



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:51 AM UTC

PDB ID : 4GMP / pdb_00004gmp
Title : Crystal structure of enterovirus 71 strain 1095 procapsid
Authors : Yoder, J.D.; Hafenstein, S.
Deposited on : 2012-08-16
Resolution : 3.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (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

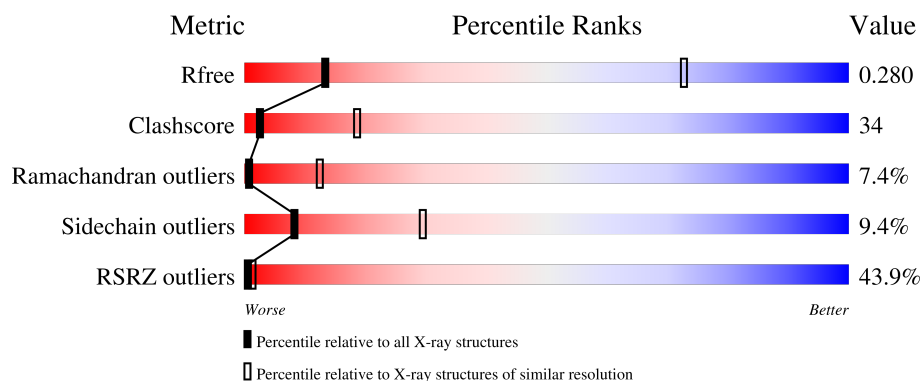
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1270 (4.10-3.70)
Clashscore	190562	1034 (4.08-3.72)
Ramachandran outliers	187476	1251 (4.10-3.70)
Sidechain outliers	187428	1243 (4.10-3.70)
RSRZ outliers	180081	1269 (4.10-3.70)

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

Mol	Chain	Length	Quality of chain
1	0	323	44% 27% 39% 7% 27%
2	1	297	22% 30% 36% 7% 27%
3	3	242	41% 41% 41% 16% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5395 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 capsid protein VP0.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	0	237	Total	C	N	O	S	0	0	0
			1833	1179	301	345	8			

- Molecule 2 is a protein called capsid protein VP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	1	218	Total	C	N	O	S	0	0	0
			1717	1101	289	316	11			

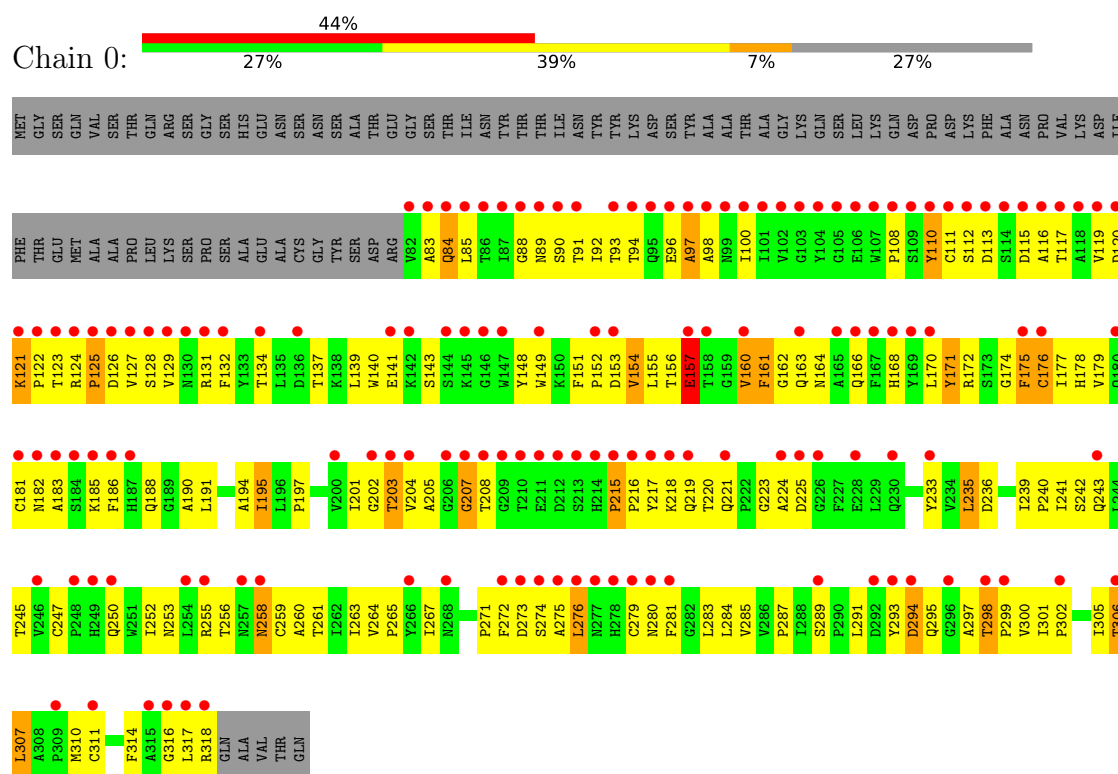
- Molecule 3 is a protein called capsid protein VP3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	3	240	Total	C	N	O	S	0	0	0
			1845	1188	304	342	11			

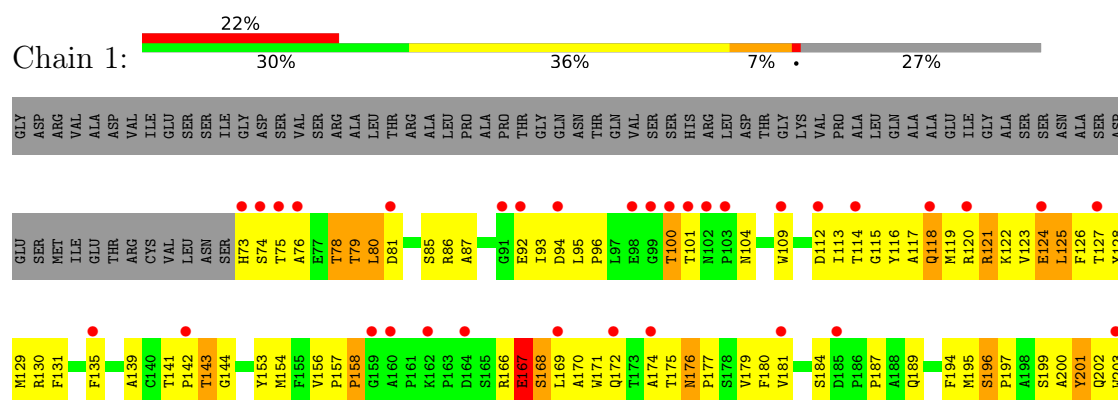
3 Residue-property plots

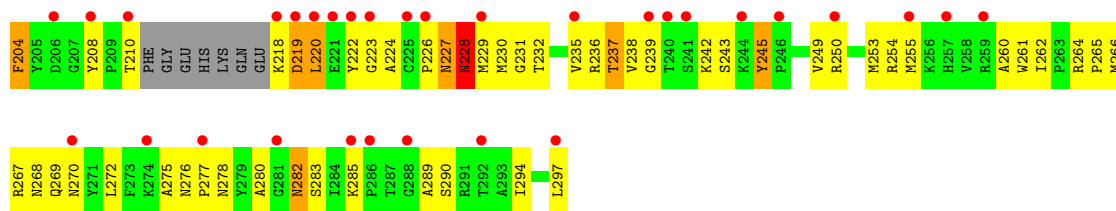
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: capsid protein VP0

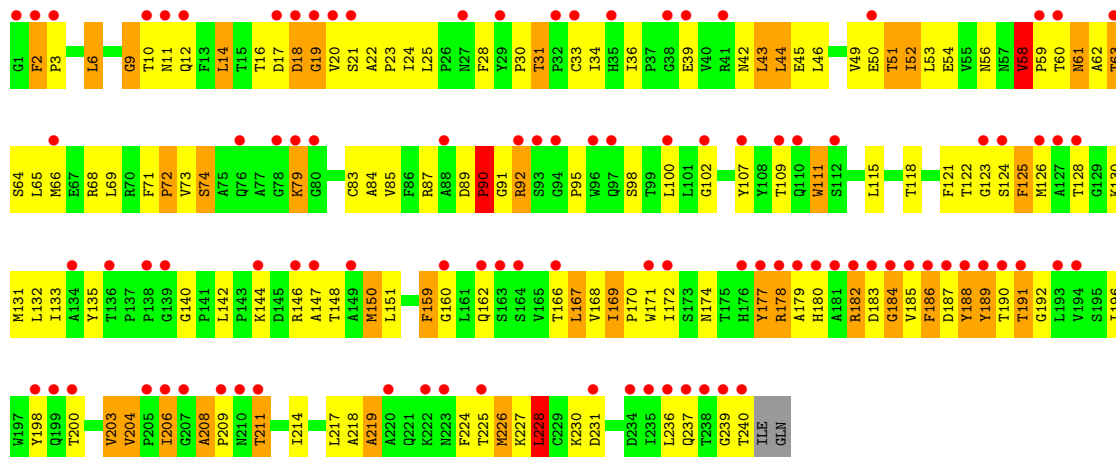


• Molecule 2: capsid protein VP1





● Molecule 3: capsid protein VP3



4 Data and refinement statistics

Property	Value	Source
Space group	P 4 ₂ 3 ₂	Depositor
Cell constants a, b, c, α , β , γ	350.25Å 350.25Å 350.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.53 – 3.90 49.53 – 3.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.53-3.90) 99.8 (49.53-3.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.81 (at 3.88Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.269 , 0.285 0.262 , 0.280	Depositor DCC
R_{free} test set	3398 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	109.8	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 102.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.37	EDS
Total number of atoms	5395	wwPDB-VP
Average B, all atoms (Å ²)	125.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.44% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	0	0.56	0/1888	1.05	11/2591 (0.4%)
2	1	0.61	0/1769	1.03	7/2411 (0.3%)
3	3	0.58	0/1897	1.09	18/2596 (0.7%)
All	All	0.59	0/5554	1.06	36/7598 (0.5%)

There are no bond length outliers.

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	161	PHE	N-CA-C	-8.57	102.26	112.89
3	3	45	GLU	N-CA-C	-8.28	102.21	111.07
3	3	18	ASP	N-CA-C	7.61	120.62	110.88
1	0	294	ASP	N-CA-C	-7.26	99.71	110.23
3	3	74	SER	N-CA-C	7.11	117.98	108.38
2	1	201	TYR	N-CA-C	-7.11	101.67	110.41
2	1	168	SER	N-CA-C	-6.95	100.15	110.23
3	3	2	PHE	CA-C-N	6.68	128.19	119.84
3	3	2	PHE	C-N-CA	6.68	128.19	119.84
3	3	169	ILE	CA-C-N	6.64	128.14	119.84
3	3	169	ILE	C-N-CA	6.64	128.14	119.84
2	1	125	LEU	N-CA-C	-6.39	104.96	112.89
3	3	31	THR	CA-C-N	6.27	126.28	119.89
3	3	31	THR	C-N-CA	6.27	126.28	119.89
1	0	84	GLN	N-CA-C	6.20	118.28	108.67
1	0	126	ASP	N-CA-C	-6.17	105.70	113.72
1	0	221	GLN	CA-C-N	6.14	127.51	119.84
1	0	221	GLN	C-N-CA	6.14	127.51	119.84
1	0	175	PHE	N-CA-C	6.08	116.03	108.19
2	1	176	ASN	CA-C-N	6.04	127.39	119.84
2	1	176	ASN	C-N-CA	6.04	127.39	119.84
3	3	111	TRP	N-CA-C	6.04	116.39	107.88
1	0	160	VAL	N-CA-C	-5.98	104.94	113.07
1	0	217	TYR	N-CA-C	-5.94	106.09	113.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	160	GLY	N-CA-C	-5.93	105.61	112.73
3	3	9	GLY	N-CA-C	-5.66	107.20	115.63
2	1	115	GLY	N-CA-C	-5.65	106.76	113.99
1	0	116	ALA	N-CA-C	-5.46	106.65	113.15
3	3	203	VAL	N-CA-C	5.44	115.69	107.75
1	0	194	ALA	N-CA-C	5.31	117.14	109.07
2	1	144	GLY	N-CA-C	-5.25	107.81	115.63
3	3	52	ILE	N-CA-C	5.24	116.01	108.93
3	3	125	PHE	N-CA-C	-5.16	105.27	112.45
3	3	208	ALA	CA-C-N	5.08	125.87	119.98
3	3	208	ALA	C-N-CA	5.08	125.87	119.98
3	3	100	LEU	N-CA-C	-5.04	105.87	111.36

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	0	1833	0	1774	134	3
2	1	1717	0	1674	135	8
3	3	1845	0	1822	141	1
All	All	5395	0	5270	366	9

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 34.

All (366) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:20:VAL:HG22	3:3:21:SER:H	1.17	1.06
3:3:206:ILE:HD12	3:3:206:ILE:H	1.23	1.01
1:0:233:TYR:HA	3:3:66:MET:HE3	1.43	0.99
2:1:229:MET:HE2	2:1:231:GLY:H	1.28	0.98
3:3:109:THR:HB	3:3:228:LEU:HB3	1.52	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:58:VAL:HG23	3:3:59:PRO:HD3	1.50	0.90
2:1:76:ALA:O	2:1:79:THR:HG23	1.73	0.88
2:1:112:ASP:OD2	2:1:114:THR:HG22	1.75	0.86
3:3:167:LEU:HD12	3:3:168:VAL:N	1.91	0.86
3:3:188:TYR:O	3:3:189:TYR:HB3	1.75	0.85
3:3:172:ILE:HD12	3:3:172:ILE:O	1.75	0.85
2:1:141:THR:OG1	2:1:143:THR:HG23	1.79	0.83
2:1:121:ARG:HG2	2:1:121:ARG:HH11	1.43	0.82
1:0:241:ILE:HG21	3:3:66:MET:HE1	1.61	0.82
2:1:218:LYS:HD3	2:1:219:ASP:N	1.96	0.81
3:3:85:VAL:HG21	3:3:142:LEU:HD12	1.62	0.81
2:1:218:LYS:HD3	2:1:219:ASP:H	1.43	0.81
3:3:58:VAL:HG23	3:3:59:PRO:CD	2.10	0.81
1:0:117:THR:HB	1:0:120:ASP:HB3	1.63	0.80
2:1:276:ASN:HB2	2:1:277:PRO:HD2	1.64	0.79
3:3:178:ARG:NH1	3:3:187:ASP:HB3	1.97	0.79
2:1:197:PRO:HD2	2:1:227:ASN:HB2	1.65	0.78
2:1:112:ASP:CG	2:1:114:THR:HG22	2.09	0.78
2:1:139:ALA:HB2	2:1:249:VAL:HG22	1.65	0.77
1:0:233:TYR:CA	3:3:66:MET:HE3	2.15	0.76
3:3:179:ALA:HA	3:3:184:GLY:HA2	1.66	0.76
3:3:20:VAL:HG22	3:3:21:SER:N	1.95	0.76
1:0:188:GLN:NE2	3:3:209:PRO:HB2	2.01	0.75
3:3:84:ALA:HB3	3:3:196:ILE:HD11	1.66	0.75
3:3:73:VAL:HA	3:3:198:TYR:OH	1.87	0.74
3:3:20:VAL:CG2	3:3:21:SER:H	1.98	0.74
1:0:125:PRO:HB3	1:0:129:VAL:HG21	1.71	0.73
2:1:100:THR:HG23	2:1:101:THR:H	1.52	0.73
1:0:139:LEU:HD22	1:0:300:VAL:HB	1.70	0.72
2:1:121:ARG:HD2	2:1:267:ARG:HB3	1.70	0.72
3:3:131:MET:HG2	3:3:159:PHE:HE1	1.53	0.72
3:3:42:ASN:OD1	3:3:44:LEU:HB2	1.89	0.72
2:1:177:PRO:HB2	3:3:24:ILE:HD11	1.70	0.71
3:3:83:CYS:HB3	3:3:196:ILE:HG13	1.73	0.71
2:1:229:MET:HE3	2:1:230:MET:H	1.55	0.71
2:1:168:SER:C	2:1:170:ALA:H	1.99	0.71
3:3:178:ARG:HH11	3:3:178:ARG:HB2	1.54	0.71
1:0:201:ILE:HG22	1:0:202:GLY:N	2.05	0.70
2:1:141:THR:HB	2:1:142:PRO:HD2	1.73	0.70
3:3:239:GLY:O	3:3:240:THR:C	2.33	0.70
1:0:128:SER:OG	1:0:160:VAL:HG11	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:229:MET:HE2	2:1:231:GLY:N	2.04	0.68
2:1:218:LYS:O	2:1:219:ASP:HB2	1.93	0.68
2:1:121:ARG:HG2	2:1:121:ARG:NH1	2.08	0.67
2:1:158:PRO:HD3	2:1:231:GLY:HA2	1.76	0.67
2:1:194:PHE:CZ	2:1:200:ALA:HA	2.31	0.66
2:1:229:MET:HE3	2:1:230:MET:N	2.10	0.66
2:1:153:TYR:CD1	2:1:235:VAL:HG13	2.31	0.65
3:3:6:LEU:HD12	3:3:10:THR:HG21	1.77	0.65
3:3:204:VAL:HG13	3:3:208:ALA:HB3	1.79	0.64
2:1:168:SER:O	2:1:170:ALA:N	2.31	0.64
3:3:206:ILE:H	3:3:206:ILE:CD1	1.98	0.63
2:1:104:ASN:HA	2:1:242:LYS:NZ	2.14	0.63
1:0:179:VAL:HG22	1:0:305:ILE:HG12	1.79	0.63
1:0:203:THR:H	1:0:215:PRO:HG3	1.62	0.63
2:1:78:THR:HG22	3:3:43:LEU:HB2	1.79	0.63
1:0:171:TYR:CG	1:0:275:ALA:HB2	2.34	0.63
2:1:85:SER:O	2:1:86:ARG:HB2	1.97	0.63
3:3:50:GLU:HA	3:3:219:ALA:HB2	1.80	0.62
2:1:156:VAL:HB	2:1:232:THR:HB	1.81	0.62
2:1:112:ASP:OD1	2:1:114:THR:HG22	1.99	0.62
3:3:115:LEU:HD11	3:3:172:ILE:HG12	1.82	0.61
2:1:153:TYR:HD1	2:1:235:VAL:HG13	1.64	0.61
3:3:178:ARG:HH11	3:3:187:ASP:HB3	1.64	0.61
2:1:128:TYR:HB2	2:1:261:TRP:HB2	1.82	0.61
3:3:225:THR:HG22	3:3:226:MET:N	2.15	0.61
1:0:88:GLY:C	1:0:90:SER:H	2.08	0.60
2:1:130:ARG:NE	3:3:33:CYS:HB3	2.16	0.60
3:3:2:PHE:CD1	3:3:3:PRO:HD2	2.36	0.60
3:3:225:THR:O	3:3:226:MET:HG2	2.00	0.60
1:0:129:VAL:HG13	1:0:161:PHE:HD1	1.65	0.60
3:3:10:THR:HG22	3:3:11:ASN:ND2	2.16	0.60
3:3:131:MET:HG2	3:3:159:PHE:CE1	2.37	0.60
2:1:189:GLN:HG3	3:3:21:SER:HB3	1.82	0.60
1:0:120:ASP:O	1:0:122:PRO:HD3	2.03	0.59
2:1:189:GLN:HG3	3:3:21:SER:CB	2.32	0.59
1:0:148:TYR:HB3	1:0:284:LEU:HD23	1.85	0.58
1:0:168:HIS:CD2	1:0:314:PHE:HB3	2.38	0.58
2:1:158:PRO:HD3	2:1:231:GLY:CA	2.33	0.58
2:1:276:ASN:HB2	2:1:277:PRO:CD	2.34	0.58
1:0:171:TYR:CB	1:0:275:ALA:HB2	2.33	0.58
3:3:178:ARG:HG2	3:3:179:ALA:H	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:177:ILE:HG21	1:0:283:LEU:CD1	2.33	0.57
2:1:135:PHE:CD1	2:1:253:MET:HB2	2.40	0.57
1:0:195:ILE:HG13	1:0:281:PHE:CE2	2.39	0.57
2:1:168:SER:C	2:1:170:ALA:N	2.62	0.57
1:0:201:ILE:CG2	1:0:202:GLY:N	2.68	0.57
1:0:171:TYR:HB3	1:0:275:ALA:HB2	1.85	0.56
3:3:14:LEU:HB3	3:3:17:ASP:HB2	1.86	0.56
2:1:254:ARG:HB3	2:1:254:ARG:HH11	1.70	0.56
1:0:92:ILE:HG13	1:0:92:ILE:O	2.04	0.56
1:0:178:HIS:HE1	1:0:259:CYS:HB2	1.69	0.56
2:1:139:ALA:CB	2:1:249:VAL:HG22	2.33	0.56
2:1:254:ARG:HB3	2:1:254:ARG:NH1	2.20	0.56
3:3:150:MET:HE2	3:3:150:MET:O	2.05	0.56
1:0:119:VAL:HG12	1:0:119:VAL:O	2.06	0.56
2:1:154:MET:HE1	2:1:171:TRP:HA	1.87	0.56
3:3:52:ILE:HA	3:3:217:LEU:HD23	1.87	0.56
2:1:93:ILE:HD11	2:1:109:TRP:HB2	1.86	0.56
2:1:280:ALA:CB	2:1:283:SER:HB3	2.36	0.56
3:3:65:LEU:O	3:3:68:ARG:HG3	2.06	0.56
1:0:155:LEU:C	1:0:157:GLU:N	2.62	0.56
2:1:120:ARG:HH11	3:3:237:GLN:HE22	1.53	0.56
1:0:90:SER:OG	1:0:132:PHE:HB2	2.06	0.56
1:0:239:ILE:O	1:0:239:ILE:HG13	2.06	0.55
2:1:174:ALA:C	2:1:176:ASN:H	2.14	0.55
1:0:240:PRO:HG3	1:0:243:GLN:NE2	2.22	0.55
1:0:241:ILE:CG2	3:3:66:MET:HE1	2.35	0.55
2:1:94:ASP:O	2:1:95:LEU:HD23	2.07	0.55
2:1:195:MET:O	2:1:196:SER:O	2.25	0.55
3:3:9:GLY:HA2	3:3:12:GLN:OE1	2.08	0.54
3:3:50:GLU:HA	3:3:218:ALA:O	2.06	0.54
1:0:115:ASP:C	1:0:117:THR:H	2.14	0.54
1:0:125:PRO:HG2	1:0:314:PHE:CD2	2.42	0.54
1:0:155:LEU:C	1:0:157:GLU:H	2.14	0.54
2:1:123:VAL:HG23	2:1:124:GLU:N	2.22	0.54
1:0:162:GLY:O	1:0:166:GLN:HG3	2.07	0.54
1:0:177:ILE:HG21	1:0:283:LEU:HD11	1.89	0.54
2:1:92:GLU:HG3	2:1:250:ARG:HG2	1.89	0.54
3:3:6:LEU:CD1	3:3:10:THR:HG21	2.37	0.54
3:3:30:PRO:O	3:3:31:THR:C	2.49	0.54
3:3:167:LEU:HD12	3:3:168:VAL:H	1.72	0.54
1:0:134:THR:HG23	1:0:306:THR:HG23	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:137:THR:HG21	1:0:302:PRO:HB2	1.88	0.54
3:3:91:GLY:HA3	3:3:111:TRP:CZ2	2.43	0.54
1:0:188:GLN:HB3	3:3:124:SER:HA	1.89	0.54
1:0:235:LEU:HD12	1:0:239:ILE:CD1	2.37	0.54
1:0:271:PRO:HG2	1:0:272:PHE:H	1.73	0.54
2:1:261:TRP:NE1	3:3:39:GLU:HB2	2.23	0.54
1:0:233:TYR:HA	3:3:66:MET:CE	2.30	0.54
2:1:93:ILE:HG13	2:1:235:VAL:HG21	1.89	0.54
1:0:125:PRO:HB3	1:0:129:VAL:CG2	2.37	0.53
3:3:174:ASN:OD1	3:3:174:ASN:O	2.25	0.53
1:0:111:CYS:SG	1:0:115:ASP:OD1	2.67	0.53
1:0:250:GLN:HG2	1:0:260:ALA:HB1	1.89	0.53
1:0:140:TRP:CE2	1:0:291:LEU:HB2	2.44	0.53
3:3:225:THR:HG22	3:3:226:MET:H	1.74	0.53
1:0:84:GLN:HB3	1:0:93:THR:HA	1.90	0.53
2:1:204:PHE:CD1	2:1:204:PHE:N	2.77	0.53
3:3:61:ASN:ND2	3:3:64:SER:OG	2.42	0.53
3:3:56:ASN:O	3:3:68:ARG:HA	2.09	0.53
2:1:171:TRP:CZ3	2:1:236:ARG:HG2	2.44	0.53
3:3:18:ASP:O	3:3:19:GLY:O	2.27	0.53
1:0:100:ILE:HG22	1:0:261:THR:HB	1.90	0.52
1:0:183:ALA:HB2	1:0:301:ILE:HG21	1.91	0.52
2:1:208:TYR:HE1	2:1:222:TYR:HB2	1.75	0.52
1:0:208:THR:HA	2:1:282:ASN:OD1	2.08	0.52
3:3:54:GLU:O	3:3:95:PRO:HB3	2.10	0.52
2:1:158:PRO:HB3	2:1:229:MET:HG3	1.91	0.52
1:0:197:PRO:HG2	2:1:262:ILE:HG21	1.91	0.52
3:3:74:SER:HB2	3:3:211:THR:OG1	2.10	0.52
2:1:180:PHE:CD1	2:1:180:PHE:N	2.78	0.52
2:1:80:LEU:HD21	2:1:260:ALA:HB3	1.92	0.52
3:3:54:GLU:HG3	3:3:98:SER:CB	2.40	0.52
3:3:91:GLY:HA3	3:3:111:TRP:HZ2	1.75	0.52
3:3:79:LYS:HB2	3:3:79:LYS:NZ	2.25	0.51
2:1:194:PHE:HZ	2:1:200:ALA:HA	1.73	0.51
2:1:166:ARG:HG2	2:1:166:ARG:HH11	1.74	0.51
3:3:167:LEU:HD12	3:3:167:LEU:C	2.36	0.51
3:3:218:ALA:O	3:3:219:ALA:HB2	2.11	0.51
3:3:44:LEU:HD21	3:3:224:PHE:HB3	1.92	0.51
3:3:128:THR:HG23	3:3:203:VAL:HB	1.93	0.51
1:0:123:THR:O	1:0:125:PRO:HD3	2.11	0.50
2:1:87:ALA:HA	2:1:254:ARG:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:260:ALA:O	3:3:39:GLU:HG3	2.11	0.50
1:0:188:GLN:HG2	3:3:209:PRO:HG2	1.92	0.50
1:0:204:VAL:O	1:0:205:ALA:HB3	2.12	0.50
1:0:265:PRO:O	1:0:267:ILE:HG13	2.11	0.50
1:0:154:VAL:HG23	1:0:224:ALA:HA	1.92	0.50
2:1:156:VAL:HG22	2:1:176:ASN:ND2	2.26	0.50
2:1:166:ARG:NH2	2:1:237:THR:OG1	2.45	0.50
2:1:203:TRP:HB2	2:1:204:PHE:CD1	2.47	0.50
1:0:182:ASN:O	1:0:301:ILE:HG23	2.11	0.50
1:0:255:ARG:HG3	1:0:256:THR:HG23	1.93	0.50
1:0:307:LEU:N	1:0:307:LEU:HD23	2.27	0.50
2:1:135:PHE:CE1	2:1:253:MET:HB2	2.46	0.50
1:0:201:ILE:HG22	1:0:202:GLY:H	1.75	0.49
2:1:280:ALA:HB1	2:1:283:SER:HB3	1.95	0.49
3:3:142:LEU:HD23	3:3:142:LEU:O	2.12	0.49
1:0:252:ILE:HG22	1:0:252:ILE:O	2.12	0.49
2:1:104:ASN:HA	2:1:242:LYS:HZ2	1.78	0.49
2:1:220:LEU:N	2:1:220:LEU:HD23	2.28	0.49
1:0:293:TYR:CE1	1:0:299:PRO:HA	2.48	0.48
2:1:127:THR:OG1	2:1:264:ARG:NH2	2.46	0.48
2:1:113:ILE:HG22	2:1:253:MET:SD	2.53	0.48
1:0:125:PRO:CB	1:0:129:VAL:HG21	2.43	0.48
1:0:129:VAL:HG22	1:0:164:ASN:ND2	2.29	0.48
2:1:73:HIS:HA	3:3:225:THR:HG21	1.94	0.48
2:1:129:MET:HE2	2:1:131:PHE:CD2	2.48	0.48
2:1:203:TRP:C	2:1:204:PHE:CD1	2.91	0.48
1:0:92:ILE:HG12	1:0:132:PHE:CE1	2.47	0.48
2:1:210:THR:O	2:1:210:THR:HG22	2.14	0.48
3:3:92:ARG:HD3	3:3:188:TYR:HD2	1.78	0.48
1:0:216:PRO:HD2	1:0:219:GLN:OE1	2.14	0.48
2:1:122:LYS:HG3	3:3:107:TYR:CE1	2.49	0.48
1:0:243:GLN:HA	3:3:51:THR:HG22	1.95	0.48
1:0:276:LEU:HD12	1:0:276:LEU:N	2.29	0.48
1:0:92:ILE:HG21	1:0:306:THR:HG21	1.96	0.48
1:0:129:VAL:CG1	1:0:161:PHE:HD1	2.27	0.48
1:0:185:LYS:HD3	3:3:125:PHE:CD1	2.48	0.48
2:1:238:VAL:HG12	2:1:239:GLY:N	2.29	0.48
1:0:125:PRO:HG2	1:0:314:PHE:CE2	2.49	0.47
3:3:130:LYS:HB2	3:3:200:THR:HG23	1.95	0.47
1:0:108:PRO:CB	1:0:174:GLY:HA3	2.44	0.47
2:1:167:GLU:N	2:1:167:GLU:CD	2.71	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:268:ASN:OD1	2:1:269:GLN:HG2	2.14	0.47
3:3:170:PRO:HG2	3:3:171:TRP:H	1.79	0.47
2:1:123:VAL:C	2:1:125:LEU:H	2.20	0.47
3:3:109:THR:OG1	3:3:228:LEU:HD12	2.15	0.47
2:1:94:ASP:C	2:1:95:LEU:HD23	2.39	0.47
3:3:204:VAL:CG1	3:3:208:ALA:HB3	2.44	0.47
1:0:176:CYS:SG	1:0:263:ILE:HD13	2.55	0.47
1:0:201:ILE:CG2	1:0:202:GLY:H	2.27	0.47
1:0:235:LEU:HD12	1:0:239:ILE:HD12	1.97	0.47
2:1:266:MET:O	2:1:267:ARG:C	2.57	0.47
3:3:71:PHE:CE1	3:3:214:ILE:HB	2.50	0.47
3:3:182:ARG:NH2	3:3:182:ARG:HG3	2.29	0.47
1:0:96:GLU:O	1:0:97:ALA:HB2	2.15	0.47
1:0:110:TYR:O	1:0:111:CYS:HB2	2.15	0.47
1:0:195:ILE:HG12	1:0:264:VAL:CG2	2.44	0.47
2:1:290:SER:OG	3:3:68:ARG:NH2	2.48	0.47
1:0:100:ILE:HD12	1:0:100:ILE:O	2.15	0.46
2:1:229:MET:HE3	2:1:229:MET:HA	1.97	0.46
2:1:154:MET:CE	2:1:171:TRP:HA	2.45	0.46
3:3:121:PHE:CE2	3:3:123:GLY:HA3	2.50	0.46
1:0:258:ASN:CG	1:0:259:CYS:N	2.74	0.46
3:3:148:THR:HA	3:3:151:LEU:HD12	1.97	0.46
1:0:258:ASN:CG	1:0:259:CYS:H	2.24	0.46
3:3:22:ALA:HB1	3:3:23:PRO:HD2	1.97	0.46
3:3:146:ARG:NH1	3:3:146:ARG:HG2	2.31	0.46
3:3:115:LEU:HB2	3:3:169:ILE:HB	1.97	0.46
3:3:188:TYR:C	3:3:190:THR:H	2.24	0.46
1:0:250:GLN:CG	1:0:260:ALA:HB1	2.47	0.45
2:1:126:PHE:CG	2:1:260:ALA:HB1	2.50	0.45
3:3:58:VAL:H	3:3:59:PRO:HD2	1.81	0.45
1:0:172:ARG:HB3	1:0:272:PHE:CE1	2.50	0.45
2:1:156:VAL:O	2:1:156:VAL:HG12	2.17	0.45
2:1:157:PRO:O	2:1:158:PRO:C	2.60	0.45
3:3:14:LEU:HD22	3:3:16:THR:H	1.82	0.45
1:0:128:SER:CB	1:0:160:VAL:HG11	2.46	0.45
3:3:90:PRO:HD2	3:3:188:TYR:OH	2.17	0.45
1:0:88:GLY:C	1:0:90:SER:N	2.74	0.45
1:0:310:MET:O	1:0:311:CYS:HB2	2.17	0.45
3:3:6:LEU:N	3:3:6:LEU:HD23	2.32	0.45
1:0:89:ASN:ND2	1:0:131:ARG:HH21	2.14	0.45
1:0:191:LEU:HD23	1:0:287:PRO:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:238:VAL:CG1	2:1:239:GLY:N	2.79	0.45
2:1:261:TRP:CD1	3:3:36:ILE:HB	2.52	0.45
3:3:84:ALA:HB3	3:3:196:ILE:CD1	2.43	0.45
1:0:129:VAL:CG2	1:0:164:ASN:ND2	2.81	0.44
1:0:183:ALA:HB2	1:0:301:ILE:CG2	2.47	0.44
1:0:283:LEU:C	1:0:283:LEU:HD23	2.42	0.44
1:0:83:ALA:HB3	1:0:96:GLU:HA	1.98	0.44
1:0:141:GLU:C	1:0:143:SER:N	2.75	0.44
2:1:74:SER:C	2:1:76:ALA:H	2.24	0.44
2:1:174:ALA:C	2:1:176:ASN:N	2.73	0.44
3:3:61:ASN:OD1	3:3:62:ALA:N	2.50	0.44
2:1:125:LEU:HD23	2:1:126:PHE:CZ	2.52	0.44
2:1:242:LYS:HG3	2:1:243:SER:N	2.32	0.44
3:3:24:ILE:HG23	3:3:25:LEU:HD13	1.98	0.44
3:3:54:GLU:HG2	3:3:69:LEU:HD23	1.99	0.44
1:0:197:PRO:HG2	2:1:262:ILE:CG2	2.48	0.44
1:0:317:LEU:HD23	1:0:318:ARG:N	2.32	0.44
3:3:118:THR:HG23	3:3:166:THR:OG1	2.17	0.44
3:3:227:LYS:HB3	3:3:227:LYS:HE2	1.80	0.44
1:0:152:PRO:HD2	1:0:279:CYS:HA	2.00	0.44
2:1:80:LEU:HD12	2:1:80:LEU:HA	1.79	0.44
2:1:116:TYR:HE2	2:1:118:GLN:HE21	1.66	0.44
2:1:195:MET:O	2:1:196:SER:C	2.60	0.44
1:0:273:ASP:OD1	1:0:274:SER:N	2.51	0.44
2:1:229:MET:CE	2:1:230:MET:N	2.79	0.44
2:1:261:TRP:CD1	3:3:39:GLU:HB2	2.53	0.44
1:0:156:THR:HA	1:0:162:GLY:HA2	1.99	0.44
2:1:245:TYR:CD1	2:1:245:TYR:N	2.85	0.43
3:3:60:THR:O	3:3:61:ASN:C	2.60	0.43
1:0:190:ALA:HB3	1:0:289:SER:HB3	1.99	0.43
2:1:104:ASN:O	2:1:166:ARG:HD2	2.18	0.43
2:1:119:MET:CE	2:1:255:MET:HE3	2.48	0.43
2:1:201:TYR:HA	2:1:228:ASN:HD21	1.81	0.43
2:1:294:ILE:CD1	3:3:71:PHE:HB3	2.47	0.43
1:0:100:ILE:HD12	1:0:100:ILE:C	2.43	0.43
1:0:233:TYR:CD2	3:3:65:LEU:HB3	2.53	0.43
2:1:78:THR:HB	3:3:42:ASN:HD21	1.83	0.43
2:1:294:ILE:HD12	3:3:56:ASN:HA	1.99	0.43
3:3:132:LEU:C	3:3:132:LEU:HD23	2.44	0.43
3:3:46:LEU:O	3:3:49:VAL:HG23	2.18	0.43
2:1:197:PRO:CD	2:1:227:ASN:HB2	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:178:ARG:HG2	3:3:179:ALA:N	2.34	0.43
1:0:129:VAL:CG2	1:0:164:ASN:HD21	2.32	0.43
1:0:141:GLU:C	1:0:143:SER:H	2.27	0.43
2:1:297:LEU:HD23	3:3:85:VAL:CG2	2.49	0.43
3:3:135:TYR:CD1	3:3:169:ILE:HD12	2.54	0.43
1:0:84:GLN:NE2	1:0:91:THR:HG21	2.34	0.43
1:0:245:THR:C	1:0:247:CYS:H	2.27	0.43
1:0:195:ILE:HG12	1:0:264:VAL:HG21	2.00	0.43
1:0:85:LEU:HD12	1:0:94:THR:HG21	2.01	0.42
2:1:123:VAL:CG2	2:1:124:GLU:N	2.81	0.42
1:0:121:LYS:HD2	1:0:121:LYS:H	1.84	0.42
1:0:235:LEU:O	1:0:236:ASP:HB2	2.19	0.42
1:0:253:ASN:HD21	3:3:122:THR:HA	1.84	0.42
2:1:156:VAL:HA	2:1:157:PRO:HD2	1.84	0.42
1:0:84:GLN:CB	1:0:93:THR:HA	2.49	0.42
1:0:121:LYS:HB3	1:0:121:LYS:HE3	1.79	0.42
1:0:175:PHE:HB3	1:0:176:CYS:H	1.67	0.42
2:1:222:TYR:C	2:1:224:ALA:H	2.27	0.42
1:0:203:THR:N	1:0:215:PRO:HG3	2.34	0.42
3:3:133:ILE:HG12	3:3:196:ILE:HG22	2.02	0.42
2:1:81:ASP:O	2:1:85:SER:HB3	2.20	0.42
3:3:182:ARG:HG3	3:3:182:ARG:HH21	1.84	0.42
2:1:177:PRO:HB2	3:3:24:ILE:CD1	2.45	0.42
1:0:110:TYR:CE1	1:0:124:ARG:HB3	2.55	0.42
1:0:160:VAL:O	1:0:163:GLN:HB3	2.19	0.42
3:3:25:LEU:HB3	3:3:28:PHE:HB2	2.02	0.42
3:3:89:ASP:HA	3:3:188:TYR:CZ	2.55	0.42
1:0:185:LYS:HB3	3:3:125:PHE:HD1	1.85	0.42
2:1:73:HIS:O	2:1:74:SER:C	2.63	0.42
2:1:114:THR:C	2:1:116:TYR:N	2.78	0.42
3:3:187:ASP:O	3:3:188:TYR:C	2.63	0.42
1:0:149:TRP:HZ3	1:0:285:VAL:CG1	2.33	0.41
2:1:126:PHE:CD2	2:1:260:ALA:HB1	2.55	0.41
1:0:90:SER:CB	1:0:132:PHE:HB2	2.51	0.41
3:3:79:LYS:HB2	3:3:79:LYS:HZ2	1.84	0.41
3:3:84:ALA:CB	3:3:196:ILE:HD11	2.45	0.41
3:3:90:PRO:O	3:3:102:GLY:HA2	2.20	0.41
1:0:216:PRO:C	1:0:218:LYS:H	2.28	0.41
2:1:116:TYR:HE2	2:1:118:GLN:NE2	2.17	0.41
3:3:63:THR:O	3:3:63:THR:OG1	2.37	0.41
1:0:220:THR:HG23	2:1:222:TYR:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:117:ALA:HB1	3:3:236:LEU:HD22	2.03	0.41
2:1:199:SER:OG	3:3:34:ILE:HG12	2.20	0.41
1:0:186:PHE:CE1	3:3:126:MET:HG3	2.55	0.41
1:0:239:ILE:HB	2:1:265:PRO:HB2	2.00	0.41
2:1:120:ARG:HH11	3:3:237:GLN:NE2	2.16	0.41
2:1:180:PHE:HD1	2:1:180:PHE:H	1.69	0.41
3:3:24:ILE:HD12	3:3:24:ILE:HA	1.90	0.41
1:0:151:PHE:N	1:0:151:PHE:CD1	2.88	0.41
3:3:177:TYR:HA	3:3:186:PHE:HA	2.03	0.41
3:3:170:PRO:O	3:3:171:TRP:HB2	2.20	0.41
3:3:183:ASP:O	3:3:185:VAL:N	2.50	0.41
1:0:153:ASP:O	1:0:154:VAL:C	2.64	0.41
1:0:155:LEU:HD23	1:0:155:LEU:HA	1.94	0.41
2:1:235:VAL:HG11	2:1:249:VAL:HG21	2.01	0.41
2:1:297:LEU:HD23	3:3:85:VAL:HG22	2.03	0.41
3:3:144:LYS:HD3	3:3:148:THR:HG21	2.02	0.41
1:0:92:ILE:HG12	1:0:132:PHE:HE1	1.85	0.41
1:0:108:PRO:HB3	1:0:174:GLY:HA3	2.03	0.41
2:1:118:GLN:HG3	3:3:231:ASP:HB3	2.03	0.41
2:1:157:PRO:HA	2:1:158:PRO:HD2	1.97	0.41
2:1:266:MET:HE1	3:3:107:TYR:CE2	2.56	0.41
3:3:74:SER:CB	3:3:211:THR:OG1	2.69	0.41
3:3:162:GLN:O	3:3:162:GLN:HG3	2.21	0.41
1:0:297:ALA:O	1:0:298:THR:C	2.62	0.40
2:1:94:ASP:C	2:1:96:PRO:HD3	2.47	0.40
2:1:272:LEU:HD23	2:1:272:LEU:HA	1.89	0.40
1:0:115:ASP:C	1:0:117:THR:N	2.79	0.40
3:3:191:THR:C	3:3:192:GLY:O	2.61	0.40
1:0:168:HIS:CG	1:0:314:PHE:HB3	2.56	0.40
1:0:177:ILE:HG22	1:0:178:HIS:N	2.37	0.40
1:0:170:LEU:HB3	1:0:272:PHE:HB3	2.04	0.40
1:0:205:ALA:HB2	2:1:278:ASN:HD22	1.86	0.40
3:3:90:PRO:HG2	3:3:115:LEU:HD11	2.02	0.40

All (9) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:208:THR:CG2	2:1:283:SER:OG[13_454]	1.16	1.04
1:0:208:THR:CG2	2:1:283:SER:CB[13_454]	1.57	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:282:ASN:ND2	2:1:283:SER:N[13_454]	1.68	0.52
3:3:63:THR:CG2	3:3:63:THR:CG2[13_454]	1.71	0.49
2:1:282:ASN:O	2:1:282:ASN:CB[13_454]	1.75	0.45
1:0:207:GLY:CA	2:1:285:LYS:NZ[13_454]	1.88	0.32
2:1:282:ASN:C	2:1:282:ASN:CB[13_454]	1.96	0.24
2:1:282:ASN:CG	2:1:282:ASN:ND2[13_454]	1.99	0.21
2:1:282:ASN:OD1	2:1:282:ASN:ND2[13_454]	2.03	0.17

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	0	235/323 (73%)	175 (74%)	42 (18%)	18 (8%)	1	12
2	1	214/297 (72%)	171 (80%)	27 (13%)	16 (8%)	1	12
3	3	238/242 (98%)	187 (79%)	34 (14%)	17 (7%)	1	13
All	All	687/862 (80%)	533 (78%)	103 (15%)	51 (7%)	1	12

All (51) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	0	97	ALA
1	0	112	SER
1	0	127	VAL
2	1	169	LEU
2	1	196	SER
2	1	226	PRO
2	1	227	ASN
2	1	275	ALA
3	3	92	ARG
3	3	180	HIS
3	3	186	PHE
1	0	98	ALA

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Mol	Chain	Res	Type
1	0	316	GLY
2	1	282	ASN
2	1	289	ALA
3	3	19	GLY
3	3	140	GLY
3	3	177	TYR
1	0	110	TYR
1	0	113	ASP
1	0	176	CYS
1	0	258	ASN
2	1	75	THR
3	3	147	ALA
3	3	182	ARG
3	3	188	TYR
3	3	219	ALA
3	3	228	LEU
1	0	154	VAL
1	0	157	GLU
1	0	223	GLY
1	0	280	ASN
2	1	124	GLU
2	1	167	GLU
2	1	219	ASP
2	1	228	ASN
3	3	43	LEU
1	0	203	THR
1	0	215	PRO
1	0	235	LEU
2	1	79	THR
3	3	189	TYR
1	0	207	GLY
3	3	58	VAL
1	0	125	PRO
2	1	158	PRO
3	3	72	PRO
3	3	184	GLY
3	3	90	PRO
2	1	187	PRO
2	1	223	GLY

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	0	201/272 (74%)	188 (94%)	13 (6%)	15	42
2	1	186/250 (74%)	167 (90%)	19 (10%)	7	26
3	3	200/202 (99%)	177 (88%)	23 (12%)	5	22
All	All	587/724 (81%)	532 (91%)	55 (9%)	8	29

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	121	LYS
1	0	157	GLU
1	0	171	TYR
1	0	181	CYS
1	0	195	ILE
1	0	225	ASP
1	0	242	SER
1	0	276	LEU
1	0	294	ASP
1	0	295	GLN
1	0	298	THR
1	0	306	THR
1	0	307	LEU
2	1	78	THR
2	1	80	LEU
2	1	100	THR
2	1	118	GLN
2	1	121	ARG
2	1	143	THR
2	1	167	GLU
2	1	172	GLN
2	1	175	THR
2	1	179	VAL
2	1	181	VAL
2	1	184	SER
2	1	202	GLN

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Mol	Chain	Res	Type
2	1	204	PHE
2	1	220	LEU
2	1	228	ASN
2	1	237	THR
2	1	245	TYR
2	1	270	ASN
3	3	6	LEU
3	3	14	LEU
3	3	44	LEU
3	3	51	THR
3	3	53	LEU
3	3	58	VAL
3	3	61	ASN
3	3	63	THR
3	3	72	PRO
3	3	79	LYS
3	3	87	ARG
3	3	90	PRO
3	3	150	MET
3	3	159	PHE
3	3	167	LEU
3	3	178	ARG
3	3	191	THR
3	3	204	VAL
3	3	206	ILE
3	3	211	THR
3	3	226	MET
3	3	228	LEU
3	3	230	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	130	ASN
1	0	164	ASN
1	0	168	HIS
1	0	188	GLN
1	0	214	HIS
1	0	257	ASN
2	1	118	GLN
2	1	172	GLN
2	1	176	ASN

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Mol	Chain	Res	Type
2	1	202	GLN
2	1	278	ASN
3	3	110	GLN
3	3	176	HIS

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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	0	237/323 (73%)	3.01	142 (59%) 0 1	89, 133, 217, 234	0
2	1	218/297 (73%)	1.75	64 (29%) 1 3	84, 110, 155, 200	0
3	3	240/242 (99%)	2.06	99 (41%) 0 1	80, 112, 189, 230	0
All	All	695/862 (80%)	2.29	305 (43%) 0 1	80, 114, 211, 234	0

All (305) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	0	97	ALA	16.0
1	0	96	GLU	13.4
3	3	179	ALA	10.9
1	0	126	ASP	9.2
1	0	130	ASN	9.1
1	0	112	SER	9.1
1	0	99	ASN	8.8
1	0	121	LYS	8.8
1	0	113	ASP	8.7
1	0	211	GLU	8.4
1	0	123	THR	8.2
2	1	99	GLY	7.7
1	0	98	ALA	7.7
2	1	218	LYS	7.6
1	0	110	TYR	7.5
3	3	182	ARG	7.5
1	0	84	GLN	7.2
1	0	88	GLY	7.2
3	3	178	ARG	7.1
3	3	234	ASP	7.1
1	0	120	ASP	7.1
1	0	212	ASP	7.1
1	0	83	ALA	7.0

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Mol	Chain	Res	Type	RSRZ
3	3	181	ALA	7.0
1	0	111	CYS	6.8
3	3	189	TYR	6.7
1	0	86	THR	6.7
1	0	206	GLY	6.5
1	0	95	GLN	6.5
1	0	116	ALA	6.4
1	0	210	THR	6.4
2	1	219	ASP	6.3
1	0	119	VAL	6.2
1	0	129	VAL	6.2
1	0	87	ILE	6.2
3	3	177	TYR	6.1
1	0	115	ASP	6.0
3	3	183	ASP	5.9
1	0	125	PRO	5.8
3	3	186	PHE	5.8
3	3	180	HIS	5.8
2	1	73	HIS	5.8
2	1	100	THR	5.8
2	1	92	GLU	5.6
1	0	316	GLY	5.5
1	0	114	SER	5.5
1	0	318	ARG	5.4
1	0	128	SER	5.3
3	3	63	THR	5.3
1	0	209	GLY	5.3
1	0	217	TYR	5.2
1	0	279	CYS	5.2
2	1	223	GLY	5.1
1	0	109	SER	5.1
3	3	240	THR	5.1
1	0	136	ASP	5.1
1	0	82	VAL	5.1
1	0	101	ILE	5.1
1	0	296	GLY	5.0
3	3	222	LYS	4.9
1	0	118	ALA	4.9
1	0	163	GLN	4.8
1	0	117	THR	4.8
1	0	127	VAL	4.8
1	0	317	LEU	4.7

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Mol	Chain	Res	Type	RSRZ
1	0	122	PRO	4.7
3	3	184	GLY	4.7
1	0	207	GLY	4.7
1	0	157	GLU	4.7
2	1	98	GLU	4.7
3	3	128	THR	4.7
1	0	167	PHE	4.6
1	0	146	GLY	4.6
3	3	1	GLY	4.5
1	0	144	SER	4.5
1	0	124	ARG	4.4
3	3	190	THR	4.4
2	1	220	LEU	4.4
3	3	185	VAL	4.4
3	3	27	ASN	4.3
3	3	187	ASP	4.3
1	0	85	LEU	4.2
2	1	74	SER	4.2
1	0	228	GLU	4.2
1	0	105	GLY	4.2
1	0	183	ALA	4.1
3	3	176	HIS	4.1
1	0	108	PRO	4.1
2	1	162	LYS	4.1
2	1	172	GLN	4.1
3	3	32	PRO	4.1
1	0	102	VAL	4.1
2	1	94	ASP	4.0
1	0	213	SER	4.0
3	3	19	GLY	3.9
3	3	162	GLN	3.9
2	1	221	GLU	3.9
1	0	203	THR	3.9
1	0	134	THR	3.9
2	1	210	THR	3.9
3	3	20	VAL	3.9
3	3	123	GLY	3.9
3	3	160	GLY	3.9
1	0	166	GLN	3.8
3	3	239	GLY	3.8
1	0	225	ASP	3.8
1	0	219	GLN	3.8

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Mol	Chain	Res	Type	RSRZ
1	0	93	THR	3.8
2	1	159	GLY	3.8
1	0	298	THR	3.7
1	0	185	LYS	3.7
1	0	107	TRP	3.7
3	3	66	MET	3.6
3	3	237	GLN	3.6
1	0	145	LYS	3.6
1	0	147	TRP	3.6
1	0	106	GLU	3.6
1	0	218	LYS	3.6
2	1	208	TYR	3.6
1	0	132	PHE	3.6
2	1	257	HIS	3.6
3	3	76	GLN	3.6
1	0	142	LYS	3.6
3	3	172	ILE	3.5
3	3	97	GLN	3.5
1	0	216	PRO	3.5
1	0	276	LEU	3.5
2	1	124	GLU	3.5
1	0	91	THR	3.5
1	0	158	THR	3.5
1	0	184	SER	3.5
1	0	258	ASN	3.4
1	0	249	HIS	3.4
3	3	220	ALA	3.4
2	1	102	ASN	3.4
3	3	210	ASN	3.4
1	0	215	PRO	3.4
1	0	275	ALA	3.4
3	3	171	TRP	3.4
3	3	225	THR	3.3
2	1	250	ARG	3.3
3	3	92	ARG	3.3
3	3	50	GLU	3.3
1	0	89	ASN	3.3
1	0	141	GLU	3.3
3	3	60	THR	3.3
1	0	299	PRO	3.2
1	0	278	HIS	3.2
3	3	223	ASN	3.2

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Mol	Chain	Res	Type	RSRZ
1	0	268	ASN	3.2
2	1	127	THR	3.2
2	1	160	ALA	3.2
1	0	131	ARG	3.1
2	1	244	LYS	3.1
1	0	169	TYR	3.1
3	3	199	GLN	3.1
3	3	78	GLY	3.1
3	3	80	GLY	3.1
1	0	230	GLN	3.0
2	1	222	TYR	3.0
3	3	79	LYS	3.0
3	3	35	HIS	3.0
2	1	255	MET	3.0
1	0	309	PRO	3.0
1	0	175	PHE	3.0
3	3	93	SER	2.9
2	1	286	PRO	2.9
1	0	226	GLY	2.9
1	0	94	THR	2.9
1	0	292	ASP	2.9
1	0	168	HIS	2.9
3	3	146	ARG	2.9
2	1	101	THR	2.9
1	0	273	ASP	2.9
2	1	120	ARG	2.9
3	3	188	TYR	2.9
1	0	204	VAL	2.8
3	3	147	ALA	2.8
3	3	238	THR	2.8
3	3	88	ALA	2.8
1	0	104	TYR	2.8
1	0	182	ASN	2.8
3	3	18	ASP	2.8
2	1	206	ASP	2.8
3	3	38	GLY	2.8
2	1	174	ALA	2.8
3	3	164	SER	2.7
1	0	165	ALA	2.7
2	1	75	THR	2.7
2	1	240	THR	2.7
2	1	109	TRP	2.7

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Mol	Chain	Res	Type	RSRZ
2	1	164	ASP	2.7
3	3	163	SER	2.7
2	1	281	GLY	2.7
3	3	41	ARG	2.7
1	0	90	SER	2.7
1	0	202	GLY	2.7
1	0	100	ILE	2.7
1	0	243	GLN	2.7
2	1	135	PHE	2.7
3	3	11	ASN	2.6
2	1	288	GLY	2.6
3	3	12	GLN	2.6
1	0	281	PHE	2.6
3	3	211	THR	2.6
2	1	235	VAL	2.6
2	1	259	ARG	2.6
2	1	142	PRO	2.6
2	1	277	PRO	2.6
3	3	10	THR	2.5
1	0	176	CYS	2.5
1	0	274	SER	2.5
3	3	127	ALA	2.5
3	3	209	PRO	2.5
3	3	96	TRP	2.5
3	3	94	GLY	2.5
2	1	114	THR	2.5
3	3	200	THR	2.5
1	0	149	TRP	2.5
3	3	33	CYS	2.5
2	1	246	PRO	2.5
3	3	138	PRO	2.5
1	0	152	PRO	2.5
2	1	103	PRO	2.5
2	1	91	GLY	2.5
3	3	231	ASP	2.5
2	1	292	THR	2.5
3	3	166	THR	2.5
2	1	241	SER	2.5
3	3	149	ALA	2.4
2	1	226	PRO	2.4
2	1	81	ASP	2.4
3	3	3	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
3	3	136	THR	2.4
1	0	103	GLY	2.4
2	1	169	LEU	2.4
2	1	112	ASP	2.4
2	1	225	CYS	2.4
1	0	255	ARG	2.4
1	0	302	PRO	2.3
1	0	250	GLN	2.3
1	0	214	HIS	2.3
3	3	112	SER	2.3
1	0	277	ASN	2.3
3	3	126	MET	2.3
2	1	118	GLN	2.3
3	3	206	ILE	2.3
1	0	221	GLN	2.3
3	3	2	PHE	2.3
3	3	59	PRO	2.3
1	0	170	LEU	2.3
1	0	254	LEU	2.3
3	3	107	TYR	2.3
1	0	248	PRO	2.3
1	0	181	CYS	2.3
2	1	185	ASP	2.3
2	1	285	LYS	2.2
3	3	100	LEU	2.2
1	0	257	ASN	2.2
1	0	315	ALA	2.2
2	1	297	LEU	2.2
3	3	102	GLY	2.2
1	0	186	PHE	2.2
1	0	294	ASP	2.2
1	0	289	SER	2.2
3	3	39	GLU	2.2
3	3	124	SER	2.2
1	0	233	TYR	2.2
3	3	29	TYR	2.2
3	3	198	TYR	2.2
3	3	194	VAL	2.2
2	1	203	TRP	2.2
3	3	110	GLN	2.2
2	1	239	GLY	2.2
3	3	205	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
3	3	191	THR	2.2
2	1	270	ASN	2.2
1	0	306	THR	2.1
3	3	193	LEU	2.1
3	3	236	LEU	2.1
1	0	224	ALA	2.1
1	0	311	CYS	2.1
2	1	274	LYS	2.1
1	0	280	ASN	2.1
3	3	134	ALA	2.1
1	0	160	VAL	2.1
3	3	17	ASP	2.1
3	3	109	THR	2.1
3	3	235	ILE	2.1
1	0	180	GLN	2.1
1	0	187	HIS	2.1
2	1	229	MET	2.1
1	0	293	TYR	2.1
1	0	153	ASP	2.1
3	3	144	LYS	2.1
1	0	266	TYR	2.0
3	3	207	GLY	2.0
1	0	208	THR	2.0
1	0	272	PHE	2.0
3	3	139	GLY	2.0
2	1	76	ALA	2.0
3	3	21	SER	2.0
1	0	200	VAL	2.0
1	0	246	VAL	2.0
2	1	181	VAL	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.