 2004-02-03
Resolution : 3.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

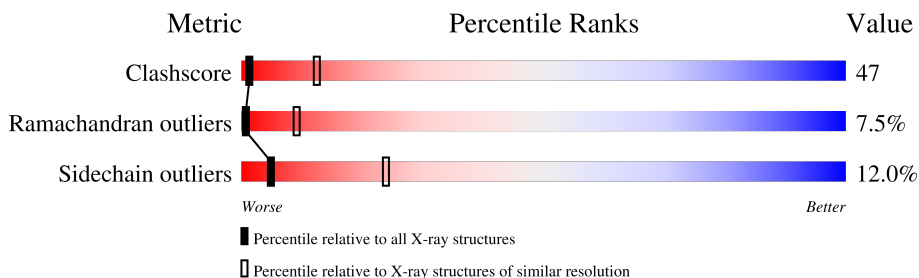
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	1	289	35% 41% 16% 7%
2	2	261	33% 46% 17% .
3	3	237	35% 49% 14% .
4	4	68	15% 10% 12% 63%
5	5	41	68% 24% 5%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6451 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 Coat protein VP1.

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

- Molecule 2 is a protein called Coat protein VP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	2	250	Total	C	N	O	S	8	0	0
			1961	1245	339	369	8			

- Molecule 3 is a protein called Coat protein VP3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	3	237	Total	C	N	O	S	0	0	0
			1834	1172	304	346	12			

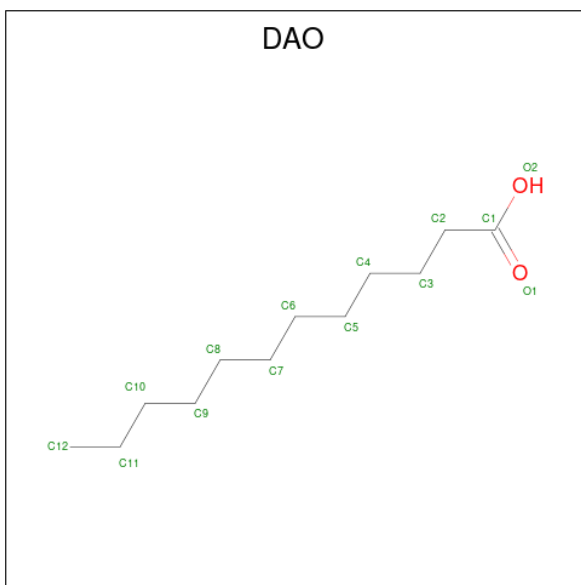
- Molecule 4 is a protein called Coat protein VP4.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	4	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	5	39	Total	C	N	O	S	0	0	0
			292	166	54	66	6			

- Molecule 6 is LAURIC ACID (CCD ID: DAO) (formula: C₁₂H₂₄O₂).



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

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

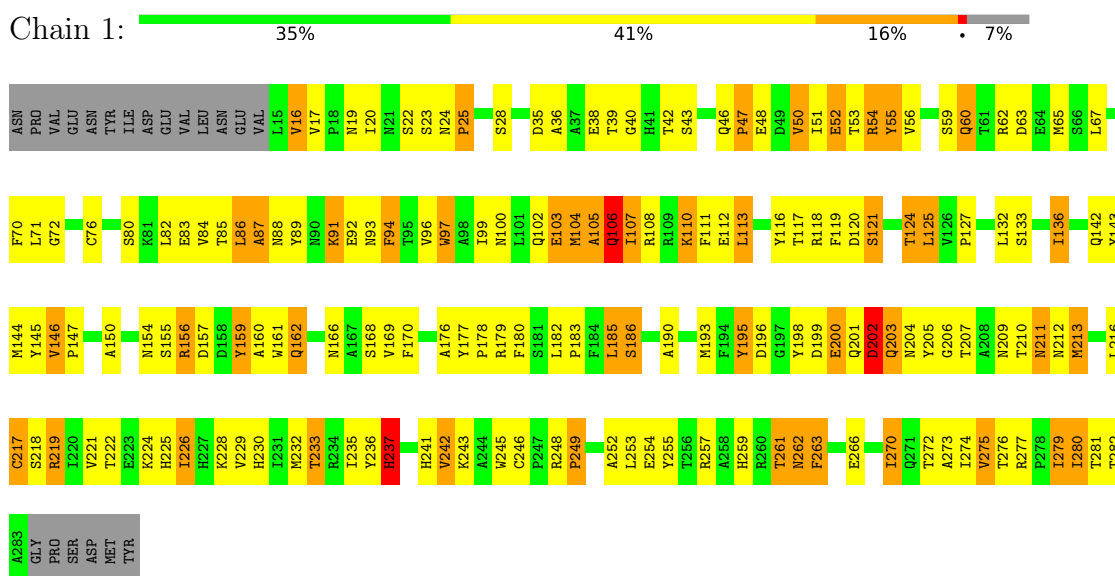
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	5	1	Total	Ca	0	0
			1	1		

3 Residue-property plots

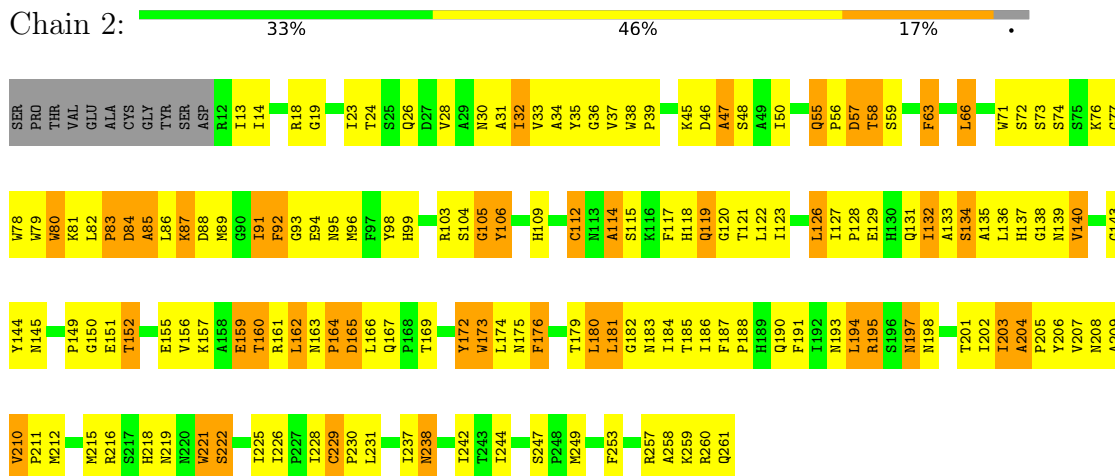
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

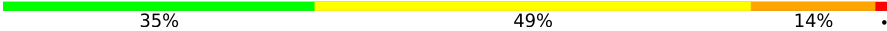
• Molecule 1: Coat protein VP1

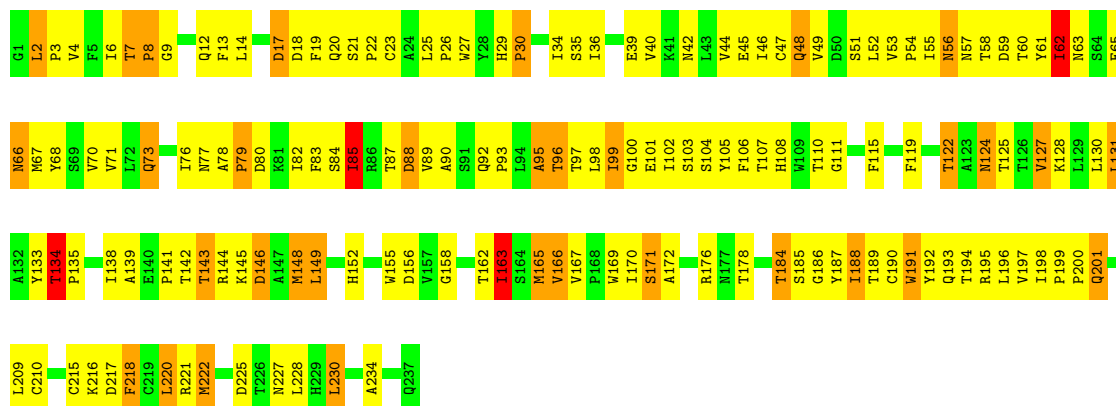


• Molecule 2: Coat protein VP2



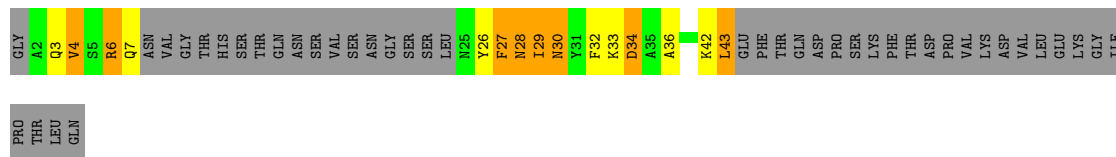
• Molecule 3: Coat protein VP3

Chain 3:  35% 49% 14% .



• Molecule 4: Coat protein VP4

Chain 4:  15% 10% 12% 63%



• Molecule 5: LDL-receptor class A 3

Chain 5:  68% 24% 5%



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 2 21	Depositor
Cell constants a, b, c, α , β , γ	313.10Å 348.79Å 380.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.60	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-3.60)	Depositor
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.285 , 0.295	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6451	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

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	1	0.73	0/2211	1.15	20/3011 (0.7%)
2	2	0.79	0/2016	1.23	21/2752 (0.8%)
3	3	0.78	1/1884 (0.1%)	1.16	10/2579 (0.4%)
4	4	1.02	0/196	1.27	4/261 (1.5%)
5	5	1.12	1/296 (0.3%)	1.14	0/399
All	All	0.79	2/6603 (0.0%)	1.18	55/9002 (0.6%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	5	118	ILE	CA-CB	6.51	1.61	1.54
3	3	85	ILE	CA-CB	-5.46	1.49	1.55

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	163	ASN	CA-C-N	10.59	133.07	119.84
2	2	163	ASN	C-N-CA	10.59	133.07	119.84
1	1	242	VAL	N-CA-C	10.32	125.20	109.20
2	2	183	ASN	N-CA-C	-9.69	98.58	113.02
3	3	7	THR	N-CA-C	8.18	122.49	110.14
1	1	16	VAL	N-CA-C	8.03	120.54	109.46
3	3	134	THR	CA-C-N	8.02	128.64	120.38
3	3	134	THR	C-N-CA	8.02	128.64	120.38
2	2	181	LEU	N-CA-C	-7.87	98.81	110.23
3	3	166	VAL	N-CA-C	7.87	119.81	108.48
1	1	226	ILE	N-CA-C	7.60	121.71	113.43
2	2	204	ALA	CA-C-N	7.51	129.02	120.98
2	2	204	ALA	C-N-CA	7.51	129.02	120.98
3	3	62	ILE	N-CA-C	7.43	124.80	109.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	166	LEU	N-CA-C	-7.31	102.36	112.30
1	1	103	GLU	N-CA-C	7.28	121.87	112.92
2	2	48	SER	N-CA-C	-7.25	103.54	113.18
1	1	146	VAL	CA-C-N	6.84	127.42	120.38
1	1	146	VAL	C-N-CA	6.84	127.42	120.38
1	1	28	SER	N-CA-C	6.83	119.34	110.53
4	4	34	ASP	N-CA-C	6.80	120.60	109.72
3	3	53	VAL	N-CA-C	6.74	114.56	107.76
1	1	225	HIS	N-CA-C	6.43	116.94	108.07
4	4	4	VAL	N-CA-C	6.17	122.17	109.34
1	1	104	MET	N-CA-C	6.12	120.81	109.24
1	1	162	GLN	N-CA-C	-6.08	104.73	111.36
2	2	55	GLN	CA-C-N	6.08	127.44	119.84
2	2	55	GLN	C-N-CA	6.08	127.44	119.84
1	1	86	LEU	N-CA-C	-5.97	101.44	110.28
4	4	36	ALA	N-CA-C	5.83	118.39	111.33
2	2	28	VAL	N-CA-C	5.80	116.53	108.23
2	2	57	ASP	N-CA-C	5.78	116.55	108.00
3	3	191	TRP	N-CA-C	5.77	117.37	109.18
3	3	152	HIS	N-CA-C	5.67	116.57	108.74
2	2	105	GLY	N-CA-C	-5.64	102.49	111.18
1	1	40	GLY	N-CA-C	-5.59	107.30	115.63
1	1	237	HIS	N-CA-C	5.58	117.53	108.26
3	3	188	ILE	CB-CA-C	-5.58	104.57	111.32
4	4	32	PHE	N-CA-C	5.55	118.86	109.76
1	1	200	GLU	N-CA-C	-5.47	106.56	113.18
1	1	235	ILE	N-CA-C	5.46	115.72	107.75
2	2	182	GLY	N-CA-C	-5.43	107.52	114.85
2	2	221	TRP	N-CA-C	5.30	116.76	109.29
1	1	97	TRP	N-CA-C	5.28	116.64	107.93
1	1	121	SER	N-CA-C	5.24	117.78	109.50
1	1	50	VAL	N-CA-C	5.21	118.15	113.10
3	3	216	LYS	N-CA-C	-5.17	105.13	111.75
1	1	249	PRO	N-CA-C	-5.17	105.05	110.58
2	2	210	VAL	CA-C-N	5.14	126.27	119.84
2	2	210	VAL	C-N-CA	5.14	126.27	119.84
2	2	92	PHE	N-CA-C	-5.14	105.57	111.07
2	2	104	SER	N-CA-C	5.12	116.31	108.42
2	2	229	CYS	CA-C-N	5.07	126.17	119.84
2	2	229	CYS	C-N-CA	5.07	126.17	119.84
1	1	133	SER	N-CA-C	-5.02	102.03	109.96

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	1	2155	0	2080	218	0
2	2	1961	0	1902	193	0
3	3	1834	0	1817	177	0
4	4	194	0	180	32	0
5	5	292	0	238	6	0
6	1	14	0	23	0	0
7	5	1	0	0	0	0
All	All	6451	0	6240	592	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 47.

All (592) 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)
2:2:91:ILE:H	2:2:91:ILE:HD12	1.14	1.13
3:3:143:THR:HG23	3:3:146:ASP:HB2	1.32	1.06
3:3:138:ILE:HG12	3:3:139:ALA:H	1.18	1.03
2:2:13:ILE:HG22	2:2:14:ILE:H	1.23	1.01
1:1:136:ILE:HD13	1:1:136:ILE:H	1.27	0.99
2:2:193:ASN:H	2:2:197:ASN:HD21	1.02	0.99
3:3:122:THR:HG23	3:3:124:ASN:H	1.26	0.98
3:3:127:VAL:HG22	3:3:128:LYS:H	1.25	0.97
1:1:106:GLN:HA	1:1:106:GLN:HE21	1.31	0.95
1:1:54:ARG:HD3	1:1:55:TYR:H	1.30	0.94
2:2:91:ILE:HD12	2:2:91:ILE:N	1.83	0.93
2:2:135:ALA:HB2	2:2:169:THR:HA	1.46	0.92
3:3:162:THR:HG22	3:3:163:ILE:H	1.35	0.92
3:3:42:ASN:HD22	3:3:44:VAL:HG12	1.33	0.91
3:3:122:THR:HG22	3:3:125:THR:OG1	1.71	0.90
3:3:162:THR:HG22	3:3:163:ILE:N	1.85	0.90
1:1:270:ILE:HD12	1:1:270:ILE:H	1.35	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:257:ARG:HG2	2:2:258:ALA:H	1.36	0.88
1:1:143:TYR:OH	1:1:233:THR:HG21	1.72	0.88
2:2:13:ILE:HG22	2:2:14:ILE:N	1.89	0.88
2:2:82:LEU:HA	2:2:83:PRO:O	1.74	0.87
3:3:127:VAL:HG22	3:3:128:LYS:N	1.88	0.87
2:2:172:TYR:HA	2:2:176:PHE:CE2	2.10	0.87
2:2:257:ARG:HG2	2:2:258:ALA:N	1.89	0.87
1:1:193:MET:HE2	1:1:193:MET:HA	1.58	0.84
4:4:6:ARG:H	4:4:6:ARG:HE	1.25	0.84
1:1:277:ARG:HD3	3:3:57:ASN:HD21	1.42	0.84
3:3:162:THR:CG2	3:3:163:ILE:H	1.89	0.83
2:2:155:GLU:HB3	2:2:157:LYS:HE3	1.57	0.83
2:2:238:ASN:HD22	2:2:238:ASN:H	1.26	0.83
5:5:125:THR:HG22	5:5:126:GLN:H	1.44	0.82
3:3:138:ILE:HG12	3:3:139:ALA:N	1.96	0.81
4:4:29:ILE:HD13	4:4:29:ILE:H	1.46	0.81
2:2:91:ILE:H	2:2:91:ILE:CD1	1.80	0.81
1:1:16:VAL:HG12	1:1:17:VAL:N	1.94	0.80
2:2:84:ASP:O	2:2:86:LEU:N	2.15	0.80
3:3:122:THR:HG23	3:3:124:ASN:N	1.96	0.80
1:1:16:VAL:HG12	1:1:17:VAL:H	1.47	0.80
3:3:155:TRP:CD2	3:3:163:ILE:HG21	2.17	0.79
2:2:136:LEU:CD1	2:2:165:ASP:HA	2.10	0.79
1:1:132:LEU:HB2	1:1:228:LYS:O	1.84	0.78
1:1:198:TYR:CE1	1:1:205:TYR:HB2	2.18	0.77
2:2:38:TRP:CD1	2:2:39:PRO:HD2	2.19	0.77
1:1:199:ASP:HB2	1:1:203:GLN:O	1.84	0.77
1:1:145:TYR:HE1	1:1:147:PRO:HG3	1.48	0.77
4:4:6:ARG:HG2	4:4:7:GLN:H	1.47	0.77
2:2:123:ILE:HG12	2:2:191:PHE:HE1	1.50	0.76
2:2:138:GLY:O	2:2:140:VAL:HG13	1.85	0.76
2:2:203:ILE:HD12	2:2:203:ILE:N	2.01	0.76
2:2:63:PHE:CD2	2:2:247:SER:HB2	2.21	0.76
3:3:127:VAL:CG2	3:3:128:LYS:H	1.99	0.76
2:2:115:SER:HB3	2:2:118:HIS:CE1	2.20	0.75
2:2:136:LEU:HD12	2:2:165:ASP:HA	1.65	0.75
2:2:197:ASN:N	2:2:197:ASN:HD22	1.84	0.75
2:2:23:ILE:HD13	2:2:63:PHE:CD1	2.21	0.74
1:1:276:THR:HG22	3:3:62:ILE:HD11	1.68	0.74
4:4:33:LYS:O	4:4:33:LYS:HG2	1.87	0.74
4:4:43:LEU:N	4:4:43:LEU:HD12	2.02	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:280:ILE:HD13	1:1:280:ILE:H	1.51	0.73
2:2:13:ILE:CG2	2:2:14:ILE:H	2.00	0.73
4:4:29:ILE:HD13	4:4:29:ILE:N	2.03	0.73
3:3:141:PRO:HG2	3:3:189:THR:HG21	1.69	0.73
1:1:145:TYR:CE1	1:1:147:PRO:HG3	2.23	0.72
1:1:76:CYS:HB2	1:1:236:TYR:CE2	2.24	0.72
3:3:110:THR:HA	3:3:169:TRP:CZ3	2.25	0.71
2:2:221:TRP:O	2:2:222:SER:HB2	1.91	0.71
4:4:6:ARG:HG2	4:4:7:GLN:N	2.05	0.70
3:3:51:SER:HB3	3:3:98:LEU:HD12	1.72	0.70
1:1:25:PRO:HD3	1:1:52:GLU:OE2	1.91	0.70
2:2:59:SER:O	2:2:91:ILE:HD13	1.91	0.70
1:1:146:VAL:HG13	1:1:150:ALA:HB3	1.74	0.70
1:1:83:GLU:HG2	1:1:230:HIS:NE2	2.07	0.69
4:4:27:PHE:C	4:4:27:PHE:CD2	2.69	0.69
1:1:54:ARG:CD	1:1:55:TYR:H	2.05	0.69
1:1:242:VAL:HG12	1:1:243:LYS:N	2.06	0.69
3:3:39:GLU:HG2	3:3:40:VAL:H	1.57	0.69
3:3:95:ALA:HB1	3:3:228:LEU:HD21	1.75	0.69
3:3:65:GLU:HG2	3:3:66:ASN:N	2.06	0.69
1:1:102:GLN:HA	1:1:108:ARG:HD2	1.72	0.69
3:3:42:ASN:ND2	3:3:44:VAL:HG12	2.07	0.69
1:1:124:THR:HG21	3:3:13:PHE:CE1	2.28	0.69
1:1:125:LEU:HB2	1:1:178:PRO:HG2	1.74	0.69
3:3:141:PRO:CG	3:3:189:THR:HG21	2.23	0.68
1:1:94:PHE:C	1:1:94:PHE:CD2	2.71	0.68
3:3:90:ALA:HB3	3:3:178:THR:O	1.93	0.68
3:3:138:ILE:CG1	3:3:139:ALA:H	1.97	0.68
1:1:16:VAL:CG1	1:1:17:VAL:H	2.06	0.68
1:1:199:ASP:OD1	1:1:200:GLU:N	2.27	0.68
2:2:95:ASN:HB3	2:2:253:PHE:CE2	2.28	0.68
1:1:89:TYR:CE1	1:1:224:LYS:HA	2.29	0.68
1:1:50:VAL:HG12	1:1:50:VAL:O	1.95	0.67
1:1:203:GLN:O	1:1:204:ASN:HB2	1.94	0.67
1:1:206:GLY:O	1:1:209:ASN:HB2	1.94	0.67
1:1:111:PHE:C	1:1:113:LEU:H	2.02	0.67
2:2:86:LEU:O	2:2:88:ASP:N	2.28	0.67
3:3:77:ASN:O	3:3:78:ALA:HB2	1.95	0.66
2:2:123:ILE:HG12	2:2:191:PHE:CE1	2.29	0.66
1:1:120:ASP:OD1	1:1:183:PRO:HA	1.95	0.66
1:1:54:ARG:HD3	1:1:55:TYR:N	2.09	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:201:GLN:HE21	3:3:201:GLN:HA	1.60	0.66
1:1:159:TYR:O	1:1:162:GLN:HG3	1.96	0.66
4:4:6:ARG:CG	4:4:7:GLN:N	2.57	0.66
1:1:263:PHE:N	1:1:263:PHE:CD2	2.64	0.65
1:1:279:ILE:HD13	1:1:280:ILE:H	1.61	0.65
2:2:84:ASP:O	2:2:87:LYS:N	2.23	0.65
2:2:162:LEU:C	2:2:164:PRO:N	2.52	0.65
3:3:227:ASN:OD1	3:3:228:LEU:HD12	1.96	0.65
2:2:121:THR:HB	2:2:229:CYS:HB2	1.79	0.65
3:3:124:ASN:N	3:3:124:ASN:HD22	1.93	0.65
1:1:277:ARG:HD3	3:3:57:ASN:ND2	2.09	0.65
3:3:209:LEU:HD12	3:3:209:LEU:N	2.11	0.65
1:1:245:TRP:NE1	3:3:36:ILE:HB	2.12	0.65
4:4:3:GLN:HB3	4:4:27:PHE:HA	1.77	0.65
3:3:9:GLY:O	3:3:12:GLN:HG2	1.96	0.65
1:1:105:ALA:O	1:1:106:GLN:C	2.40	0.64
4:4:3:GLN:HB2	4:4:26:TYR:O	1.97	0.64
3:3:230:LEU:H	3:3:230:LEU:HD22	1.60	0.64
1:1:136:ILE:H	1:1:136:ILE:CD1	2.06	0.64
2:2:157:LYS:HD2	2:2:161:ARG:HH12	1.61	0.64
3:3:54:PRO:HG2	3:3:93:PRO:HB2	1.78	0.64
1:1:142:GLN:HG3	1:1:170:PHE:CE1	2.32	0.64
1:1:16:VAL:CG1	1:1:17:VAL:N	2.60	0.64
1:1:232:MET:HE3	1:1:232:MET:HA	1.79	0.63
2:2:238:ASN:HD22	2:2:238:ASN:N	1.94	0.63
1:1:94:PHE:C	1:1:94:PHE:HD2	2.06	0.63
1:1:279:ILE:HD13	1:1:280:ILE:HD13	1.81	0.63
3:3:143:THR:CG2	3:3:146:ASP:HB2	2.19	0.63
1:1:210:THR:O	1:1:212:ASN:N	2.31	0.63
4:4:42:LYS:C	4:4:43:LEU:HD12	2.24	0.63
3:3:148:MET:SD	3:3:149:LEU:HD23	2.38	0.63
1:1:84:VAL:HG23	1:1:229:VAL:O	1.98	0.62
2:2:66:LEU:HD12	2:2:244:ILE:HB	1.80	0.62
3:3:130:LEU:C	3:3:130:LEU:HD23	2.25	0.62
1:1:263:PHE:N	1:1:263:PHE:HD2	1.98	0.62
1:1:161:TRP:CE2	1:1:219:ARG:HG2	2.34	0.62
1:1:23:SER:HB3	1:1:53:THR:HG22	1.82	0.61
2:2:180:LEU:N	2:2:180:LEU:HD12	2.15	0.61
1:1:252:ALA:HB2	2:2:180:LEU:HD11	1.83	0.61
2:2:238:ASN:H	2:2:238:ASN:ND2	1.97	0.61
2:2:83:PRO:HD2	2:2:219:ASN:HA	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:228:LEU:HD12	3:3:228:LEU:N	2.16	0.61
5:5:121:GLY:O	5:5:144:GLU:HB3	2.01	0.61
2:2:132:ILE:HG23	2:2:176:PHE:HB3	1.83	0.60
2:2:218:HIS:HD2	2:2:219:ASN:N	1.99	0.60
1:1:216:LEU:HD12	1:1:217:CYS:N	2.16	0.60
2:2:172:TYR:CD2	2:2:173:TRP:N	2.68	0.60
1:1:106:GLN:HA	1:1:106:GLN:NE2	2.11	0.60
1:1:198:TYR:C	1:1:209:ASN:HD21	2.09	0.60
3:3:138:ILE:HG23	3:3:139:ALA:N	2.16	0.60
1:1:277:ARG:CD	3:3:57:ASN:HD21	2.14	0.60
2:2:19:GLY:HA2	2:2:58:THR:HG22	1.83	0.60
2:2:181:LEU:O	3:3:68:TYR:CE1	2.55	0.60
4:4:6:ARG:HE	4:4:6:ARG:N	1.99	0.60
1:1:161:TRP:HB2	1:1:219:ARG:HH21	1.66	0.60
2:2:197:ASN:ND2	2:2:197:ASN:H	1.98	0.60
3:3:107:THR:CB	3:3:222:MET:HG2	2.31	0.60
2:2:193:ASN:H	2:2:197:ASN:ND2	1.86	0.59
1:1:35:ASP:CG	1:1:36:ALA:H	2.10	0.59
1:1:38:GLU:HA	2:2:191:PHE:HB2	1.84	0.59
1:1:19:ASN:HB3	1:1:56:VAL:O	2.01	0.59
3:3:122:THR:HG22	3:3:125:THR:N	2.17	0.59
3:3:62:ILE:HG23	3:3:63:ASN:OD1	2.01	0.59
1:1:86:LEU:O	1:1:87:ALA:HB3	2.03	0.59
1:1:274:ILE:HD13	3:3:67:MET:HE1	1.84	0.59
3:3:99:ILE:HG23	3:3:100:GLY:H	1.66	0.59
3:3:165:MET:HG2	3:3:166:VAL:N	2.15	0.59
1:1:50:VAL:O	1:1:51:ILE:HG23	2.02	0.59
1:1:110:LYS:O	1:1:113:LEU:HB2	2.03	0.59
3:3:125:THR:CG2	3:3:196:LEU:HD11	2.33	0.59
2:2:122:LEU:HD11	2:2:242:ILE:HD11	1.84	0.58
2:2:260:ARG:HG3	2:2:261:GLN:N	2.18	0.58
2:2:197:ASN:HD22	2:2:197:ASN:H	1.48	0.58
2:2:203:ILE:HD12	2:2:203:ILE:H	1.69	0.58
3:3:61:TYR:O	3:3:63:ASN:N	2.36	0.58
1:1:242:VAL:CG1	1:1:243:LYS:N	2.66	0.58
3:3:200:PRO:O	3:3:201:GLN:HB2	2.03	0.58
4:4:30:ASN:N	4:4:30:ASN:HD22	2.00	0.58
1:1:213:MET:HA	1:1:213:MET:HE2	1.86	0.58
3:3:2:LEU:HD23	3:3:3:PRO:N	2.19	0.58
3:3:122:THR:HG22	3:3:125:THR:H	1.69	0.58
4:4:30:ASN:N	4:4:30:ASN:ND2	2.52	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:84:ASP:OD1	2:2:85:ALA:N	2.37	0.57
1:1:277:ARG:NH1	1:1:280:ILE:HG22	2.19	0.57
2:2:181:LEU:O	3:3:68:TYR:HE1	1.87	0.57
3:3:7:THR:HG23	3:3:8:PRO:HD2	1.86	0.57
5:5:118:ILE:HA	5:5:129:PRO:HA	1.86	0.57
3:3:107:THR:HB	3:3:222:MET:HG2	1.86	0.57
1:1:262:ASN:HA	2:2:133:ALA:HB1	1.87	0.57
2:2:127:ILE:HG23	2:2:187:PHE:CE2	2.39	0.57
3:3:196:LEU:HD12	3:3:197:VAL:H	1.68	0.57
2:2:132:ILE:HG22	2:2:133:ALA:H	1.69	0.57
1:1:144:MET:HE3	1:1:166:ASN:HD22	1.69	0.57
1:1:270:ILE:H	1:1:270:ILE:CD1	2.08	0.57
2:2:50:ILE:O	2:2:50:ILE:HG13	2.04	0.57
2:2:162:LEU:C	2:2:164:PRO:HD3	2.29	0.56
3:3:39:GLU:HG2	3:3:40:VAL:N	2.20	0.56
3:3:163:ILE:HG23	3:3:163:ILE:O	2.05	0.56
1:1:55:TYR:C	1:1:55:TYR:CD2	2.82	0.56
2:2:225:ILE:O	2:2:226:ILE:HD13	2.05	0.56
1:1:156:ARG:O	1:1:156:ARG:HG2	2.04	0.56
1:1:161:TRP:CG	1:1:219:ARG:HE	2.23	0.56
1:1:161:TRP:CD2	1:1:219:ARG:HG2	2.39	0.56
1:1:195:TYR:HE2	2:2:218:HIS:CE1	2.23	0.56
2:2:118:HIS:O	2:2:119:GLN:HB3	2.04	0.56
3:3:101:GLU:O	3:3:104:SER:HB2	2.05	0.56
4:4:3:GLN:HE21	4:4:27:PHE:CB	2.19	0.56
2:2:218:HIS:CD2	2:2:219:ASN:N	2.74	0.56
1:1:257:ARG:HH11	1:1:257:ARG:HB3	1.70	0.56
2:2:180:LEU:HD12	2:2:180:LEU:H	1.71	0.56
2:2:193:ASN:N	2:2:197:ASN:HD21	1.86	0.56
2:2:135:ALA:HB2	2:2:169:THR:CA	2.29	0.56
2:2:203:ILE:CG2	2:2:249:MET:HE1	2.36	0.56
1:1:39:THR:O	2:2:190:GLN:HG2	2.06	0.56
1:1:195:TYR:HE2	2:2:218:HIS:ND1	2.04	0.56
2:2:164:PRO:HA	2:2:167:GLN:HG2	1.87	0.56
4:4:6:ARG:H	4:4:6:ARG:NE	2.00	0.55
3:3:198:ILE:HB	3:3:199:PRO:HD2	1.89	0.55
1:1:99:ILE:O	1:1:100:ASN:HB3	2.05	0.55
1:1:144:MET:HE3	1:1:166:ASN:ND2	2.21	0.55
1:1:198:TYR:CZ	2:2:144:TYR:HA	2.42	0.55
1:1:51:ILE:O	1:1:53:THR:N	2.40	0.55
1:1:226:ILE:HG22	1:1:226:ILE:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:120:GLY:N	2:2:194:LEU:HD12	2.20	0.55
2:2:176:PHE:N	2:2:176:PHE:CD2	2.74	0.55
3:3:111:GLY:O	3:3:169:TRP:HB2	2.06	0.55
1:1:55:TYR:C	1:1:55:TYR:HD2	2.15	0.55
3:3:51:SER:HB3	3:3:98:LEU:CD1	2.36	0.55
3:3:65:GLU:N	3:3:65:GLU:OE1	2.39	0.55
1:1:257:ARG:HB3	1:1:257:ARG:NH1	2.22	0.55
1:1:277:ARG:HH12	1:1:280:ILE:HG22	1.71	0.55
2:2:86:LEU:O	2:2:89:MET:HG2	2.06	0.55
2:2:98:TYR:CE1	2:2:259:LYS:HB2	2.42	0.55
2:2:257:ARG:CG	2:2:258:ALA:N	2.62	0.55
2:2:126:LEU:HD13	2:2:221:TRP:CE3	2.42	0.54
3:3:111:GLY:HA3	3:3:218:PHE:HA	1.88	0.54
3:3:191:TRP:CD1	3:3:191:TRP:N	2.74	0.54
1:1:207:THR:OG1	1:1:259:HIS:ND1	2.41	0.54
3:3:128:LYS:HB2	3:3:194:THR:OG1	2.06	0.54
3:3:171:SER:OG	3:3:172:ALA:N	2.38	0.54
1:1:50:VAL:O	1:1:50:VAL:CG1	2.55	0.54
1:1:198:TYR:HA	1:1:209:ASN:HD21	1.72	0.54
3:3:131:LEU:N	3:3:131:LEU:HD22	2.23	0.54
3:3:6:ILE:HG22	3:3:7:THR:N	2.23	0.54
3:3:99:ILE:HG23	3:3:100:GLY:N	2.23	0.54
3:3:171:SER:HB2	3:3:176:ARG:CZ	2.37	0.54
2:2:127:ILE:HG23	2:2:128:PRO:HD2	1.89	0.54
2:2:237:ILE:N	2:2:237:ILE:HD12	2.23	0.54
2:2:32:ILE:HD13	2:2:33:VAL:H	1.73	0.53
2:2:80:TRP:CE3	2:2:80:TRP:N	2.76	0.53
1:1:110:LYS:O	1:1:113:LEU:CB	2.57	0.53
1:1:249:PRO:HD3	2:2:187:PHE:CE1	2.43	0.53
2:2:91:ILE:N	2:2:91:ILE:CD1	2.53	0.53
2:2:103:ARG:HB2	2:2:212:MET:HG2	1.90	0.53
2:2:175:ASN:O	2:2:176:PHE:HB2	2.08	0.53
1:1:111:PHE:HD1	1:1:111:PHE:H	1.57	0.53
2:2:115:SER:HB3	2:2:118:HIS:ND1	2.23	0.53
3:3:92:GLN:OE1	3:3:93:PRO:HA	2.09	0.53
3:3:148:MET:SD	3:3:148:MET:C	2.91	0.53
1:1:80:SER:C	1:1:232:MET:HE1	2.34	0.53
3:3:221:ARG:O	3:3:222:MET:HB3	2.08	0.53
1:1:84:VAL:HG21	1:1:229:VAL:HG23	1.91	0.53
2:2:149:PRO:HG2	2:2:150:GLY:H	1.73	0.53
1:1:96:VAL:HG12	1:1:97:TRP:N	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:159:TYR:CD2	1:1:160:ALA:N	2.77	0.53
2:2:162:LEU:C	2:2:164:PRO:CD	2.81	0.53
1:1:204:ASN:O	1:1:205:TYR:C	2.51	0.53
2:2:84:ASP:O	2:2:85:ALA:C	2.52	0.53
1:1:103:GLU:O	1:1:104:MET:HG2	2.09	0.52
1:1:155:SER:C	1:1:157:ASP:H	2.16	0.52
2:2:84:ASP:CG	2:2:85:ALA:N	2.67	0.52
3:3:54:PRO:HG3	3:3:96:THR:CG2	2.40	0.52
3:3:122:THR:CG2	3:3:125:THR:H	2.22	0.52
1:1:155:SER:C	1:1:157:ASP:N	2.66	0.52
2:2:237:ILE:HD12	2:2:237:ILE:H	1.75	0.52
1:1:277:ARG:NH2	1:1:280:ILE:HA	2.25	0.52
4:4:6:ARG:CG	4:4:7:GLN:H	2.13	0.52
1:1:161:TRP:CB	1:1:219:ARG:HH21	2.22	0.52
2:2:172:TYR:CD2	2:2:172:TYR:N	2.77	0.52
2:2:193:ASN:O	2:2:195:ARG:N	2.43	0.52
1:1:88:ASN:O	1:1:89:TYR:C	2.52	0.52
1:1:237:HIS:ND1	1:1:237:HIS:C	2.68	0.52
1:1:20:ILE:N	1:1:20:ILE:HD12	2.25	0.52
1:1:193:MET:HE2	1:1:193:MET:CA	2.34	0.52
3:3:52:LEU:HD23	3:3:210:CYS:O	2.09	0.52
3:3:184:THR:HG22	3:3:185:SER:H	1.75	0.52
2:2:94:GLU:O	2:2:95:ASN:C	2.53	0.51
3:3:82:ILE:HG12	3:3:192:TYR:CE1	2.45	0.51
4:4:27:PHE:C	4:4:27:PHE:HD2	2.17	0.51
1:1:161:TRP:CZ2	1:1:219:ARG:HG2	2.46	0.51
2:2:23:ILE:HG21	2:2:109:HIS:CD2	2.45	0.51
3:3:2:LEU:C	3:3:2:LEU:CD2	2.83	0.51
3:3:131:LEU:CB	3:3:165:MET:HE3	2.39	0.51
1:1:86:LEU:O	1:1:87:ALA:CB	2.58	0.51
1:1:270:ILE:HD12	1:1:270:ILE:N	2.17	0.51
1:1:276:THR:HG22	3:3:62:ILE:CD1	2.40	0.51
2:2:23:ILE:HD13	2:2:63:PHE:CE1	2.44	0.51
2:2:115:SER:C	2:2:117:PHE:H	2.17	0.51
1:1:71:LEU:N	1:1:71:LEU:HD23	2.25	0.51
5:5:125:THR:HG22	5:5:126:GLN:N	2.21	0.51
2:2:175:ASN:C	2:2:176:PHE:HD2	2.18	0.51
4:4:43:LEU:N	4:4:43:LEU:CD1	2.72	0.51
1:1:92:GLU:O	1:1:156:ARG:HB2	2.11	0.51
2:2:76:LYS:HB3	2:2:172:TYR:CE1	2.46	0.51
3:3:107:THR:OG1	3:3:222:MET:HG2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:24:ASN:HB3	1:1:25:PRO:HD2	1.93	0.51
1:1:261:THR:HB	2:2:133:ALA:HB2	1.93	0.51
2:2:84:ASP:C	2:2:86:LEU:N	2.69	0.51
3:3:70:VAL:HG12	3:3:71:VAL:N	2.26	0.51
4:4:3:GLN:NE2	4:4:27:PHE:HB3	2.26	0.51
1:1:136:ILE:HD13	1:1:136:ILE:N	2.11	0.51
2:2:172:TYR:N	2:2:172:TYR:HD2	2.08	0.51
3:3:54:PRO:HG3	3:3:96:THR:HG21	1.92	0.51
2:2:157:LYS:HD2	2:2:161:ARG:NH1	2.25	0.51
3:3:73:GLN:HB3	3:3:76:ILE:HG13	1.93	0.51
3:3:131:LEU:HB3	3:3:165:MET:HE3	1.92	0.50
2:2:34:ALA:HB3	2:2:205:PRO:CD	2.42	0.50
2:2:127:ILE:HD11	2:2:184:ILE:HD11	1.93	0.50
3:3:82:ILE:HG12	3:3:192:TYR:HE1	1.76	0.50
4:4:6:ARG:N	4:4:6:ARG:NE	2.58	0.50
1:1:25:PRO:HD3	1:1:52:GLU:CD	2.37	0.50
1:1:42:THR:O	1:1:43:SER:C	2.54	0.50
3:3:122:THR:HG22	3:3:125:THR:CB	2.42	0.50
3:3:193:GLN:HA	3:3:193:GLN:HE21	1.77	0.50
1:1:65:MET:HB2	3:3:42:ASN:HD21	1.77	0.50
1:1:155:SER:O	1:1:157:ASP:N	2.45	0.50
1:1:23:SER:CB	1:1:53:THR:HG22	2.42	0.50
1:1:51:ILE:O	1:1:52:GLU:C	2.55	0.49
1:1:96:VAL:CG1	1:1:97:TRP:N	2.75	0.49
2:2:173:TRP:O	2:2:174:LEU:HD23	2.12	0.49
3:3:87:THR:O	3:3:88:ASP:C	2.55	0.49
2:2:72:SER:C	2:2:74:SER:H	2.20	0.49
2:2:161:ARG:C	2:2:162:LEU:HG	2.34	0.49
1:1:83:GLU:HG2	1:1:230:HIS:CD2	2.47	0.49
1:1:104:MET:O	1:1:105:ALA:C	2.55	0.49
1:1:156:ARG:NH2	1:1:221:VAL:O	2.45	0.49
1:1:182:LEU:HD23	1:1:183:PRO:HD2	1.94	0.49
3:3:65:GLU:O	3:3:67:MET:N	2.45	0.49
3:3:144:ARG:O	3:3:145:LYS:C	2.53	0.49
1:1:124:THR:HG23	1:1:179:ARG:HB2	1.95	0.49
1:1:202:ASP:HB3	2:2:144:TYR:CD1	2.48	0.49
2:2:126:LEU:HD22	2:2:221:TRP:HE3	1.78	0.49
1:1:145:TYR:CD1	1:1:145:TYR:C	2.91	0.48
1:1:22:SER:HA	1:1:54:ARG:O	2.13	0.48
2:2:34:ALA:O	2:2:36:GLY:N	2.47	0.48
3:3:155:TRP:CE2	3:3:163:ILE:HG21	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:182:LEU:CD2	1:1:183:PRO:HD2	2.43	0.48
1:1:185:LEU:O	1:1:186:SER:O	2.31	0.48
3:3:54:PRO:HA	3:3:68:TYR:CD2	2.48	0.48
1:1:279:ILE:HG23	1:1:281:THR:H	1.79	0.48
3:3:82:ILE:HD12	3:3:190:CYS:SG	2.54	0.48
1:1:94:PHE:HE1	1:1:154:ASN:C	2.21	0.48
1:1:111:PHE:C	1:1:113:LEU:N	2.70	0.48
3:3:55:ILE:HD12	3:3:83:PHE:CD2	2.47	0.48
1:1:48:GLU:HG3	1:1:53:THR:HG21	1.96	0.48
1:1:87:ALA:O	1:1:88:ASN:HB2	2.12	0.48
1:1:241:HIS:N	1:1:241:HIS:CD2	2.79	0.48
3:3:26:PRO:O	3:3:27:TRP:HB2	2.14	0.48
1:1:103:GLU:C	1:1:104:MET:HG2	2.38	0.48
2:2:176:PHE:N	2:2:176:PHE:HD2	2.10	0.48
3:3:170:ILE:O	3:3:170:ILE:HG22	2.14	0.48
1:1:85:THR:HG23	1:1:85:THR:O	2.14	0.48
1:1:16:VAL:HG12	1:1:17:VAL:O	2.14	0.47
3:3:2:LEU:HD23	3:3:2:LEU:C	2.37	0.47
3:3:14:LEU:HB3	3:3:17:ASP:HB3	1.96	0.47
1:1:198:TYR:HA	1:1:209:ASN:ND2	2.29	0.47
1:1:198:TYR:CA	1:1:209:ASN:HD21	2.28	0.47
2:2:143:GLY:O	2:2:144:TYR:C	2.57	0.47
3:3:84:SER:O	3:3:85:ILE:HG23	2.14	0.47
3:3:155:TRP:CE3	3:3:163:ILE:HG21	2.48	0.47
1:1:252:ALA:HB2	2:2:180:LEU:CD1	2.44	0.47
2:2:186:ILE:HG13	2:2:186:ILE:O	2.14	0.47
2:2:198:ASN:OD1	2:2:198:ASN:O	2.32	0.47
2:2:55:GLN:HA	2:2:56:PRO:HD2	1.74	0.47
3:3:122:THR:CG2	3:3:125:THR:N	2.77	0.47
2:2:198:ASN:OD1	2:2:198:ASN:C	2.57	0.47
3:3:2:LEU:O	3:3:4:VAL:HG13	2.14	0.47
3:3:115:PHE:CE2	3:3:188:ILE:HD11	2.49	0.47
1:1:80:SER:C	1:1:232:MET:CE	2.87	0.47
2:2:98:TYR:CZ	2:2:259:LYS:HB2	2.49	0.47
2:2:18:ARG:O	2:2:19:GLY:C	2.57	0.47
2:2:34:ALA:HB3	2:2:204:ALA:HA	1.97	0.47
3:3:130:LEU:HD12	3:3:193:GLN:NE2	2.29	0.47
1:1:17:VAL:O	1:1:17:VAL:HG23	2.15	0.47
2:2:46:ASP:O	2:2:47:ALA:O	2.32	0.47
2:2:23:ILE:CG2	2:2:24:THR:N	2.76	0.47
2:2:197:ASN:N	2:2:197:ASN:ND2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:82:LEU:HA	2:2:83:PRO:C	2.31	0.46
3:3:155:TRP:CD1	3:3:155:TRP:C	2.92	0.46
3:3:133:TYR:HE1	3:3:186:GLY:HA3	1.80	0.46
2:2:206:TYR:CE1	2:2:208:ASN:HB3	2.50	0.46
3:3:18:ASP:O	3:3:19:PHE:CD1	2.69	0.46
1:1:201:GLN:O	1:1:202:ASP:C	2.58	0.46
1:1:262:ASN:ND2	2:2:134:SER:OG	2.44	0.46
1:1:274:ILE:CD1	3:3:67:MET:HE1	2.45	0.46
3:3:195:ARG:O	3:3:197:VAL:HG23	2.16	0.46
3:3:29:HIS:O	3:3:30:PRO:C	2.58	0.46
4:4:3:GLN:HE21	4:4:27:PHE:HB3	1.81	0.46
1:1:110:LYS:O	1:1:111:PHE:C	2.57	0.46
1:1:272:THR:OG1	1:1:273:ALA:N	2.46	0.46
2:2:115:SER:C	2:2:117:PHE:N	2.72	0.46
2:2:207:VAL:O	2:2:208:ASN:HB2	2.15	0.46
1:1:253:LEU:CD1	1:1:263:PHE:HD1	2.29	0.46
2:2:218:HIS:CD2	2:2:218:HIS:C	2.93	0.46
3:3:73:GLN:HE21	3:3:73:GLN:HB2	1.65	0.46
1:1:245:TRP:CE2	3:3:36:ILE:HB	2.51	0.46
2:2:45:LYS:O	2:2:45:LYS:HG2	2.15	0.46
2:2:79:TRP:NE1	2:2:176:PHE:CE1	2.84	0.46
3:3:58:THR:C	3:3:60:THR:N	2.73	0.46
2:2:126:LEU:HD22	2:2:221:TRP:CE3	2.51	0.46
4:4:27:PHE:HD2	4:4:27:PHE:O	1.99	0.46
4:4:27:PHE:O	4:4:28:ASN:HB3	2.15	0.46
2:2:34:ALA:C	2:2:36:GLY:N	2.74	0.45
2:2:105:GLY:O	2:2:249:MET:N	2.50	0.45
2:2:165:ASP:N	2:2:165:ASP:OD1	2.49	0.45
1:1:46:GLN:HB3	1:1:47:PRO:HD2	1.97	0.45
1:1:143:TYR:O	1:1:168:SER:HA	2.17	0.45
3:3:77:ASN:O	3:3:78:ALA:CB	2.62	0.45
3:3:215:CYS:C	3:3:217:ASP:N	2.71	0.45
1:1:89:TYR:CD1	1:1:224:LYS:HA	2.52	0.45
1:1:180:PHE:CD1	1:1:180:PHE:C	2.95	0.45
2:2:95:ASN:OD1	2:2:99:HIS:HE1	1.98	0.45
4:4:4:VAL:HG23	4:4:26:TYR:CE1	2.52	0.45
1:1:46:GLN:O	1:1:47:PRO:C	2.60	0.45
2:2:172:TYR:O	2:2:175:ASN:N	2.48	0.45
2:2:231:LEU:O	2:2:231:LEU:HG	2.16	0.45
1:1:67:LEU:HD23	1:1:67:LEU:HA	1.78	0.45
2:2:71:TRP:CE2	2:2:231:LEU:HB2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:79:TRP:HE1	2:2:176:PHE:HE1	1.64	0.45
2:2:193:ASN:HD22	2:2:193:ASN:C	2.23	0.45
2:2:215:MET:HE2	2:2:215:MET:HA	1.98	0.45
3:3:54:PRO:HB3	3:3:68:TYR:CE2	2.51	0.45
3:3:166:VAL:CG1	3:3:167:VAL:N	2.79	0.45
1:1:207:THR:HG23	2:2:131:GLN:HE22	1.80	0.45
2:2:260:ARG:CG	2:2:261:GLN:N	2.80	0.45
3:3:46:ILE:C	3:3:48:GLN:N	2.72	0.45
2:2:79:TRP:CD1	2:2:176:PHE:CE1	3.05	0.45
3:3:98:LEU:O	3:3:99:ILE:C	2.60	0.45
2:2:144:TYR:C	2:2:144:TYR:CD2	2.95	0.45
2:2:106:TYR:HB3	2:2:247:SER:O	2.17	0.45
1:1:196:ASP:OD1	2:2:81:LYS:HD3	2.16	0.44
2:2:34:ALA:HB3	2:2:205:PRO:HD3	1.99	0.44
4:4:29:ILE:N	4:4:29:ILE:CD1	2.74	0.44
2:2:32:ILE:O	2:2:203:ILE:HD12	2.18	0.44
3:3:196:LEU:HD12	3:3:197:VAL:N	2.30	0.44
1:1:161:TRP:CE3	1:1:219:ARG:HG2	2.51	0.44
1:1:212:ASN:C	1:1:213:MET:HE3	2.43	0.44
1:1:261:THR:O	1:1:262:ASN:O	2.36	0.44
3:3:122:THR:HG22	3:3:125:THR:HG1	1.78	0.44
1:1:54:ARG:HD3	1:1:55:TYR:O	2.17	0.44
1:1:224:LYS:HB3	5:5:132:TRP:HZ2	1.82	0.44
2:2:38:TRP:CD1	2:2:39:PRO:CD	2.97	0.44
2:2:132:ILE:CG2	2:2:176:PHE:HB3	2.47	0.44
1:1:24:ASN:CB	1:1:25:PRO:HD2	2.48	0.44
3:3:46:ILE:O	3:3:49:VAL:N	2.46	0.44
3:3:103:SER:HA	3:3:220:LEU:HD21	1.98	0.44
2:2:150:GLY:O	2:2:152:THR:N	2.50	0.44
3:3:128:LYS:O	3:3:193:GLN:HB3	2.18	0.44
1:1:275:VAL:CG1	1:1:276:THR:N	2.81	0.44
3:3:7:THR:O	3:3:8:PRO:C	2.61	0.44
3:3:209:LEU:HD12	3:3:209:LEU:H	1.80	0.44
1:1:59:SER:O	1:1:60:GLN:O	2.36	0.44
1:1:62:ARG:O	1:1:63:ASP:C	2.61	0.44
2:2:95:ASN:CB	2:2:253:PHE:CE2	3.00	0.44
2:2:174:LEU:HA	2:2:179:THR:O	2.18	0.44
3:3:7:THR:HG22	3:3:8:PRO:O	2.18	0.44
1:1:210:THR:OG1	1:1:211:ASN:N	2.51	0.43
1:1:245:TRP:CD1	3:3:36:ILE:HG22	2.53	0.43
1:1:261:THR:O	1:1:262:ASN:C	2.60	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:229:CYS:HA	2:2:230:PRO:HD2	1.70	0.43
2:2:162:LEU:O	2:2:164:PRO:N	2.47	0.43
5:5:115:ILE:HG22	5:5:115:ILE:O	2.18	0.43
1:1:177:TYR:CD2	1:1:177:TYR:N	2.81	0.43
3:3:46:ILE:O	3:3:48:GLN:N	2.51	0.43
3:3:128:LYS:HD2	3:3:194:THR:HG21	2.01	0.43
3:3:134:THR:HA	3:3:135:PRO:HD3	1.79	0.43
2:2:34:ALA:C	2:2:36:GLY:H	2.27	0.43
1:1:85:THR:N	1:1:93:ASN:OD1	2.48	0.43
1:1:107:ILE:HG22	1:1:108:ARG:N	2.33	0.43
4:4:6:ARG:HD2	4:4:6:ARG:C	2.44	0.43
2:2:210:VAL:HB	2:2:211:PRO:HD2	1.99	0.43
3:3:155:TRP:CD1	3:3:156:ASP:N	2.87	0.43
1:1:253:LEU:O	1:1:254:GLU:C	2.62	0.43
2:2:114:ALA:CB	2:2:194:LEU:HD22	2.49	0.43
2:2:216:ARG:HG3	2:2:216:ARG:HH11	1.82	0.43
2:2:86:LEU:C	2:2:88:ASP:H	2.27	0.43
2:2:172:TYR:O	2:2:174:LEU:N	2.51	0.43
2:2:203:ILE:HG23	2:2:249:MET:HE1	1.99	0.43
3:3:25:LEU:HD23	3:3:25:LEU:HA	1.76	0.43
3:3:200:PRO:O	3:3:201:GLN:CB	2.67	0.43
2:2:106:TYR:C	2:2:249:MET:HE2	2.44	0.43
2:2:150:GLY:C	2:2:152:THR:H	2.26	0.43
2:2:175:ASN:C	2:2:176:PHE:CD2	2.96	0.43
3:3:78:ALA:HB1	3:3:79:PRO:HD2	2.00	0.43
3:3:108:HIS:HA	3:3:176:ARG:O	2.19	0.43
4:4:3:GLN:CB	4:4:26:TYR:O	2.67	0.43
1:1:53:THR:OG1	1:1:54:ARG:N	2.52	0.42
1:1:94:PHE:CE1	1:1:154:ASN:C	2.97	0.42
1:1:202:ASP:OD2	1:1:202:ASP:N	2.52	0.42
2:2:91:ILE:O	2:2:92:PHE:C	2.62	0.42
3:3:26:PRO:HA	4:4:34:ASP:OD1	2.19	0.42
3:3:97:THR:O	3:3:98:LEU:C	2.62	0.42
1:1:118:ARG:O	1:1:119:PHE:HB3	2.19	0.42
1:1:183:PRO:HD3	3:3:23:CYS:SG	2.59	0.42
1:1:221:VAL:O	1:1:222:THR:C	2.62	0.42
3:3:65:GLU:C	3:3:67:MET:N	2.77	0.42
1:1:201:GLN:O	1:1:203:GLN:HB2	2.19	0.42
2:2:228:ILE:HD12	2:2:228:ILE:HA	1.89	0.42
3:3:58:THR:C	3:3:62:ILE:HD13	2.44	0.42
3:3:83:PHE:CE1	3:3:190:CYS:HB3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:59:SER:O	1:1:60:GLN:C	2.62	0.42
2:2:37:VAL:O	2:2:205:PRO:HB3	2.19	0.42
1:1:108:ARG:NE	1:1:255:TYR:CE2	2.88	0.42
1:1:116:TYR:OH	2:2:208:ASN:HA	2.19	0.42
1:1:161:TRP:CB	1:1:219:ARG:NH2	2.83	0.42
1:1:176:ALA:O	1:1:177:TYR:C	2.63	0.42
2:2:77:GLY:C	2:2:156:VAL:HG23	2.44	0.42
2:2:193:ASN:C	2:2:193:ASN:ND2	2.76	0.42
3:3:48:GLN:HE21	3:3:48:GLN:HB2	1.51	0.42
2:2:159:GLU:O	2:2:160:THR:O	2.37	0.42
2:2:126:LEU:HD23	2:2:126:LEU:HA	1.64	0.42
3:3:57:ASN:OD1	3:3:57:ASN:N	2.52	0.42
3:3:83:PHE:CE1	3:3:190:CYS:CB	3.03	0.42
3:3:230:LEU:HD13	3:3:230:LEU:N	2.35	0.42
1:1:110:LYS:O	1:1:113:LEU:N	2.52	0.42
2:2:71:TRP:CZ2	2:2:231:LEU:HB2	2.55	0.42
3:3:119:PHE:CD1	3:3:119:PHE:C	2.97	0.42
3:3:199:PRO:HB2	3:3:200:PRO:CD	2.50	0.42
4:4:3:GLN:HB2	4:4:26:TYR:C	2.44	0.42
1:1:161:TRP:CH2	1:1:219:ARG:HG2	2.55	0.42
2:2:34:ALA:HB3	2:2:205:PRO:HD2	2.01	0.42
2:2:128:PRO:O	2:2:129:GLU:C	2.62	0.42
2:2:209:ALA:C	2:2:210:VAL:CG1	2.93	0.42
3:3:42:ASN:O	3:3:45:GLU:HG3	2.19	0.42
2:2:93:GLY:O	2:2:94:GLU:C	2.63	0.41
3:3:65:GLU:C	3:3:67:MET:H	2.28	0.41
1:1:161:TRP:HB2	1:1:219:ARG:NH2	2.34	0.41
3:3:34:ILE:HG13	3:3:35:SER:N	2.34	0.41
3:3:190:CYS:C	3:3:191:TRP:CD1	2.98	0.41
3:3:209:LEU:N	3:3:209:LEU:CD1	2.83	0.41
1:1:127:PRO:HG3	1:1:233:THR:CG2	2.50	0.41
1:1:146:VAL:HA	1:1:147:PRO:HD3	1.80	0.41
1:1:198:TYR:C	1:1:209:ASN:ND2	2.77	0.41
4:4:4:VAL:HG21	4:4:42:LYS:NZ	2.36	0.41
1:1:132:LEU:HD23	1:1:132:LEU:HA	1.79	0.41
2:2:46:ASP:O	2:2:47:ALA:C	2.62	0.41
3:3:54:PRO:HB3	3:3:68:TYR:HE2	1.85	0.41
1:1:199:ASP:HB3	1:1:203:GLN:H	1.84	0.41
2:2:187:PHE:HB3	2:2:188:PRO:CD	2.49	0.41
3:3:56:ASN:HB3	3:3:67:MET:HA	2.02	0.41
3:3:106:PHE:O	3:3:178:THR:HG21	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:166:VAL:HG12	3:3:167:VAL:N	2.34	0.41
3:3:193:GLN:HA	3:3:193:GLN:NE2	2.36	0.41
1:1:70:PHE:CD2	1:1:71:LEU:HD21	2.56	0.41
2:2:99:HIS:CG	2:2:253:PHE:HB3	2.56	0.41
2:2:112:CYS:O	2:2:112:CYS:SG	2.78	0.41
3:3:228:LEU:N	3:3:228:LEU:CD1	2.83	0.41
1:1:19:ASN:N	1:1:19:ASN:HD22	2.16	0.41
1:1:117:THR:O	1:1:190:ALA:HB1	2.21	0.41
1:1:179:ARG:HG2	1:1:180:PHE:N	2.35	0.41
1:1:111:PHE:CD1	1:1:111:PHE:N	2.89	0.41
2:2:57:ASP:CG	2:2:58:THR:H	2.28	0.41
2:2:118:HIS:O	3:3:122:THR:HA	2.21	0.41
3:3:184:THR:HG21	3:3:187:TYR:CE1	2.56	0.41
1:1:142:GLN:O	1:1:218:SER:HA	2.20	0.41
1:1:145:TYR:O	1:1:147:PRO:HD3	2.21	0.41
1:1:203:GLN:O	1:1:204:ASN:CB	2.67	0.41
1:1:245:TRP:CD1	3:3:36:ILE:CG2	3.04	0.41
2:2:93:GLY:O	2:2:96:MET:HB3	2.20	0.41
2:2:173:TRP:C	2:2:174:LEU:HD23	2.46	0.41
3:3:58:THR:O	3:3:60:THR:N	2.53	0.41
1:1:111:PHE:O	1:1:113:LEU:N	2.51	0.41
3:3:102:ILE:O	3:3:105:TYR:HB2	2.20	0.41
1:1:179:ARG:CG	1:1:180:PHE:N	2.82	0.40
1:1:257:ARG:HH11	1:1:257:ARG:CB	2.33	0.40
3:3:51:SER:HB3	3:3:98:LEU:CG	2.51	0.40
3:3:55:ILE:HG22	3:3:56:ASN:N	2.37	0.40
1:1:91:LYS:O	1:1:91:LYS:HG2	2.21	0.40
1:1:248:ARG:HB3	1:1:249:PRO:HD2	2.03	0.40
2:2:185:THR:C	2:2:187:PHE:H	2.29	0.40
3:3:54:PRO:HA	3:3:68:TYR:HD2	1.85	0.40
3:3:58:THR:C	3:3:60:THR:H	2.29	0.40
3:3:58:THR:O	3:3:62:ILE:HD13	2.21	0.40
3:3:184:THR:HG22	3:3:185:SER:N	2.36	0.40
1:1:70:PHE:C	1:1:72:GLY:H	2.29	0.40
1:1:113:LEU:HD12	1:1:113:LEU:O	2.22	0.40
2:2:77:GLY:O	2:2:156:VAL:HG23	2.21	0.40
1:1:198:TYR:HB3	1:1:199:ASP:H	1.72	0.40
2:2:78:TRP:O	2:2:79:TRP:HB3	2.22	0.40
1:1:35:ASP:CG	1:1:36:ALA:N	2.79	0.40
1:1:84:VAL:HA	1:1:93:ASN:OD1	2.22	0.40
1:1:263:PHE:HD2	1:1:263:PHE:H	1.66	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:209:ALA:O	2:2:210:VAL:HG12	2.21	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	1	267/289 (92%)	208 (78%)	38 (14%)	21 (8%)	1	8
2	2	248/261 (95%)	179 (72%)	47 (19%)	22 (9%)	0	7
3	3	235/237 (99%)	180 (77%)	39 (17%)	16 (7%)	1	11
4	4	21/68 (31%)	15 (71%)	5 (24%)	1 (5%)	2	16
5	5	37/41 (90%)	24 (65%)	12 (32%)	1 (3%)	4	27
All	All	808/896 (90%)	606 (75%)	141 (18%)	61 (8%)	1	9

All (61) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	60	GLN
1	1	91	LYS
1	1	105	ALA
1	1	185	LEU
1	1	186	SER
1	1	211	ASN
1	1	262	ASN
2	2	31	ALA
2	2	47	ALA
2	2	83	PRO
2	2	85	ALA
2	2	87	LYS
2	2	159	GLU

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Mol	Chain	Res	Type
2	2	160	THR
2	2	194	LEU
2	2	222	SER
3	3	17	ASP
3	3	62	ILE
3	3	89	VAL
3	3	163	ILE
3	3	218	PHE
3	3	234	ALA
1	1	106	GLN
1	1	282	THR
2	2	73	SER
2	2	112	CYS
3	3	66	ASN
3	3	88	ASP
3	3	95	ALA
3	3	158	GLY
1	1	87	ALA
1	1	202	ASP
2	2	35	TYR
2	2	84	ASP
2	2	145	ASN
2	2	151	GLU
2	2	165	ASP
2	2	173	TRP
1	1	25	PRO
1	1	112	GLU
1	1	156	ARG
1	1	266	GLU
2	2	30	ASN
2	2	66	LEU
2	2	139	ASN
3	3	79	PRO
3	3	222	MET
4	4	28	ASN
1	1	52	GLU
1	1	110	LYS
2	2	114	ALA
2	2	119	GLN
3	3	30	PRO
3	3	47	CYS
1	1	107	ILE

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Mol	Chain	Res	Type
1	1	195	TYR
3	3	22	PRO
1	1	246	CYS
5	5	150	GLY
1	1	47	PRO
3	3	127	VAL

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	1	238/257 (93%)	213 (90%)	25 (10%)	6	29
2	2	216/226 (96%)	192 (89%)	24 (11%)	6	27
3	3	210/210 (100%)	180 (86%)	30 (14%)	3	19
4	4	19/59 (32%)	14 (74%)	5 (26%)	0	3
5	5	34/36 (94%)	32 (94%)	2 (6%)	18	45
All	All	717/788 (91%)	631 (88%)	86 (12%)	5	24

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	54	ARG
1	1	55	TYR
1	1	82	LEU
1	1	94	PHE
1	1	106	GLN
1	1	113	LEU
1	1	121	SER
1	1	124	THR
1	1	125	LEU
1	1	136	ILE
1	1	159	TYR
1	1	169	VAL
1	1	202	ASP

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Mol	Chain	Res	Type
1	1	203	GLN
1	1	213	MET
1	1	217	CYS
1	1	219	ARG
1	1	233	THR
1	1	237	HIS
1	1	261	THR
1	1	263	PHE
1	1	270	ILE
1	1	275	VAL
1	1	279	ILE
1	1	280	ILE
2	2	26	GLN
2	2	32	ILE
2	2	58	THR
2	2	63	PHE
2	2	80	TRP
2	2	91	ILE
2	2	106	TYR
2	2	126	LEU
2	2	132	ILE
2	2	134	SER
2	2	137	HIS
2	2	140	VAL
2	2	152	THR
2	2	162	LEU
2	2	164	PRO
2	2	172	TYR
2	2	176	PHE
2	2	180	LEU
2	2	195	ARG
2	2	197	ASN
2	2	201	THR
2	2	202	ILE
2	2	203	ILE
2	2	238	ASN
3	3	2	LEU
3	3	8	PRO
3	3	20	GLN
3	3	21	SER
3	3	48	GLN
3	3	56	ASN

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Mol	Chain	Res	Type
3	3	59	ASP
3	3	62	ILE
3	3	73	GLN
3	3	80	ASP
3	3	85	ILE
3	3	96	THR
3	3	99	ILE
3	3	122	THR
3	3	124	ASN
3	3	131	LEU
3	3	134	THR
3	3	142	THR
3	3	143	THR
3	3	146	ASP
3	3	148	MET
3	3	149	LEU
3	3	163	ILE
3	3	165	MET
3	3	171	SER
3	3	184	THR
3	3	201	GLN
3	3	220	LEU
3	3	225	ASP
3	3	230	LEU
4	4	6	ARG
4	4	27	PHE
4	4	29	ILE
4	4	30	ASN
4	4	43	LEU
5	5	113	CYS
5	5	120	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	19	ASN
1	1	24	ASN
1	1	106	GLN
1	1	138	HIS
1	1	162	GLN
1	1	166	ASN
1	1	175	GLN

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Mol	Chain	Res	Type
1	1	201	GLN
1	1	209	ASN
1	1	241	HIS
2	2	15	GLN
2	2	26	GLN
2	2	55	GLN
2	2	95	ASN
2	2	99	HIS
2	2	109	HIS
2	2	131	GLN
2	2	137	HIS
2	2	175	ASN
2	2	193	ASN
2	2	197	ASN
2	2	219	ASN
2	2	238	ASN
3	3	12	GLN
3	3	20	GLN
3	3	42	ASN
3	3	48	GLN
3	3	56	ASN
3	3	73	GLN
3	3	108	HIS
3	3	124	ASN
3	3	174	HIS
3	3	193	GLN
3	3	201	GLN
4	4	3	GLN
4	4	25	ASN
4	4	30	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [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	1	290	-	13,13,13	1.68	2 (15%)	13,13,13	0.89	1 (7%)

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	1	290	-	-	8/11/11/11	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	1	290	DAO	C2-C1	4.11	1.60	1.50
6	1	290	DAO	C3-C2	2.23	1.60	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	1	290	DAO	O2-C1-C2	2.09	120.61	114.00

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	1	290	DAO	C2-C3-C4-C5
6	1	290	DAO	C11-C10-C9-C8
6	1	290	DAO	C5-C6-C7-C8
6	1	290	DAO	C9-C10-C11-C12
6	1	290	DAO	C3-C4-C5-C6
6	1	290	DAO	C1-C2-C3-C4
6	1	290	DAO	O1-C1-C2-C3
6	1	290	DAO	O2-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 [i](#)

There are no chain breaks in this entry.

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

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.