



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:55 PM GMT

PDB ID : 4GMP
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

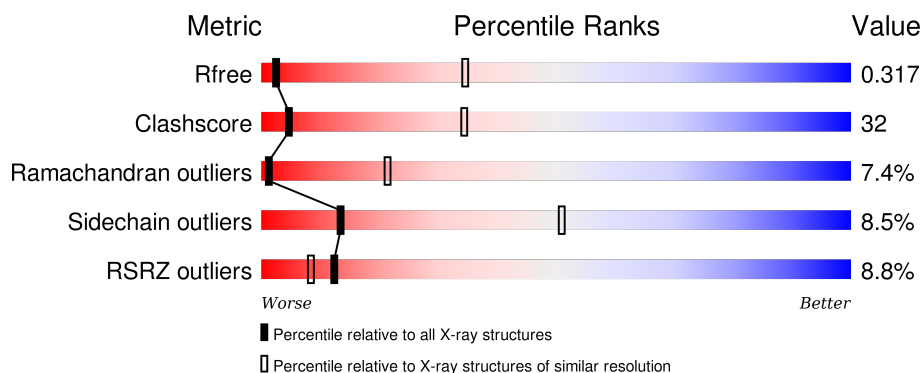
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.90 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}	91344	1014 (4.28-3.52)
Clashscore	102246	1031 (4.24-3.56)
Ramachandran outliers	100387	1012 (4.26-3.54)
Sidechain outliers	100360	1004 (4.26-3.54)
RSRZ outliers	91569	1018 (4.28-3.52)

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

Mol	Chain	Length	Quality of chain
1	0	323	
2	1	297	
3	3	242	

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			

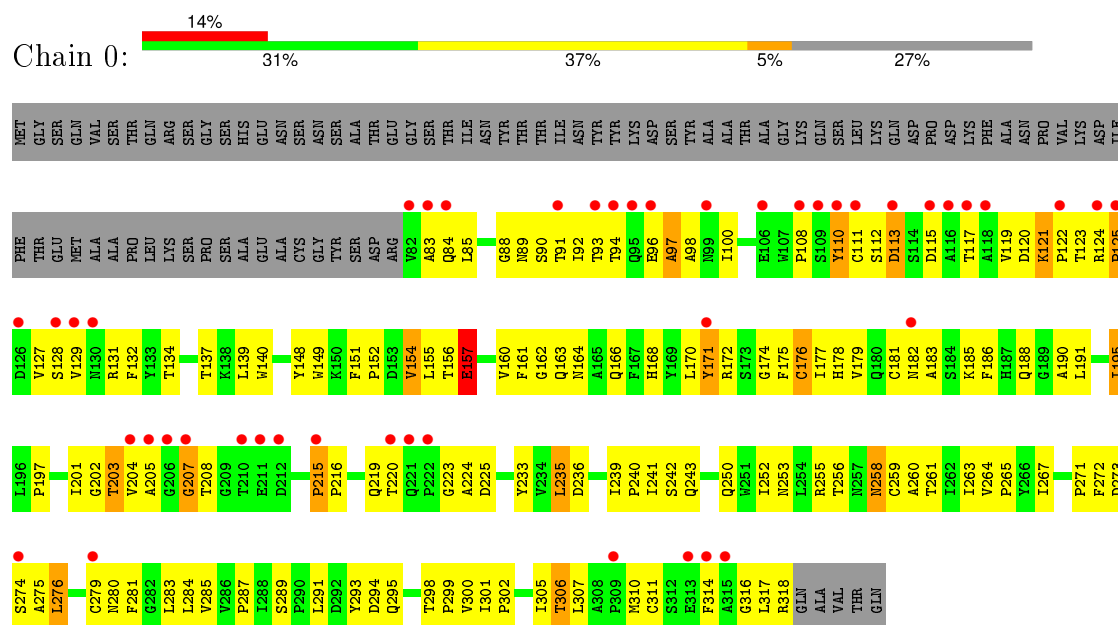
- Molecule 3 is a protein called capsid protein VP3.

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

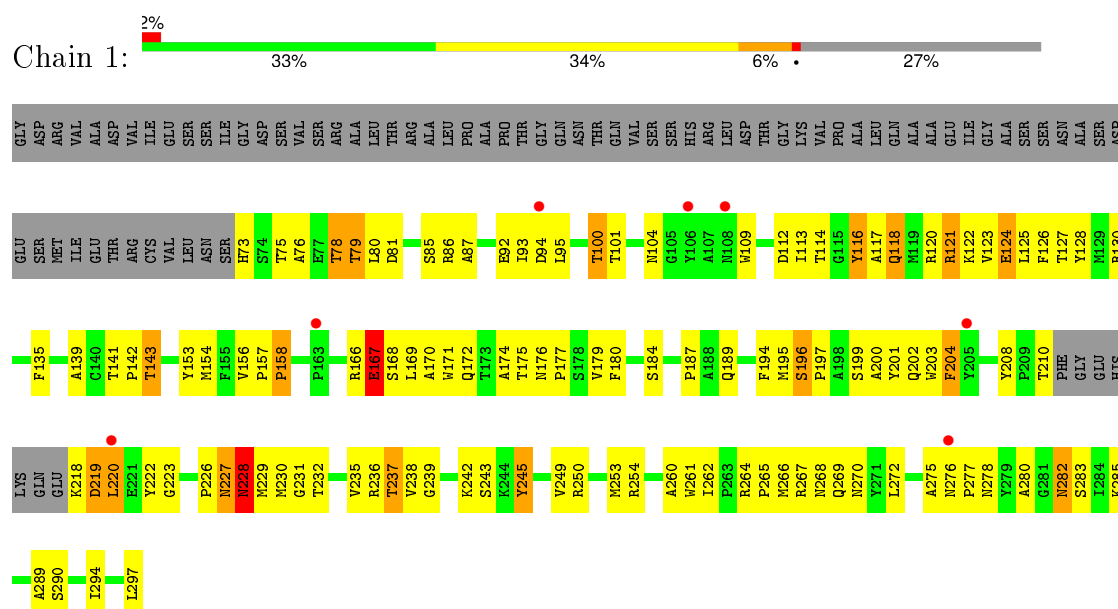
3 Residue-property plots

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

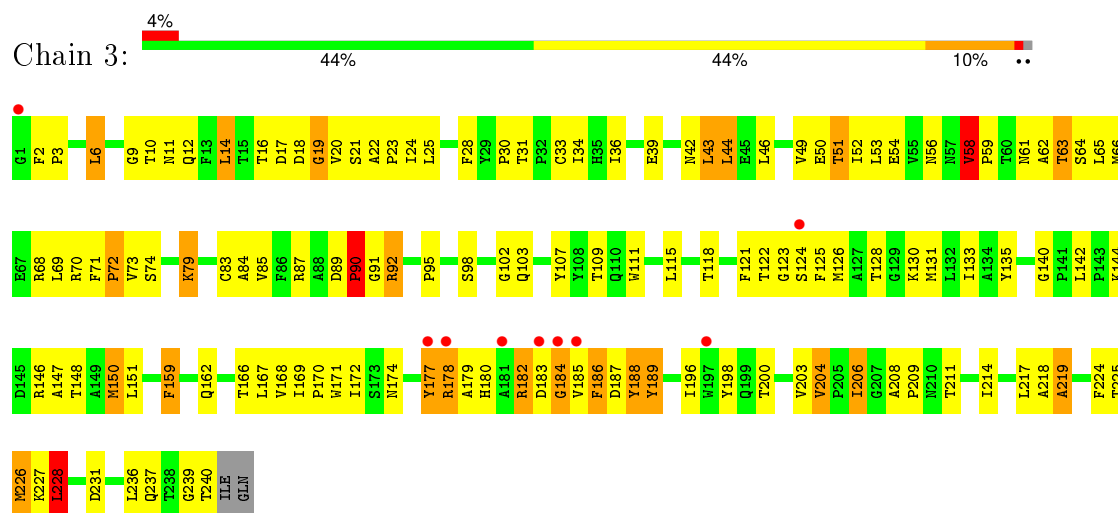
• Molecule 1: capsid protein VP0



• 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) 99.9 (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 0.299 , 0.317	Depositor DCC
R_{free} test set	3398 reflections (5.35%)	DCC
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 , 88.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 66880 reflections	Xtriage
F_o, F_c correlation	0.71	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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.44	0/1888	0.67	0/2591
2	1	0.46	0/1769	0.68	0/2411
3	3	0.49	0/1897	0.71	0/2596
All	All	0.47	0/5554	0.69	0/7598

There are no bond length outliers.

There are no bond angle outliers.

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	124	3
2	1	1717	0	1674	125	8
3	3	1845	0	1822	134	1
All	All	5395	0	5270	341	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 32.

All (341) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:229:MET:HE2	2:1:231:GLY:H	1.24	1.02
3:3:206:ILE:HD12	3:3:206:ILE:H	1.23	1.01
3:3:109:THR:HB	3:3:228:LEU:HB3	1.52	0.91
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:O	3:3:172:ILE:HD12	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
3:3:85:VAL:HG21	3:3:142:LEU:HD12	1.62	0.81
2:1:218:LYS:HD3	2:1:219:ASP:N	1.96	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
3:3:20:VAL:HG22	3:3:21:SER:N	1.95	0.80
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
2:1:139:ALA:HB2	2:1:249:VAL:HG22	1.65	0.77
3:3:179:ALA:HA	3:3:184:GLY:HA2	1.66	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
2:1:112:ASP:CG	2:1:114:THR:HG22	2.09	0.73
2:1:100:THR:HG23	2:1:101:THR:H	1.52	0.73
1:0:125:PRO:HB3	1:0:129:VAL:HG21	1.71	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
3:3:178:ARG:HB2	3:3:178:ARG:HH11	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
1:0:128:SER:OG	1:0:160:VAL:HG11	1.91	0.70
1:0:233:TYR:HA	3:3:66:MET:HE3	1.73	0.69
2:1:229:MET:HE2	2:1:231:GLY:N	2.04	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:218:LYS:O	2:1:219:ASP:HB2	1.93	0.68
2:1:121:ARG:NH1	2:1:121:ARG:HG2	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
2:1:168:SER:C	2:1:170:ALA:H	1.99	0.66
3:3:239:GLY:O	3:3:240:THR:C	2.33	0.65
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
2:1:78:THR:HG22	3:3:43:LEU:HB2	1.79	0.63
1:0:203:THR:H	1:0:215:PRO:HG3	1.62	0.63
1:0:179:VAL:HG22	1:0:305:ILE:HG12	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
1:0:233:TYR:HA	3:3:66:MET:CE	2.30	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
3:3:225:THR:O	3:3:226:MET:HG2	2.00	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
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
2:1:229:MET:HE2	2:1:230:MET:N	2.17	0.59
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
1:0:168:HIS:CD2	1:0:314:PHE:HB3	2.38	0.58
1:0:148:TYR:HB3	1:0:284:LEU:HD23	1.85	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:178:ARG:HG2	3:3:179:ALA:H	1.68	0.57
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
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
2:1:139:ALA:CB	2:1:249:VAL:HG22	2.33	0.56
1:0:178:HIS:HE1	1:0:259:CYS:HB2	1.69	0.56
2:1:254:ARG:HB3	2:1:254:ARG:NH1	2.20	0.56
1:0:92:ILE:HG13	1:0:92:ILE:O	2.04	0.56
1:0:119:VAL:O	1:0:119:VAL:HG12	2.06	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
1:0:88:GLY:C	1:0:90:SER:H	2.08	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
2:1:266:MET:HE2	3:3:103:GLN:HB3	1.87	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:HG13	1:0:239:ILE:O	2.06	0.55
1:0:240:PRO:HG3	1:0:243:GLN:NE2	2.22	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
3:3:50:GLU:HA	3:3:218:ALA:O	2.06	0.54
3:3:9:GLY:HA2	3:3:12:GLN:OE1	2.08	0.54
1:0:125:PRO:HG2	1:0:314:PHE:CD2	2.42	0.54
2:1:123:VAL:HG23	2:1:124:GLU:N	2.22	0.54
3:3:167:LEU:HD12	3:3:168:VAL:H	1.72	0.54
3:3:6:LEU:CD1	3:3:10:THR:HG21	2.37	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
1:0:162:GLY:O	1:0:166:GLN:HG3	2.07	0.54
1:0:134:THR:HG23	1:0:306:THR:HG23	1.89	0.54
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:0:155:LEU:C	1:0:157:GLU:N	2.62	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
2:1:168:SER:C	2:1:170:ALA:N	2.62	0.53
3:3:225:THR:HG22	3:3:226:MET:H	1.74	0.53
2:1:204:PHE:CD1	2:1:204:PHE:N	2.77	0.53
1:0:84:GLN:HB3	1:0:93:THR:HA	1.90	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
3:3:18:ASP:O	3:3:19:GLY:O	2.27	0.53
2:1:171:TRP:CZ3	2:1:236:ARG:HG2	2.44	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:N	2:1:180:PHE:CD1	2.78	0.52
3:3:54:GLU:HG3	3:3:98:SER:CB	2.40	0.52
2:1:80:LEU:HD21	2:1:260:ALA:HB3	1.92	0.52
3:3:91:GLY:HA3	3:3:111:TRP:HZ2	1.75	0.52
3:3:79:LYS:NZ	3:3:79:LYS:HB2	2.25	0.51
2:1:194:PHE:HZ	2:1:200:ALA:HA	1.73	0.51
2:1:166:ARG:HH11	2:1:166:ARG:HG2	1.74	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
2:1:174:ALA:C	2:1:176:ASN:H	2.14	0.50
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
2:1:156:VAL:HG22	2:1:176:ASN:ND2	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:166:ARG:NH2	2:1:237:THR:OG1	2.45	0.50
1:0:155:LEU:C	1:0:157:GLU:H	2.14	0.50
1:0:154:VAL:HG23	1:0:224:ALA:HA	1.92	0.50
1:0:115:ASP:C	1:0:117:THR:H	2.14	0.50
2:1:203:TRP:HB2	2:1:204:PHE:CD1	2.47	0.50
2:1:135:PHE:CE1	2:1:253:MET:HB2	2.46	0.50
1:0:182:ASN:O	1:0:301:ILE:HG23	2.11	0.50
1:0:307:LEU:N	1:0:307:LEU:HD23	2.27	0.50
1:0:255:ARG:HG3	1:0:256:THR:HG23	1.93	0.50
1:0:201:ILE:HG22	1:0:202:GLY:H	1.75	0.49
3:3:30:PRO:O	3:3:31:THR:C	2.49	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
1:0:241:ILE:HG21	3:3:66:MET:HE3	1.94	0.49
2:1:220:LEU:N	2:1:220:LEU:HD23	2.28	0.49
2:1:127:THR:OG1	2:1:264:ARG:NH2	2.46	0.48
1:0:293:TYR:CE1	1:0:299:PRO:HA	2.48	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
2:1:104:ASN:HA	2:1:242:LYS:HZ2	1.79	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:N	1:0:276:LEU:HD12	2.29	0.48
1:0:129:VAL:CG1	1:0:161:PHE:HD1	2.27	0.48
1:0:92:ILE:HG21	1:0:306:THR:HG21	1.96	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
2:1:268:ASN:OD1	2:1:269:GLN:HG2	2.14	0.47
1:0:108:PRO:CB	1:0:174:GLY:HA3	2.44	0.47
3:3:170:PRO:HG2	3:3:171:TRP:H	1.79	0.47
3:3:109:THR:OG1	3:3:228:LEU:HD12	2.15	0.47
3:3:204:VAL:CG1	3:3:208:ALA:HB3	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:201:ILE:CG2	1:0:202:GLY:H	2.27	0.47
3:3:71:PHE:CE1	3:3:214:ILE:HB	2.50	0.47
1:0:235:LEU:HD12	1:0:239:ILE:HD12	1.97	0.47
1:0:176:CYS:SG	1:0:263:ILE:HD13	2.55	0.47
3:3:182:ARG:HG3	3:3:182:ARG:NH2	2.29	0.47
2:1:154:MET:CE	2:1:171:TRP:HA	2.45	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
1:0:96:GLU:O	1:0:97:ALA:HB2	2.15	0.47
2:1:290:SER:OG	3:3:68:ARG:NH2	2.48	0.47
1:0:100:ILE:O	1:0:100:ILE:HD12	2.15	0.46
3:3:167:LEU:HD12	3:3:167:LEU:C	2.36	0.46
3:3:121:PHE:CE2	3:3:123:GLY:HA3	2.50	0.46
3:3:148:THR:HA	3:3:151:LEU:HD12	1.97	0.46
2:1:229:MET:CE	2:1:230:MET:N	2.79	0.46
3:3:146:ARG:NH1	3:3:146:ARG:HG2	2.31	0.46
3:3:22:ALA:HB1	3:3:23:PRO:HD2	1.97	0.46
3:3:115:LEU:HB2	3:3:169:ILE:HB	1.97	0.46
3:3:58:VAL:H	3:3:59:PRO:HD2	1.81	0.45
2:1:126:PHE:CG	2:1:260:ALA:HB1	2.50	0.45
1:0:250:GLN:CG	1:0:260:ALA:HB1	2.47	0.45
2:1:156:VAL:HG12	2:1:156:VAL:O	2.17	0.45
1:0:172:ARG:HB3	1:0:272:PHE:CE1	2.50	0.45
3:3:14:LEU:HD22	3:3:16:THR:H	1.82	0.45
3:3:90:PRO:HD2	3:3:188:TYR:OH	2.17	0.45
1:0:128:SER:CB	1:0:160:VAL:HG11	2.46	0.45
3:3:6:LEU:HD23	3:3:6:LEU:N	2.32	0.45
1:0:310:MET:O	1:0:311:CYS:HB2	2.17	0.45
3:3:84:ALA:HB3	3:3:196:ILE:CD1	2.43	0.45
2:1:261:TRP:CD1	3:3:36:ILE:HB	2.52	0.45
2:1:238:VAL:CG1	2:1:239:GLY:N	2.79	0.45
1:0:191:LEU:HD23	1:0:287:PRO:HA	1.99	0.45
1:0:89:ASN:ND2	1:0:131:ARG:HH21	2.14	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
3:3:61:ASN:OD1	3:3:62:ALA:N	2.50	0.44
1:0:83:ALA:HB3	1:0:96:GLU:HA	1.98	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
2:1:242:LYS:HG3	2:1:243:SER:N	2.32	0.44
2:1:125:LEU:HD23	2:1:126:PHE:CZ	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:197:PRO:HG2	2:1:262:ILE:CG2	2.48	0.44
3:3:227:LYS:HB3	3:3:227:LYS:HE2	1.80	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
2:1:80:LEU:HA	2:1:80:LEU:HD12	1.79	0.44
1:0:152:PRO:HD2	1:0:279:CYS:HA	2.00	0.44
2:1:116:TYR:HE2	2:1:118:GLN:HE21	1.66	0.44
2:1:261:TRP:CD1	3:3:39:GLU:HB2	2.53	0.44
1:0:273:ASP:OD1	1:0:274:SER:N	2.51	0.44
1:0:156:THR:HA	1:0:162:GLY:HA2	1.99	0.44
2:1:203:TRP:C	2:1:204:PHE:CD1	2.91	0.43
2:1:245:TYR:N	2:1:245:TYR:CD1	2.85	0.43
2:1:294:ILE:CD1	3:3:71:PHE:HB3	2.47	0.43
3:3:66:MET:HE1	3:3:69:LEU:HD11	1.99	0.43
2:1:104:ASN:O	2:1:166:ARG:HD2	2.18	0.43
1:0:190:ALA:HB3	1:0:289:SER:HB3	1.99	0.43
2:1:201:TYR:HA	2:1:228:ASN:HD21	1.81	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
1:0:233:TYR:CD2	3:3:65:LEU:HB3	2.53	0.43
2:1:123:VAL:C	2:1:125:LEU:H	2.20	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
3:3:178:ARG:HG2	3:3:179:ALA:N	2.34	0.43
3:3:135:TYR:CD1	3:3:169:ILE:HD12	2.54	0.43
2:1:297:LEU:HD23	3:3:85:VAL:CG2	2.49	0.43
1:0:129:VAL:CG2	1:0:164:ASN:HD21	2.32	0.43
1:0:84:GLN:NE2	1:0:91:THR:HG21	2.34	0.43
2:1:167:GLU:CD	2:1:167:GLU:N	2.71	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
2:1:94:ASP:C	2:1:95:LEU:HD23	2.39	0.42
3:3:150:MET:HE2	3:3:151:LEU:HA	2.01	0.42
2:1:156:VAL:HA	2:1:157:PRO:HD2	1.84	0.42
1:0:235:LEU:O	1:0:236:ASP:HB2	2.19	0.42
1:0:121:LYS:H	1:0:121:LYS:HD2	1.84	0.42
1:0:253:ASN:HD21	3:3:122:THR:HA	1.84	0.42
2:1:266:MET:O	2:1:267:ARG:C	2.57	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:175:PHE:HB3	1:0:176:CYS:H	1.67	0.42
3:3:133:ILE:HG12	3:3:196:ILE:HG22	2.02	0.42
1:0:203:THR:N	1:0:215:PRO:HG3	2.34	0.42
2:1:154:MET:HE3	2:1:171:TRP:HA	2.02	0.42
2:1:81:ASP:O	2:1:85:SER:HB3	2.20	0.42
3:3:182:ARG:HH21	3:3:182:ARG:HG3	1.84	0.42
2:1:177:PRO:HB2	3:3:24:ILE:CD1	2.45	0.42
3:3:89:ASP:HA	3:3:188:TYR:CZ	2.55	0.42
1:0:110:TYR:CE1	1:0:124:ARG:HB3	2.55	0.42
3:3:25:LEU:HB3	3:3:28:PHE:HB2	2.02	0.42
1:0:160:VAL:O	1:0:163:GLN:HB3	2.19	0.42
1:0:185:LYS:HB3	3:3:125:PHE:HD1	1.85	0.42
2:1:126:PHE:CD2	2:1:260:ALA:HB1	2.55	0.41
1:0:149:TRP:HZ3	1:0:285:VAL:CG1	2.33	0.41
3:3:90:PRO:O	3:3:102:GLY:HA2	2.20	0.41
3:3:84:ALA:CB	3:3:196:ILE:HD11	2.45	0.41
1:0:90:SER:CB	1:0:132:PHE:HB2	2.51	0.41
2:1:116:TYR:HE2	2:1:118:GLN:NE2	2.17	0.41
3:3:63:THR:OG1	3:3:63:THR:O	2.37	0.41
2:1:174:ALA:C	2:1:176:ASN:N	2.73	0.41
1:0:220:THR:HG23	2:1:222:TYR:CE1	2.55	0.41
2:1:199:SER:OG	3:3:34:ILE:HG12	2.20	0.41
2:1:117:ALA:HB1	3:3:236:LEU:HD22	2.03	0.41
1:0:258:ASN:CG	1:0:259:CYS:N	2.74	0.41
2:1:120:ARG:HH11	3:3:237:GLN:NE2	2.16	0.41
1:0:239:ILE:HB	2:1:265:PRO:HB2	2.00	0.41
1:0:186:PHE:CE1	3:3:126:MET:HG3	2.55	0.41
3:3:24:ILE:HA	3:3:24:ILE:HD12	1.90	0.41
2:1:180:PHE:H	2:1:180:PHE:HD1	1.69	0.41
3:3:170:PRO:O	3:3:171:TRP:HB2	2.20	0.41
1:0:258:ASN:CG	1:0:259:CYS:H	2.24	0.41
1:0:151:PHE:CD1	1:0:151:PHE:N	2.88	0.41
3:3:177:TYR:HA	3:3:186:PHE:HA	2.03	0.41
3:3:183:ASP:O	3:3:185:VAL:N	2.50	0.41
2:1:297:LEU:HD23	3:3:85:VAL:HG22	2.03	0.41
2:1:235:VAL:HG11	2:1:249:VAL:HG21	2.01	0.41
1:0:155:LEU:HD23	1:0:155:LEU:HA	1.94	0.41
3:3:144:LYS:HD3	3:3:148:THR:HG21	2.02	0.41
2:1:157:PRO:HA	2:1:158:PRO:HD2	1.97	0.41
1:0:92:ILE:HG12	1:0:132:PHE:HE1	1.85	0.41
3:3:74:SER:CB	3:3:211:THR:OG1	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:3:162:GLN:HG3	3:3:162:GLN:O	2.21	0.41
2:1:157:PRO:O	2:1:158:PRO:C	2.60	0.40
2:1:272:LEU:HD23	2:1:272:LEU:HA	1.89	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
1:0:283:LEU:C	1:0:283:LEU:HD23	2.42	0.40
3:3:90:PRO:HG2	3:3:115:LEU:HD11	2.02	0.40
1:0:88:GLY:C	1:0:90:SER:N	2.74	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

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
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 ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	0	235/323 (73%)	175 (74%)	42 (18%)	18 (8%)	1 20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	1	214/297 (72%)	171 (80%)	27 (13%)	16 (8%)	1	21
3	3	238/242 (98%)	187 (79%)	34 (14%)	17 (7%)	1	23
All	All	687/862 (80%)	533 (78%)	103 (15%)	51 (7%)	1	21

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
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

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Mol	Chain	Res	Type
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%)	21	61
2	1	186/250 (74%)	168 (90%)	18 (10%)	10	43
3	3	200/202 (99%)	181 (90%)	19 (10%)	11	44
All	All	587/724 (81%)	537 (92%)	50 (8%)	13	51

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	113	ASP
1	0	121	LYS
1	0	157	GLU
1	0	171	TYR
1	0	181	CYS

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Mol	Chain	Res	Type
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
2	1	78	THR
2	1	100	THR
2	1	116	TYR
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	184	SER
2	1	202	GLN
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	63	THR
3	3	70	ARG
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	178	ARG
3	3	204	VAL

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Mol	Chain	Res	Type
3	3	206	ILE
3	3	226	MET
3	3	228	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	164	ASN
1	0	168	HIS
1	0	188	GLN
1	0	214	HIS
2	1	152	GLN
2	1	176	ASN
2	1	202	GLN
2	1	278	ASN
3	3	48	GLN
3	3	110	GLN
3	3	176	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	1.09	45 (18%) 2 2	89, 133, 217, 234	0
2	1	218/297 (73%)	0.32	7 (3%) 51 38	84, 110, 155, 200	0
3	3	240/242 (99%)	0.42	9 (3%) 44 33	80, 112, 189, 230	0
All	All	695/862 (80%)	0.62	61 (8%) 12 8	80, 114, 211, 234	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	3	185	VAL	5.4
1	0	125	PRO	5.4
3	3	184	GLY	5.4
1	0	206	GLY	5.1
1	0	84	GLN	4.6
3	3	183	ASP	4.5
1	0	110	TYR	4.5
1	0	205	ALA	4.4
1	0	116	ALA	4.2
1	0	130	ASN	4.2
1	0	204	VAL	4.2
1	0	279	CYS	4.0
1	0	124	ARG	3.9
3	3	178	ARG	3.8
1	0	315	ALA	3.8
1	0	212	ASP	3.7
3	3	177	TYR	3.7
1	0	117	THR	3.7
1	0	108	PRO	3.6
3	3	181	ALA	3.6
1	0	128	SER	3.6
1	0	83	ALA	3.3
1	0	93	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	0	129	VAL	3.2
1	0	222	PRO	3.1
1	0	221	GLN	3.1
1	0	313	GLU	3.1
3	3	1	GLY	3.0
1	0	82	VAL	2.9
1	0	126	ASP	2.9
1	0	171	TYR	2.8
1	0	113	ASP	2.8
1	0	115	ASP	2.8
1	0	314	PHE	2.7
3	3	124	SER	2.7
2	1	108	ASN	2.7
1	0	118	ALA	2.6
1	0	182	ASN	2.5
1	0	99	ASN	2.5
1	0	106	GLU	2.5
1	0	94	THR	2.5
1	0	274	SER	2.5
1	0	95	GLN	2.4
2	1	106	TYR	2.4
1	0	211	GLU	2.4
1	0	109	SER	2.4
1	0	111	CYS	2.4
1	0	91	THR	2.3
1	0	215	PRO	2.3
2	1	163	PRO	2.3
2	1	94	ASP	2.3
2	1	276	ASN	2.2
1	0	220	THR	2.2
1	0	122	PRO	2.2
1	0	309	PRO	2.2
1	0	210	THR	2.1
1	0	207	GLY	2.1
2	1	220	LEU	2.1
1	0	96	GLU	2.1
3	3	197	TRP	2.0
2	1	205	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.