



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 09:16 PM UTC

PDB ID : 4JGY / pdb_00004jgy
Title : Crystal structure of human coxsackievirus A16 uncoating intermediate (space group P4232)
Authors : Ren, J.; Wang, X.; Hu, Z.; Gao, Q.; Sun, Y.; Li, X.; Porta, C.; Walter, T.S.; Gilbert, R.J.; Zhao, Y.; Axford, D.; Williams, M.; Mcauley, K.; Rowlands, D.J.; Yin, W.; Wang, J.; Stuart, D.I.; Rao, Z.; Fry, E.E.
Deposited on : 2013-03-04
Resolution : 3.00 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

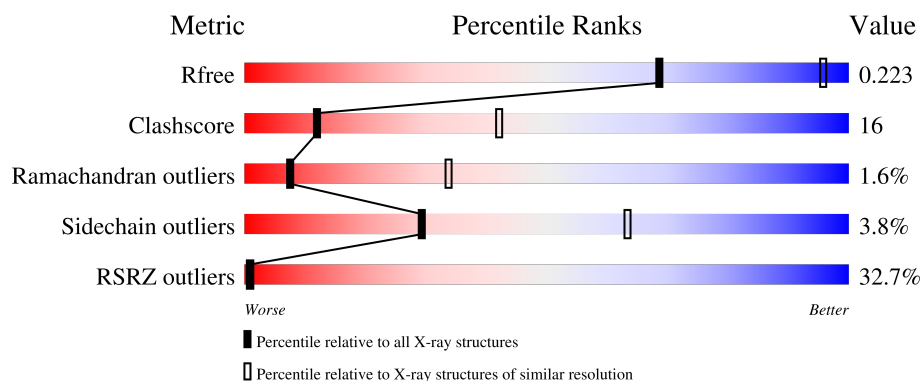
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	A	297	24% 52% 23% • 23%
2	B	254	41% 63% 27% • 6%
3	C	242	21% 67% 26% • 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5468 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 Polyprotein, capsid protein VP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	228	Total	C	N	O	S	0	0	0
			1830	1170	312	335	13			

- Molecule 2 is a protein called Polyprotein, capsid protein VP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	239	Total	C	N	O	S	0	0	0
			1844	1186	305	343	10			

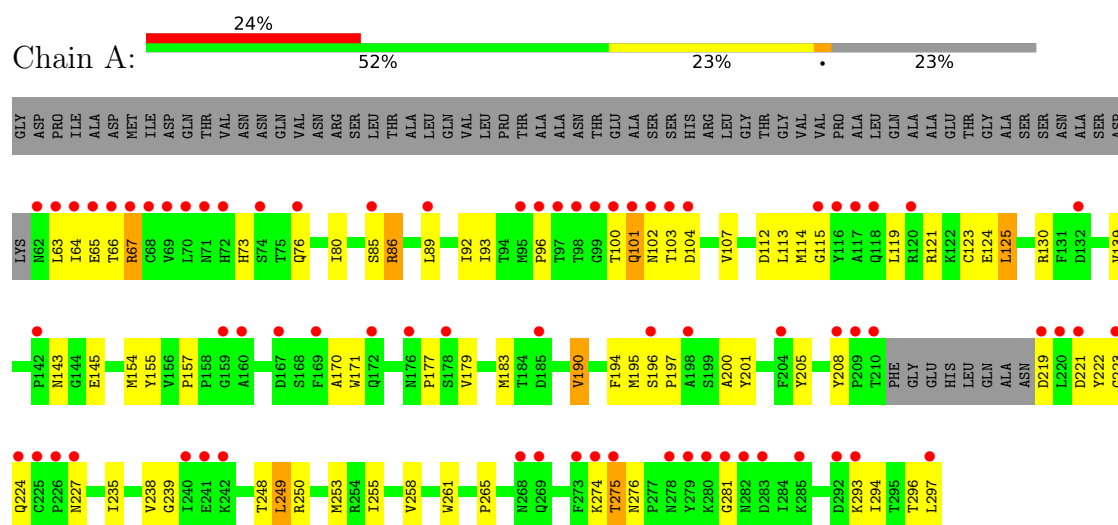
- Molecule 3 is a protein called Polyprotein, capsid protein VP3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	231	Total	C	N	O	S	0	0	0
			1794	1156	291	336	11			

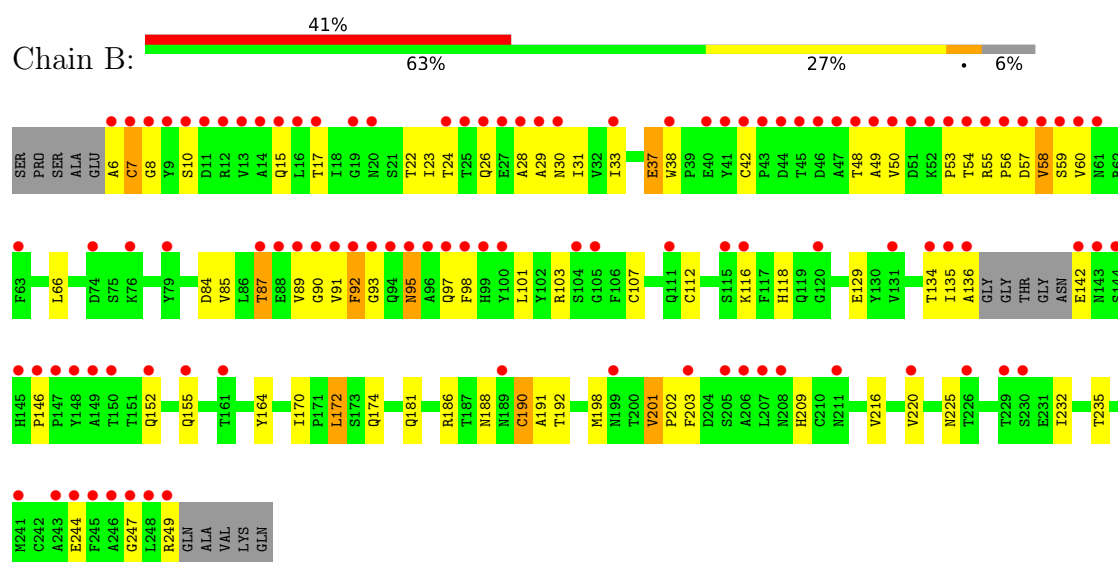
3 Residue-property plots [i](#)

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

• Molecule 1: Polyprotein, capsid protein VP1

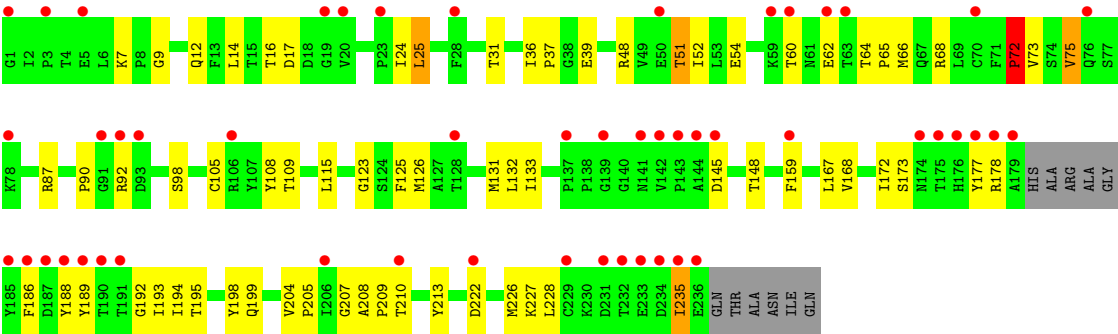


• Molecule 2: Polyprotein, capsid protein VP2



• Molecule 3: Polyprotein, 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	357.00Å 357.00Å 357.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.51 – 3.00 49.51 – 3.00	Depositor EDS
% Data completeness (in resolution range)	95.1 (49.51-3.00) 95.1 (49.51-3.00)	Depositor EDS
R_{merge}	0.60	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.16 (at 3.01Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.227 , 0.233 0.222 , 0.223	Depositor DCC
R_{free} test set	1451 reflections (0.99%)	wwPDB-VP
Wilson B-factor (Å ²)	65.9	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 38.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.45	EDS
Total number of atoms	5468	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.36% 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 [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.51	0/1883	1.01	9/2564 (0.4%)
2	B	0.51	0/1898	1.08	14/2608 (0.5%)
3	C	0.53	0/1845	0.99	5/2528 (0.2%)
All	All	0.51	0/5626	1.03	28/7700 (0.4%)

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	152	GLN	CA-C-N	10.99	130.77	119.56
2	B	152	GLN	C-N-CA	10.99	130.77	119.56
1	A	103	THR	N-CA-C	-10.66	100.30	113.20
1	A	125	LEU	N-CA-C	-8.39	103.05	113.28
2	B	220	VAL	CA-C-N	7.53	127.57	119.89
2	B	220	VAL	C-N-CA	7.53	127.57	119.89
2	B	107	CYS	N-CA-C	-7.39	96.48	108.52
1	A	195	MET	N-CA-C	6.70	119.59	111.82
2	B	190	CYS	CA-CB-SG	6.66	129.71	114.40
1	A	275	THR	N-CA-C	6.56	120.89	113.02
2	B	190	CYS	N-CA-C	6.51	119.10	108.55
2	B	50	VAL	N-CA-C	-6.24	107.17	113.47
2	B	89	VAL	N-CA-C	6.08	117.53	108.46
3	C	64	THR	CA-C-N	6.06	127.42	119.84
3	C	64	THR	C-N-CA	6.06	127.42	119.84
2	B	172	LEU	N-CA-C	-6.02	104.64	112.23
2	B	92	PHE	N-CA-C	-5.99	105.47	112.89
1	A	201	TYR	N-CA-C	-5.97	101.65	110.48
2	B	49	ALA	N-CA-C	-5.81	106.24	113.38
3	C	52	ILE	N-CA-C	5.64	116.34	108.89
1	A	276	ASN	CA-C-N	5.56	126.79	119.84
1	A	276	ASN	C-N-CA	5.56	126.79	119.84
3	C	123	GLY	N-CA-C	5.56	118.44	112.33
2	B	85	VAL	N-CA-C	5.35	116.72	110.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	199	GLN	N-CA-C	-5.26	104.98	111.40
1	A	196	SER	CA-C-N	5.12	125.57	120.04
1	A	196	SER	C-N-CA	5.12	125.57	120.04
2	B	37	GLU	N-CA-C	5.04	117.65	109.24

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1830	0	1792	74	0
2	B	1844	0	1786	62	0
3	C	1794	0	1759	61	0
All	All	5468	0	5337	170	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 16.

All (170) 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:B:54:THR:HG22	2:B:56:PRO:HD3	1.42	0.97
2:B:91:VAL:O	2:B:95:ASN:HB2	1.76	0.85
2:B:164:TYR:HA	3:C:66:MET:HE3	1.63	0.81
3:C:65:PRO:O	3:C:68:ARG:HG3	1.82	0.80
1:A:255:ILE:HG22	1:A:258:VAL:HG22	1.64	0.80
1:A:143:ASN:HD21	1:A:145:GLU:HG3	1.47	0.79
3:C:109:THR:OG1	3:C:228:LEU:HD12	1.84	0.77
2:B:6:ALA:HA	2:B:30:ASN:HB3	1.67	0.77
1:A:143:ASN:ND2	1:A:145:GLU:HG3	2.01	0.76
2:B:172:LEU:HD23	3:C:66:MET:HE1	1.66	0.74
1:A:66:THR:HG22	1:A:67:ARG:H	1.52	0.74
1:A:96:PRO:HD2	1:A:102:ASN:ND2	2.04	0.71
3:C:105:CYS:HA	3:C:226:MET:CE	2.20	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:6:ALA:HB2	2:B:181:GLN:NE2	2.07	0.70
2:B:198:MET:HG2	3:C:37:PRO:HG2	1.74	0.70
1:A:190:VAL:HG11	3:C:24:ILE:HD13	1.73	0.69
2:B:15:GLN:HG3	2:B:24:THR:HG22	1.74	0.69
2:B:42:CYS:HB2	2:B:103:ARG:HD2	1.74	0.69
1:A:154:MET:HE1	1:A:171:TRP:HA	1.75	0.69
1:A:66:THR:HG22	1:A:67:ARG:HD2	1.76	0.67
3:C:9:GLY:O	3:C:12:GLN:HG2	1.96	0.66
3:C:204:VAL:CG2	3:C:208:ALA:HB3	2.25	0.66
2:B:201:VAL:HG23	2:B:202:PRO:HD2	1.76	0.65
1:A:63:LEU:HD13	3:C:92:ARG:NH2	2.12	0.65
1:A:130:ARG:NH2	3:C:31:THR:O	2.29	0.65
2:B:181:GLN:HG2	2:B:191:ALA:HB1	1.77	0.65
3:C:115:LEU:HD11	3:C:172:ILE:HD13	1.78	0.65
1:A:113:LEU:HD21	1:A:253:MET:SD	2.38	0.64
3:C:145:ASP:OD1	3:C:148:THR:HG23	1.98	0.63
1:A:113:LEU:C	1:A:115:GLY:H	2.06	0.62
1:A:86:ARG:HG2	3:C:16:THR:HG22	1.82	0.62
1:A:113:LEU:HD21	1:A:253:MET:HE1	1.80	0.62
2:B:93:GLY:O	2:B:97:GLN:HG3	2.00	0.62
1:A:224:GLN:HE22	1:A:275:THR:HB	1.65	0.61
2:B:216:VAL:O	2:B:216:VAL:HG23	1.99	0.61
2:B:17:THR:HG22	2:B:22:THR:HG23	1.81	0.61
2:B:28:ALA:C	2:B:30:ASN:H	2.08	0.60
2:B:7:CYS:O	2:B:188:ASN:HB2	2.01	0.60
2:B:6:ALA:HB3	2:B:190:CYS:O	2.02	0.59
2:B:101:LEU:HB3	2:B:203:PHE:HB3	1.85	0.59
1:A:64:ILE:HD12	1:A:64:ILE:H	1.67	0.59
1:A:66:THR:HG22	1:A:67:ARG:N	2.17	0.59
1:A:139:VAL:HG12	1:A:249:LEU:HB2	1.85	0.59
3:C:66:MET:HA	3:C:66:MET:HE2	1.84	0.59
1:A:121:ARG:HD2	3:C:235:ILE:HD13	1.83	0.59
1:A:85:SER:O	1:A:86:ARG:HB2	2.03	0.58
1:A:102:ASN:C	1:A:104:ASP:H	2.10	0.58
3:C:105:CYS:HA	3:C:226:MET:HE3	1.85	0.58
2:B:134:THR:HG22	2:B:135:ILE:H	1.69	0.58
1:A:208:TYR:CE1	1:A:222:TYR:HB2	2.39	0.57
3:C:192:GLY:C	3:C:193:ILE:HD12	2.28	0.57
3:C:87:ARG:HD2	3:C:92:ARG:HH22	1.69	0.57
2:B:116:LYS:HD3	3:C:125:PHE:HD1	1.68	0.57
2:B:116:LYS:HD3	3:C:125:PHE:CD1	2.39	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:ARG:HH21	1:A:250:ARG:HG3	1.68	0.57
3:C:54:GLU:HG3	3:C:98:SER:CB	2.35	0.57
1:A:73:HIS:HD2	3:C:227:LYS:HE3	1.69	0.56
2:B:181:GLN:HG2	2:B:191:ALA:CB	2.35	0.56
1:A:73:HIS:CD2	3:C:227:LYS:HE3	2.40	0.56
2:B:164:TYR:CA	3:C:66:MET:HE3	2.34	0.56
1:A:64:ILE:HD12	1:A:64:ILE:N	2.20	0.56
1:A:102:ASN:C	1:A:104:ASP:N	2.64	0.55
1:A:143:ASN:HD21	1:A:145:GLU:CG	2.19	0.55
3:C:204:VAL:HG23	3:C:205:PRO:HD2	1.88	0.55
3:C:14:LEU:HB3	3:C:17:ASP:HB2	1.88	0.55
2:B:42:CYS:HB2	2:B:103:ARG:CD	2.36	0.55
1:A:255:ILE:CG2	1:A:258:VAL:HG22	2.37	0.55
1:A:113:LEU:HD21	1:A:253:MET:CE	2.37	0.55
1:A:297:LEU:C	1:A:297:LEU:HD12	2.32	0.55
3:C:108:TYR:HB2	3:C:226:MET:HE2	1.89	0.54
2:B:134:THR:HG22	2:B:135:ILE:N	2.22	0.54
1:A:238:VAL:HG12	1:A:239:GLY:N	2.22	0.54
3:C:105:CYS:HA	3:C:226:MET:HE1	1.88	0.54
1:A:235:ILE:N	1:A:235:ILE:HD12	2.22	0.54
3:C:177:TYR:C	3:C:178:ARG:HD2	2.32	0.54
1:A:194:PHE:CZ	1:A:200:ALA:HA	2.43	0.53
2:B:17:THR:HG22	2:B:22:THR:OG1	2.08	0.53
2:B:59:SER:OG	2:B:91:VAL:HG21	2.09	0.52
1:A:139:VAL:HG23	1:A:183:MET:HG3	1.91	0.52
3:C:109:THR:HB	3:C:228:LEU:HB3	1.92	0.52
1:A:139:VAL:CG1	1:A:249:LEU:HD12	2.40	0.52
3:C:75:VAL:CG2	3:C:210:THR:HB	2.40	0.52
3:C:90:PRO:HD2	3:C:189:TYR:OH	2.10	0.52
1:A:293:LYS:HD3	1:A:296:THR:HG23	1.93	0.51
2:B:134:THR:OG1	2:B:146:PRO:HG3	2.10	0.51
2:B:28:ALA:O	2:B:30:ASN:N	2.38	0.51
3:C:177:TYR:O	3:C:178:ARG:HD2	2.10	0.51
2:B:216:VAL:O	2:B:216:VAL:CG2	2.58	0.51
2:B:186:ARG:NH1	3:C:159:PHE:O	2.43	0.51
3:C:126:MET:HA	3:C:126:MET:HE2	1.92	0.51
3:C:7:LYS:HA	3:C:7:LYS:HE2	1.94	0.50
1:A:294:ILE:HG12	1:A:294:ILE:O	2.11	0.49
3:C:73:VAL:HA	3:C:198:TYR:OH	2.12	0.49
2:B:48:THR:HB	2:B:53:PRO:HD3	1.94	0.49
1:A:64:ILE:CD1	3:C:186:PHE:HB2	2.43	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:56:PRO:O	2:B:60:VAL:HB	2.13	0.49
1:A:89:LEU:HD21	1:A:92:ILE:HD11	1.93	0.49
1:A:100:THR:HG22	1:A:101:GLN:HG3	1.95	0.49
1:A:197:PRO:HG2	1:A:227:ASN:HD22	1.78	0.49
2:B:7:CYS:HB3	2:B:26:GLN:HG3	1.94	0.49
2:B:17:THR:HG22	2:B:22:THR:CG2	2.43	0.49
1:A:293:LYS:HD3	1:A:296:THR:CG2	2.43	0.48
2:B:55:ARG:HG2	2:B:244:GLU:HG2	1.94	0.48
1:A:112:ASP:OD1	1:A:274:LYS:HE2	2.14	0.48
1:A:250:ARG:HG3	1:A:250:ARG:NH2	2.29	0.48
2:B:247:GLY:HA3	2:B:249:ARG:NH1	2.29	0.48
2:B:84:ASP:O	2:B:87:THR:HB	2.14	0.48
2:B:186:ARG:HG3	2:B:186:ARG:HH21	1.79	0.48
3:C:204:VAL:CG2	3:C:205:PRO:HD2	2.44	0.47
2:B:118:HIS:CD2	2:B:232:ILE:HD11	2.48	0.47
1:A:205:TYR:O	1:A:223:GLY:HA2	2.14	0.47
1:A:238:VAL:HG12	1:A:239:GLY:H	1.78	0.47
1:A:113:LEU:C	1:A:115:GLY:N	2.72	0.47
2:B:103:ARG:HH11	2:B:103:ARG:HG3	1.79	0.47
1:A:297:LEU:HD12	1:A:297:LEU:OXT	2.15	0.47
1:A:139:VAL:HG12	1:A:249:LEU:CB	2.44	0.47
2:B:103:ARG:HG3	2:B:103:ARG:NH1	2.30	0.47
2:B:186:ARG:HG3	2:B:186:ARG:NH2	2.29	0.46
1:A:113:LEU:HD22	1:A:119:LEU:HD21	1.96	0.46
2:B:57:ASP:O	2:B:58:VAL:O	2.34	0.46
2:B:98:PHE:CE2	2:B:249:ARG:NH2	2.84	0.46
1:A:63:LEU:CD1	3:C:189:TYR:HB3	2.45	0.46
2:B:23:ILE:O	2:B:23:ILE:HG13	2.16	0.46
2:B:66:LEU:HD22	2:B:155:GLN:HG2	1.97	0.46
2:B:8:GLY:CA	2:B:188:ASN:HA	2.45	0.46
1:A:123:CYS:C	1:A:125:LEU:H	2.24	0.46
1:A:63:LEU:HD12	3:C:189:TYR:HB3	1.98	0.45
1:A:93:ILE:CG2	1:A:107:VAL:HG11	2.46	0.45
1:A:65:GLU:HG2	3:C:189:TYR:O	2.16	0.45
3:C:72:PRO:HB3	3:C:213:TYR:CE2	2.52	0.45
2:B:33:ILE:HD13	2:B:38:TRP:NE1	2.32	0.45
1:A:293:LYS:HB2	1:A:296:THR:HG23	1.99	0.44
3:C:75:VAL:HG23	3:C:210:THR:HB	1.99	0.44
1:A:154:MET:CE	1:A:171:TRP:HA	2.45	0.44
3:C:48:ARG:HE	3:C:222:ASP:HA	1.83	0.44
3:C:167:LEU:HD12	3:C:168:VAL:H	1.83	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:MET:HE1	1:A:170:ALA:O	2.17	0.44
3:C:109:THR:HG1	3:C:228:LEU:HD12	1.83	0.44
1:A:208:TYR:HE1	1:A:222:TYR:HB2	1.80	0.43
1:A:64:ILE:HD13	3:C:186:PHE:HB2	1.99	0.43
1:A:265:PRO:HB2	2:B:170:ILE:HB	2.00	0.43
2:B:28:ALA:C	2:B:30:ASN:N	2.76	0.43
2:B:37:GLU:CD	3:C:37:PRO:HB3	2.43	0.43
3:C:194:ILE:HD12	3:C:194:ILE:N	2.33	0.43
2:B:225:ASN:ND2	3:C:207:GLY:C	2.76	0.43
1:A:139:VAL:HG11	1:A:249:LEU:HD12	2.00	0.43
1:A:261:TRP:CD1	3:C:36:ILE:HB	2.54	0.43
1:A:281:GLY:HA3	2:B:135:ILE:HG12	2.00	0.43
2:B:6:ALA:HA	2:B:30:ASN:CB	2.44	0.43
2:B:129:GLU:CD	2:B:209:HIS:HE2	2.26	0.43
1:A:154:MET:HE1	1:A:171:TRP:CA	2.47	0.42
2:B:8:GLY:HA2	2:B:188:ASN:HA	2.02	0.42
3:C:131:MET:HG2	3:C:159:PHE:HE1	1.85	0.42
1:A:66:THR:CG2	1:A:67:ARG:H	2.29	0.41
1:A:197:PRO:CG	1:A:227:ASN:HD22	2.31	0.41
2:B:198:MET:HB2	2:B:198:MET:HE3	1.81	0.41
1:A:93:ILE:HG23	1:A:107:VAL:HG11	2.02	0.41
1:A:261:TRP:CD1	3:C:39:GLU:HB2	2.54	0.41
3:C:54:GLU:HG3	3:C:98:SER:HB3	2.00	0.41
3:C:109:THR:CB	3:C:228:LEU:HD12	2.51	0.41
3:C:208:ALA:HA	3:C:209:PRO:HD3	1.95	0.41
1:A:177:PRO:HG3	3:C:25:LEU:CD1	2.51	0.40
2:B:60:VAL:HG13	2:B:92:PHE:HD1	1.86	0.40
2:B:136:ALA:HB1	2:B:142:GLU:O	2.22	0.40
3:C:132:LEU:C	3:C:132:LEU:HD23	2.47	0.40
1:A:208:TYR:CE1	1:A:219:ASP:HB3	2.56	0.40
2:B:31:ILE:HG12	2:B:192:THR:HB	2.03	0.40
2:B:174:GLN:HA	3:C:51:THR:HG22	2.03	0.40
1:A:76:GLN:HE21	1:A:76:GLN:HA	1.87	0.40
1:A:155:TYR:HB3	1:A:177:PRO:HG2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	224/297 (75%)	197 (88%)	22 (10%)	5 (2%)	5	26
2	B	235/254 (92%)	210 (89%)	21 (9%)	4 (2%)	7	32
3	C	227/242 (94%)	214 (94%)	11 (5%)	2 (1%)	14	48
All	All	686/793 (86%)	621 (90%)	54 (8%)	11 (2%)	7	34

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	58	VAL
2	B	29	ALA
1	A	114	MET
3	C	62	GLU
3	C	72	PRO
1	A	67	ARG
1	A	124	GLU
1	A	157	PRO
2	B	10	SER
2	B	90	GLY
1	A	86	ARG

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	204/257 (79%)	197 (97%)	7 (3%)	32	66

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	202/212 (95%)	196 (97%)	6 (3%)	36	69
3	C	197/204 (97%)	187 (95%)	10 (5%)	21	55
All	All	603/673 (90%)	580 (96%)	23 (4%)	29	63

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	80	ILE
1	A	101	GLN
1	A	179	VAL
1	A	190	VAL
1	A	221	ASP
1	A	248	THR
1	A	249	LEU
2	B	7	CYS
2	B	87	THR
2	B	95	ASN
2	B	112	CYS
2	B	201	VAL
2	B	235	THR
3	C	25	LEU
3	C	51	THR
3	C	60	THR
3	C	72	PRO
3	C	75	VAL
3	C	133	ILE
3	C	173	SER
3	C	188	TYR
3	C	195	THR
3	C	235	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	73	HIS
1	A	76	GLN
1	A	101	GLN
1	A	108	ASN
1	A	143	ASN
1	A	189	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	224	GLN
1	A	227	ASN
1	A	268	ASN
1	A	278	ASN
2	B	15	GLN
2	B	94	GLN
2	B	99	HIS
2	B	111	GLN
2	B	143	ASN
2	B	145	HIS
2	B	181	GLN
2	B	208	ASN
2	B	211	ASN
2	B	225	ASN
3	C	11	ASN
3	C	41	HIS
3	C	56	ASN
3	C	61	ASN
3	C	67	GLN
3	C	154	HIS
3	C	174	ASN
3	C	221	GLN

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	A	228/297 (76%)	1.92	72 (31%)  	41, 62, 138, 198	0
2	B	239/254 (94%)	2.49	105 (43%)  	41, 67, 169, 200	0
3	C	231/242 (95%)	1.58	51 (22%)  	41, 58, 118, 179	0
All	All	698/793 (88%)	2.00	228 (32%)  	41, 61, 150, 200	0

All (228) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	142	GLU	13.5
3	C	236	GLU	11.2
2	B	27	GLU	11.0
2	B	143	ASN	10.6
2	B	57	ASP	10.3
1	A	103	THR	10.2
1	A	219	ASP	9.8
2	B	11	ASP	9.7
3	C	185	TYR	9.7
2	B	9	TYR	9.5
2	B	249	ARG	9.2
3	C	179	ALA	9.2
1	A	220	LEU	8.9
2	B	148	TYR	8.7
2	B	12	ARG	8.5
1	A	101	GLN	8.0
2	B	10	SER	7.7
2	B	94	GLN	7.7
2	B	91	VAL	7.6
2	B	144	SER	7.5
1	A	99	GLY	7.3
2	B	47	ALA	7.2
2	B	136	ALA	7.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	71	ASN	7.1
2	B	44	ASP	7.0
1	A	100	THR	6.9
2	B	43	PRO	6.9
1	A	98	THR	6.9
2	B	29	ALA	6.9
2	B	145	HIS	6.9
2	B	46	ASP	6.6
2	B	58	VAL	6.5
1	A	66	THR	6.5
2	B	98	PHE	6.5
2	B	147	PRO	6.4
2	B	61	ASN	6.4
2	B	8	GLY	6.3
1	A	221	ASP	6.3
1	A	210	THR	6.3
2	B	6	ALA	6.3
2	B	135	ILE	6.3
3	C	187	ASP	6.2
3	C	178	ARG	6.0
1	A	62	ASN	6.0
1	A	63	LEU	6.0
1	A	64	ILE	5.8
3	C	1	GLY	5.8
1	A	72	HIS	5.7
2	B	51	ASP	5.7
3	C	188	TYR	5.6
1	A	292	ASP	5.5
1	A	65	GLU	5.5
3	C	235	ILE	5.5
2	B	24	THR	5.4
2	B	59	SER	5.4
2	B	100	TYR	5.4
3	C	233	GLU	5.4
3	C	191	THR	5.3
1	A	68	CYS	5.3
3	C	177	TYR	5.3
3	C	141	ASN	5.2
2	B	50	VAL	5.2
2	B	134	THR	5.2
1	A	67	ARG	5.1
3	C	76	GLN	5.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	102	ASN	5.0
3	C	186	PHE	5.0
2	B	55	ARG	4.9
1	A	224	GLN	4.8
2	B	40	GLU	4.7
1	A	76	GLN	4.7
3	C	176	HIS	4.7
2	B	13	VAL	4.7
2	B	150	THR	4.7
2	B	248	LEU	4.6
2	B	15	GLN	4.6
2	B	105	GLY	4.6
2	B	20	ASN	4.4
3	C	139	GLY	4.3
2	B	52	LYS	4.3
2	B	16	LEU	4.3
2	B	90	GLY	4.3
2	B	53	PRO	4.2
3	C	5	GLU	4.2
1	A	223	GLY	4.2
2	B	56	PRO	4.1
3	C	59	LYS	4.1
1	A	283	ASP	4.1
1	A	70	LEU	4.0
2	B	41	TYR	4.0
1	A	274	LYS	4.0
2	B	14	ALA	4.0
2	B	88	GLU	3.9
2	B	208	ASN	3.9
2	B	96	ALA	3.9
3	C	234	ASP	3.9
2	B	206	ALA	3.9
3	C	190	THR	3.8
2	B	26	GLN	3.8
2	B	95	ASN	3.8
1	A	242	LYS	3.8
2	B	247	GLY	3.8
2	B	7	CYS	3.7
2	B	161	THR	3.7
1	A	280	LYS	3.7
3	C	20	VAL	3.7
1	A	97	THR	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	282	ASN	3.6
2	B	28	ALA	3.6
1	A	226	PRO	3.5
3	C	50	GLU	3.5
2	B	97	GLN	3.5
2	B	155	GLN	3.5
2	B	45	THR	3.4
2	B	207	LEU	3.4
3	C	92	ARG	3.4
2	B	89	VAL	3.4
1	A	285	LYS	3.4
1	A	169	PHE	3.3
2	B	17	THR	3.3
3	C	78	LYS	3.2
1	A	132	ASP	3.2
2	B	87	THR	3.2
1	A	116	TYR	3.2
3	C	175	THR	3.2
3	C	231	ASP	3.2
1	A	172	GLN	3.2
2	B	79	TYR	3.1
1	A	118	GLN	3.1
2	B	111	GLN	3.1
2	B	54	THR	3.1
2	B	92	PHE	3.1
2	B	60	VAL	3.0
1	A	209	PRO	3.0
1	A	74	SER	3.0
2	B	115	SER	3.0
3	C	91	GLY	3.0
2	B	38	TRP	3.0
2	B	146	PRO	3.0
1	A	281	GLY	3.0
2	B	205	SER	2.9
2	B	199	ASN	2.9
1	A	275	THR	2.9
2	B	245	PHE	2.9
1	A	117	ALA	2.9
2	B	19	GLY	2.9
1	A	160	ALA	2.9
2	B	49	ALA	2.9
1	A	96	PRO	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	149	ALA	2.9
1	A	167	ASP	2.8
2	B	42	CYS	2.8
2	B	104	SER	2.8
1	A	104	ASP	2.8
2	B	33	ILE	2.8
1	A	198	ALA	2.8
1	A	241	GLU	2.8
2	B	25	THR	2.8
1	A	240	ILE	2.8
3	C	232	THR	2.8
1	A	69	VAL	2.7
3	C	60	THR	2.7
1	A	159	GLY	2.7
3	C	19	GLY	2.7
1	A	225	CYS	2.7
2	B	74	ASP	2.7
2	B	226	THR	2.7
2	B	230	SER	2.7
1	A	115	GLY	2.6
2	B	243	ALA	2.6
3	C	229	CYS	2.6
2	B	30	ASN	2.6
3	C	106	ARG	2.6
3	C	143	PRO	2.6
2	B	93	GLY	2.6
2	B	48	THR	2.6
3	C	70	CYS	2.5
1	A	227	ASN	2.5
1	A	293	LYS	2.5
3	C	144	ALA	2.5
2	B	76	LYS	2.5
1	A	185	ASP	2.5
3	C	137	PRO	2.5
2	B	246	ALA	2.5
3	C	222	ASP	2.4
3	C	142	VAL	2.4
3	C	63	THR	2.4
1	A	204	PHE	2.4
1	A	279	TYR	2.4
3	C	93	ASP	2.4
1	A	95	MET	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	89	LEU	2.3
3	C	62	GLU	2.3
2	B	220	VAL	2.3
1	A	142	PRO	2.3
2	B	99	HIS	2.3
1	A	196	SER	2.3
2	B	116	LYS	2.3
3	C	206	ILE	2.2
1	A	297	LEU	2.2
1	A	178	SER	2.2
1	A	269	GLN	2.2
1	A	176	ASN	2.2
3	C	174	ASN	2.2
2	B	244	GLU	2.2
3	C	128	THR	2.2
2	B	120	GLY	2.2
3	C	189	TYR	2.2
1	A	85	SER	2.2
1	A	273	PHE	2.2
2	B	203	PHE	2.2
2	B	152	GLN	2.1
1	A	268	ASN	2.1
2	B	189	ASN	2.1
3	C	145	ASP	2.1
2	B	229	THR	2.1
2	B	241	MET	2.1
3	C	159	PHE	2.1
1	A	208	TYR	2.1
2	B	63	PHE	2.1
2	B	211	ASN	2.1
1	A	120	ARG	2.1
3	C	23	PRO	2.1
1	A	278	ASN	2.0
2	B	131	VAL	2.0
3	C	210	THR	2.0
3	C	28	PHE	2.0
3	C	3	PRO	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 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.