



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:26 PM UTC

PDB ID : 4QPG / pdb_00004qpg
Title : Crystal structure of empty hepatitis A virus
Authors : Wang, X.; Ren, J.; Gao, Q.; Hu, Z.; Sun, Y.; Li, X.; Rowlands, D.J.; Yin, W.;
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Deposited on : 2014-06-23
Resolution : 3.50 Å(reported)

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

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

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) : 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

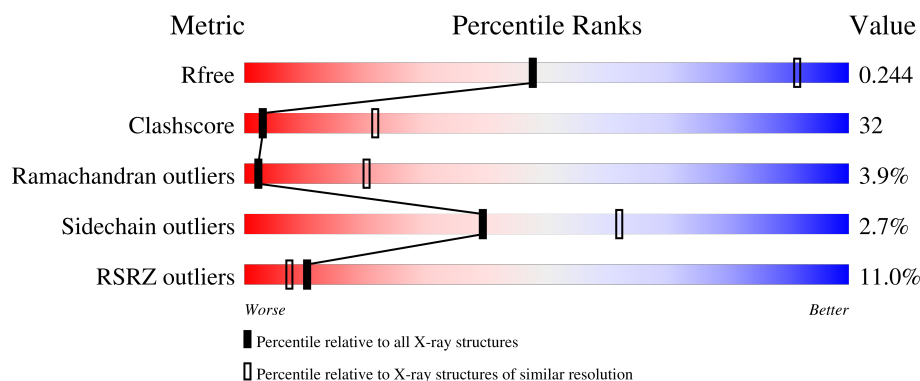
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	225	12% 45% 48% 6%
2	B	204	9% 54% 41% 5%
3	C	246	11% 49% 48% .

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5368 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 VP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	225	Total	C	N	O	S	0	0	0
			1785	1151	290	338	6			

- Molecule 2 is a protein called Capsid protein VP0.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	204	Total	C	N	O	S	0	0	0
			1615	1042	274	296	3			

- Molecule 3 is a protein called Capsid protein VP3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	246	Total	C	N	O	S	0	0	0
			1956	1248	331	363	14			

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Cl	0	0
			2	2		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).

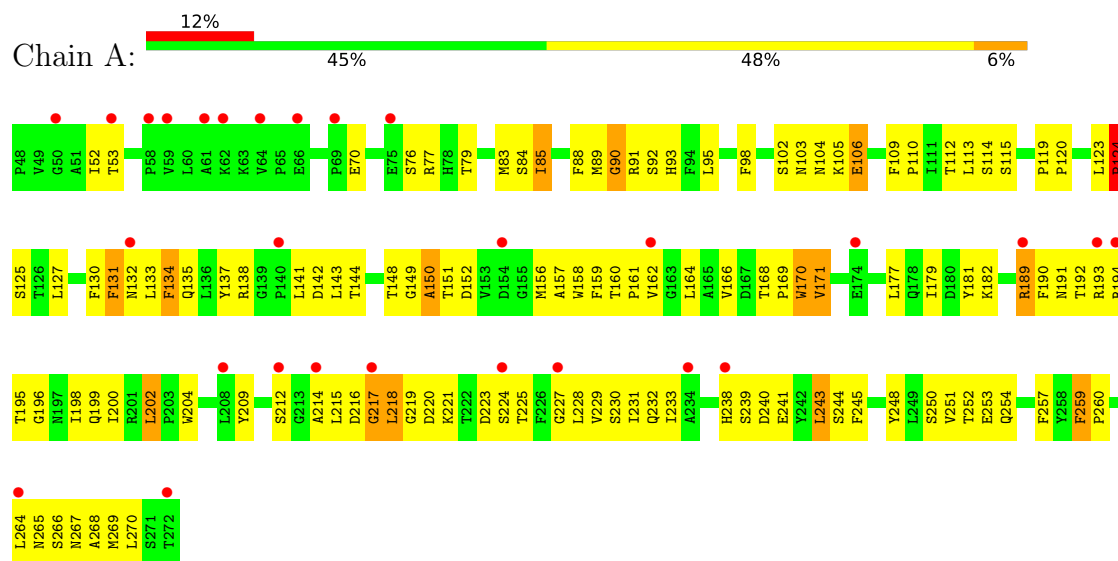


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		

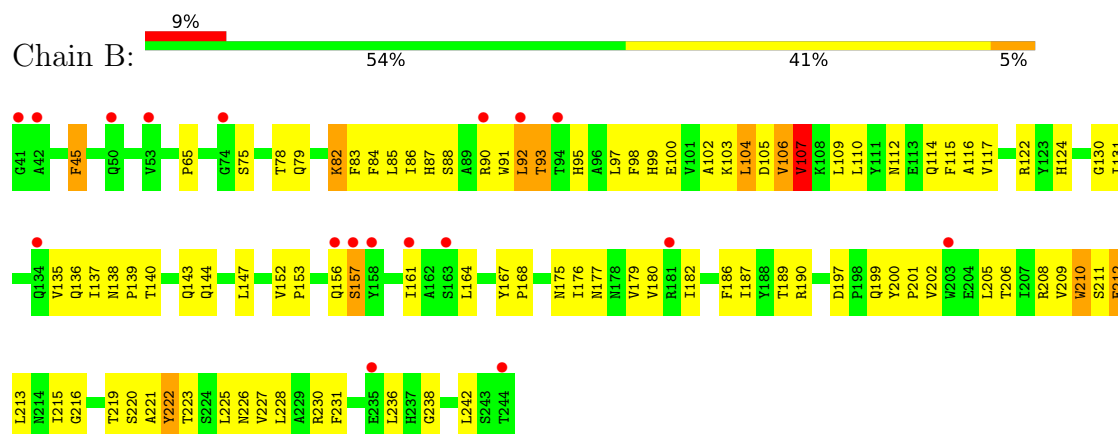
3 Residue-property plots [i](#)

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: Capsid protein VP1

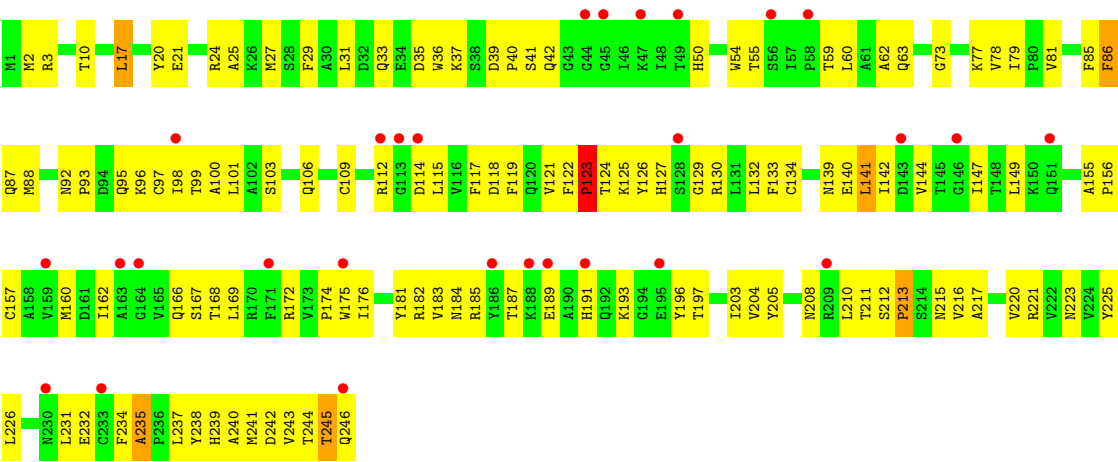


• Molecule 2: Capsid protein VP0



• Molecule 3: Capsid protein VP3





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	366.11Å 442.91Å 289.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.67 – 3.50 49.67 – 3.50	Depositor EDS
% Data completeness (in resolution range)	67.8 (49.67-3.50) 67.8 (49.67-3.50)	Depositor EDS
R_{merge}	0.36	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.08 (at 3.48Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.264 , 0.263 0.245 , 0.244	Depositor DCC
R_{free} test set	3996 reflections (0.67%)	wwPDB-VP
Wilson B-factor (Å ²)	175.5	Xtriage
Anisotropy	0.189	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 86.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.59	EDS
Total number of atoms	5368	wwPDB-VP
Average B, all atoms (Å ²)	180.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.63% 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

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, CL

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	0.32	0/1838	0.87	8/2506 (0.3%)
2	B	0.35	0/1659	0.83	5/2260 (0.2%)
3	C	0.32	0/2007	0.81	0/2733
All	All	0.33	0/5504	0.84	13/7499 (0.2%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	239	SER	N-CA-C	-6.77	104.89	113.01
1	A	202	LEU	CA-C-N	6.28	126.19	119.85
1	A	202	LEU	C-N-CA	6.28	126.19	119.85
1	A	168	THR	CA-C-N	6.06	127.41	119.84
1	A	168	THR	C-N-CA	6.06	127.41	119.84
2	B	93	THR	N-CA-C	-6.05	104.60	112.23
2	B	65	PRO	N-CA-C	-5.95	105.77	113.57
1	A	90	GLY	N-CA-C	-5.74	106.64	113.99
2	B	157	SER	CB-CA-C	-5.74	109.94	116.54
1	A	115	SER	N-CA-C	-5.34	106.03	112.54
2	B	197	ASP	CA-C-N	5.06	125.04	120.03
2	B	197	ASP	C-N-CA	5.06	125.04	120.03
1	A	171	VAL	N-CA-C	5.05	115.54	108.17

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	1785	0	1730	133	0
2	B	1615	0	1598	94	0
3	C	1956	0	1911	146	0
4	A	2	0	0	1	0
5	A	5	0	0	0	0
5	B	5	0	0	0	0
All	All	5368	0	5239	337	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 32.

All (337) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:ARG:NH2	4:A:301:CL:CL	2.32	0.98
3:C:62:ALA:HA	3:C:88:MET:HE3	1.46	0.98
2:B:92:LEU:H	2:B:95:HIS:HD2	1.14	0.92
2:B:92:LEU:H	2:B:95:HIS:CD2	1.89	0.91
1:A:265:ASN:HD21	1:A:267:ASN:HB2	1.38	0.89
3:C:241:MET:HE3	3:C:242:ASP:H	1.42	0.84
2:B:102:ALA:HB1	2:B:104:LEU:HD11	1.57	0.84
3:C:144:VAL:HG21	3:C:203:ILE:HD11	1.60	0.83
3:C:41:SER:HB3	3:C:42:GLN:NE2	1.95	0.80
3:C:144:VAL:HG23	3:C:147:ILE:HD12	1.61	0.80
1:A:195:THR:HG23	1:A:196:GLY:H	1.48	0.77
3:C:231:LEU:HD12	3:C:232:GLU:H	1.49	0.77
1:A:251:VAL:HG21	1:A:257:PHE:HZ	1.49	0.77
1:A:266:SER:HA	1:A:269:MET:HE3	1.66	0.75
1:A:150:ALA:HB3	1:A:243:LEU:HG	1.70	0.74
1:A:105:LYS:H	1:A:233:ILE:HD11	1.53	0.74
1:A:265:ASN:ND2	1:A:267:ASN:HB2	2.02	0.73
3:C:121:VAL:HG11	3:C:160:MET:HE1	1.70	0.73
1:A:265:ASN:ND2	3:C:95:GLN:HB2	2.03	0.73
2:B:104:LEU:N	2:B:104:LEU:HD12	2.03	0.73
1:A:143:LEU:HD12	1:A:144:THR:H	1.55	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:PHE:HD2	1:A:260:PRO:HD2	1.55	0.72
3:C:130:ARG:HD2	3:C:208:ASN:HD22	1.54	0.71
1:A:52:ILE:HG13	3:C:166:GLN:HG2	1.72	0.70
3:C:17:LEU:HD12	3:C:17:LEU:H	1.55	0.70
2:B:147:LEU:HD23	2:B:209:VAL:HA	1.74	0.70
1:A:91:ARG:HG3	3:C:17:LEU:O	1.92	0.69
3:C:103:SER:HA	3:C:106:GLN:NE2	2.07	0.69
2:B:82:LYS:HG3	2:B:83:PHE:N	2.08	0.69
1:A:259:PHE:HZ	2:B:168:PRO:HD3	1.57	0.68
2:B:107:VAL:HG21	2:B:202:VAL:HB	1.75	0.68
3:C:79:ILE:HD12	3:C:85:PHE:CZ	2.28	0.68
1:A:144:THR:HG21	1:A:199:GLN:HE21	1.58	0.67
1:A:112:THR:HG22	1:A:114:SER:H	1.60	0.66
3:C:87:GLN:HA	3:C:243:VAL:HG13	1.77	0.66
3:C:124:THR:C	3:C:126:TYR:H	2.04	0.66
1:A:191:ASN:HB3	1:A:194:ARG:HD2	1.78	0.66
2:B:122:ARG:HG2	2:B:122:ARG:HH11	1.61	0.66
1:A:209:TYR:CE2	3:C:41:SER:HB2	2.32	0.65
2:B:137:ILE:HG13	2:B:139:PRO:HD3	1.79	0.65
3:C:210:LEU:HD21	3:C:220:VAL:HG23	1.78	0.65
3:C:77:LYS:HE2	3:C:79:ILE:HD11	1.78	0.64
3:C:231:LEU:HD12	3:C:232:GLU:N	2.11	0.64
2:B:91:TRP:CZ2	2:B:213:LEU:HB2	2.32	0.64
3:C:112:ARG:HD2	3:C:181:TYR:CE2	2.32	0.64
1:A:113:LEU:HA	1:A:123:LEU:HD12	1.80	0.64
2:B:92:LEU:N	2:B:95:HIS:HD2	1.93	0.63
3:C:172:ARG:O	3:C:174:PRO:HD3	1.98	0.63
3:C:160:MET:HE2	3:C:162:ILE:HD13	1.80	0.63
3:C:109:CYS:SG	3:C:237:LEU:HD23	2.38	0.63
1:A:218:LEU:HD23	2:B:199:GLN:O	1.99	0.62
3:C:160:MET:HB2	3:C:169:LEU:HD12	1.81	0.62
3:C:241:MET:HE3	3:C:242:ASP:N	2.13	0.62
2:B:225:LEU:C	2:B:225:LEU:HD23	2.25	0.62
3:C:121:VAL:CG1	3:C:160:MET:HE1	2.30	0.62
3:C:169:LEU:C	3:C:169:LEU:HD23	2.25	0.61
2:B:103:LYS:C	2:B:104:LEU:HD12	2.25	0.61
3:C:129:GLY:O	3:C:162:ILE:HG12	1.99	0.61
3:C:130:ARG:HD2	3:C:208:ASN:ND2	2.16	0.61
1:A:143:LEU:HD12	1:A:144:THR:N	2.15	0.61
1:A:265:ASN:CG	3:C:95:GLN:HB2	2.26	0.61
3:C:77:LYS:HE3	3:C:246:GLN:OE1	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:92:ASN:HA	3:C:93:PRO:C	2.25	0.60
1:A:77:ARG:HA	1:A:77:ARG:NE	2.16	0.60
2:B:161:ILE:H	3:C:95:GLN:HE22	1.47	0.60
3:C:155:ALA:HB1	3:C:156:PRO:HD2	1.84	0.60
1:A:227:GLY:C	1:A:228:LEU:HD12	2.27	0.60
2:B:105:ASP:OD2	2:B:201:PRO:HB3	2.02	0.60
3:C:17:LEU:HD12	3:C:17:LEU:N	2.16	0.60
1:A:105:LYS:H	1:A:233:ILE:CD1	2.15	0.60
2:B:143:GLN:HA	2:B:215:ILE:HG22	1.83	0.59
2:B:84:PHE:CD2	2:B:115:PHE:HB3	2.37	0.59
3:C:144:VAL:CG2	3:C:203:ILE:HD11	2.30	0.59
3:C:189:GLU:CD	3:C:189:GLU:H	2.10	0.59
3:C:234:PHE:O	3:C:235:ALA:HB3	2.03	0.59
2:B:205:LEU:HD23	2:B:206:THR:N	2.18	0.58
3:C:124:THR:O	3:C:126:TYR:N	2.36	0.58
3:C:118:ASP:HB2	3:C:225:TYR:HB2	1.84	0.58
3:C:144:VAL:CG2	3:C:147:ILE:HD12	2.33	0.58
2:B:112:ASN:ND2	2:B:114:GLN:HB2	2.19	0.58
3:C:78:VAL:O	3:C:79:ILE:HD13	2.02	0.58
3:C:193:LYS:HD3	3:C:196:TYR:OH	2.03	0.58
1:A:259:PHE:CZ	2:B:168:PRO:HD3	2.36	0.58
1:A:144:THR:HG22	1:A:199:GLN:HG2	1.85	0.58
2:B:136:GLN:HB3	2:B:179:VAL:HG22	1.86	0.58
3:C:139:ASN:OD1	3:C:142:ILE:HG23	2.04	0.57
2:B:135:VAL:HG22	2:B:227:VAL:HG22	1.86	0.57
1:A:190:PHE:CG	1:A:198:ILE:HD11	2.40	0.57
1:A:182:LYS:HE2	1:A:232:GLN:OE1	2.05	0.56
2:B:92:LEU:N	2:B:92:LEU:HD12	2.20	0.56
3:C:237:LEU:HD12	3:C:237:LEU:C	2.30	0.56
3:C:134:CYS:HA	3:C:157:CYS:HB3	1.87	0.56
3:C:185:ARG:H	3:C:197:THR:HG22	1.71	0.56
2:B:117:VAL:HG21	2:B:231:PHE:CE2	2.40	0.56
1:A:156:MET:HB2	1:A:189:ARG:HD3	1.87	0.56
3:C:121:VAL:HG11	3:C:162:ILE:HG23	1.88	0.56
1:A:195:THR:HG23	1:A:196:GLY:N	2.18	0.56
2:B:105:ASP:O	2:B:106:VAL:C	2.49	0.56
1:A:144:THR:CG2	1:A:199:GLN:HG2	2.36	0.55
1:A:150:ALA:HA	1:A:241:GLU:HG3	1.89	0.55
1:A:159:PHE:HD2	1:A:202:LEU:HD22	1.70	0.55
3:C:81:VAL:HG12	3:C:115:LEU:HD12	1.87	0.55
1:A:92:SER:CB	1:A:250:SER:HB2	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:SER:HB2	1:A:250:SER:HB2	1.87	0.55
1:A:157:ALA:HA	1:A:230:SER:O	2.05	0.55
3:C:132:LEU:HD23	3:C:132:LEU:C	2.32	0.54
1:A:142:ASP:OD2	1:A:252:THR:HG22	2.07	0.54
3:C:101:LEU:HD23	3:C:226:LEU:HG	1.87	0.54
3:C:185:ARG:HD2	3:C:191:HIS:HA	1.88	0.54
3:C:21:GLU:CD	3:C:21:GLU:H	2.15	0.54
2:B:130:GLY:O	2:B:131:ILE:HD13	2.08	0.54
1:A:102:SER:OG	1:A:105:LYS:HG3	2.08	0.54
2:B:88:SER:HB3	2:B:226:ASN:OD1	2.08	0.54
3:C:160:MET:HB2	3:C:169:LEU:CD1	2.38	0.54
1:A:243:LEU:HD22	1:A:245:PHE:CE1	2.42	0.54
3:C:62:ALA:HB2	3:C:87:GLN:HG2	1.90	0.53
3:C:237:LEU:HD12	3:C:238:TYR:N	2.23	0.53
3:C:112:ARG:HA	3:C:175:TRP:CZ3	2.43	0.53
1:A:95:LEU:O	1:A:124:PRO:HG3	2.09	0.53
2:B:97:LEU:HD12	2:B:98:PHE:H	1.73	0.53
3:C:174:PRO:O	3:C:176:ILE:HG12	2.08	0.53
1:A:135:GLN:OE1	2:B:153:PRO:HG2	2.08	0.53
1:A:52:ILE:CG1	3:C:166:GLN:HG2	2.39	0.53
1:A:113:LEU:HA	1:A:123:LEU:CD1	2.39	0.53
1:A:259:PHE:HD2	1:A:260:PRO:CD	2.21	0.53
2:B:225:LEU:HD23	2:B:226:ASN:N	2.23	0.53
1:A:112:THR:HG23	1:A:224:SER:O	2.09	0.53
2:B:104:LEU:N	2:B:104:LEU:CD1	2.72	0.53
3:C:185:ARG:O	3:C:185:ARG:HG2	2.09	0.53
1:A:52:ILE:HD12	3:C:168:THR:O	2.09	0.52
3:C:41:SER:HB3	3:C:42:GLN:HE21	1.72	0.52
1:A:251:VAL:HG21	1:A:257:PHE:CZ	2.38	0.52
2:B:87:HIS:HB3	2:B:104:LEU:HD21	1.90	0.52
2:B:210:TRP:HA	2:B:210:TRP:CE3	2.45	0.52
3:C:185:ARG:HG2	3:C:185:ARG:HH11	1.73	0.52
1:A:77:ARG:HA	1:A:77:ARG:HE	1.74	0.52
1:A:160:THR:HG21	1:A:166:VAL:HB	1.92	0.52
1:A:228:LEU:HD12	1:A:228:LEU:N	2.25	0.52
1:A:199:GLN:HB3	3:C:25:ALA:HA	1.92	0.52
2:B:124:HIS:CD2	2:B:236:LEU:HB3	2.45	0.52
1:A:204:TRP:HB3	3:C:36:TRP:NE1	2.25	0.51
3:C:212:SER:HB2	3:C:213:PRO:HD2	1.93	0.51
2:B:189:THR:HG23	2:B:200:TYR:OH	2.09	0.51
3:C:88:MET:HE2	3:C:88:MET:HA	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:132:LEU:HD13	3:C:149:LEU:HD11	1.92	0.51
1:A:85:ILE:HG23	1:A:130:PHE:HE2	1.75	0.51
1:A:134:PHE:CD1	1:A:134:PHE:N	2.78	0.51
1:A:259:PHE:HZ	2:B:168:PRO:CD	2.23	0.51
1:A:112:THR:HG22	1:A:114:SER:N	2.26	0.51
3:C:142:ILE:O	3:C:142:ILE:HG13	2.11	0.51
2:B:140:THR:CG2	2:B:143:GLN:HG3	2.40	0.51
1:A:267:ASN:HD21	3:C:96:LYS:HE3	1.76	0.51
2:B:86:ILE:HD11	2:B:110:LEU:CD2	2.40	0.51
1:A:214:ALA:HB1	2:B:157:SER:HB2	1.91	0.51
3:C:114:ASP:OD1	3:C:174:PRO:HA	2.11	0.51
3:C:124:THR:C	3:C:126:TYR:N	2.68	0.51
1:A:113:LEU:HD22	1:A:131:PHE:CG	2.45	0.51
1:A:138:ARG:HB2	1:A:204:TRP:CZ2	2.46	0.50
3:C:117:PHE:CE1	3:C:226:LEU:HD13	2.46	0.50
1:A:259:PHE:HD1	2:B:187:ILE:HG21	1.76	0.50
1:A:238:HIS:C	1:A:240:ASP:N	2.70	0.50
2:B:136:GLN:CB	2:B:179:VAL:HG22	2.41	0.50
1:A:93:HIS:HB2	1:A:127:LEU:HD21	1.93	0.50
1:A:216:ASP:O	1:A:217:GLY:C	2.53	0.50
2:B:86:ILE:HD11	2:B:110:LEU:HD21	1.92	0.49
3:C:121:VAL:C	3:C:123:PRO:HD3	2.37	0.49
3:C:160:MET:HE2	3:C:162:ILE:CD1	2.42	0.49
3:C:117:PHE:CD1	3:C:226:LEU:HD13	2.47	0.49
2:B:87:HIS:HB3	2:B:104:LEU:CD2	2.43	0.49
1:A:119:PRO:HA	1:A:120:PRO:C	2.37	0.49
1:A:132:ASN:ND2	1:A:264:LEU:HD11	2.28	0.49
1:A:191:ASN:CB	1:A:194:ARG:HH11	2.26	0.49
2:B:220:SER:HB3	2:B:222:TYR:CE1	2.48	0.49
3:C:86:PHE:CE1	3:C:243:VAL:HG22	2.48	0.49
2:B:176:ILE:HD11	3:C:167:SER:HB3	1.95	0.48
2:B:117:VAL:HG21	2:B:231:PHE:CD2	2.48	0.48
2:B:161:ILE:O	2:B:164:LEU:HG	2.14	0.48
3:C:185:ARG:C	3:C:187:THR:H	2.22	0.48
3:C:55:THR:HB	3:C:231:LEU:HD23	1.96	0.48
1:A:109:PHE:CE1	1:A:229:VAL:HB	2.49	0.47
2:B:45:PHE:CD1	2:B:45:PHE:C	2.92	0.47
2:B:161:ILE:H	3:C:95:GLN:NE2	2.11	0.47
1:A:177:LEU:O	1:A:182:LYS:NZ	2.46	0.47
3:C:60:LEU:HG	3:C:88:MET:HG3	1.97	0.47
1:A:158:TRP:CE2	1:A:230:SER:HB2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:75:SER:H	2:B:78:THR:HB	1.80	0.47
2:B:84:PHE:HB3	2:B:115:PHE:CD2	2.49	0.47
1:A:233:ILE:C	1:A:233:ILE:HD12	2.38	0.47
1:A:53:THR:O	3:C:168:THR:HB	2.15	0.47
1:A:84:SER:O	1:A:85:ILE:C	2.58	0.47
1:A:161:PRO:HB2	1:A:164:LEU:HD12	1.95	0.47
1:A:200:ILE:HD13	3:C:29:PHE:CD2	2.50	0.47
2:B:45:PHE:HD1	2:B:45:PHE:O	1.97	0.47
3:C:130:ARG:HA	3:C:160:MET:O	2.15	0.47
1:A:238:HIS:C	1:A:240:ASP:H	2.23	0.46
2:B:83:PHE:CD2	2:B:230:ARG:HB3	2.50	0.46
1:A:113:LEU:O	1:A:114:SER:C	2.59	0.46
1:A:166:VAL:HG11	1:A:228:LEU:HD22	1.98	0.46
1:A:204:TRP:HB3	3:C:36:TRP:CE2	2.50	0.46
1:A:77:ARG:HE	1:A:77:ARG:CA	2.28	0.46
2:B:97:LEU:HD12	2:B:209:VAL:O	2.14	0.46
3:C:106:GLN:OE1	3:C:240:ALA:HA	2.15	0.46
1:A:150:ALA:HA	1:A:241:GLU:CG	2.46	0.46
2:B:87:HIS:CG	2:B:88:SER:N	2.83	0.46
2:B:104:LEU:HB3	2:B:109:LEU:CD1	2.45	0.46
3:C:103:SER:O	3:C:106:GLN:HG2	2.16	0.46
3:C:213:PRO:HG2	3:C:216:VAL:HG22	1.98	0.46
1:A:83:MET:HB2	3:C:50:HIS:HE1	1.80	0.46
1:A:88:PHE:C	1:A:90:GLY:N	2.74	0.46
2:B:140:THR:HG22	2:B:143:GLN:HG3	1.97	0.46
2:B:223:THR:HG23	2:B:223:THR:O	2.14	0.46
3:C:2:MET:SD	3:C:2:MET:C	2.99	0.46
3:C:238:TYR:CD1	3:C:238:TYR:C	2.94	0.46
1:A:138:ARG:NH2	3:C:37:LYS:O	2.49	0.45
1:A:264:LEU:O	1:A:269:MET:HE2	2.16	0.45
2:B:100:GLU:HA	2:B:208:ARG:HG2	1.98	0.45
3:C:59:THR:OG1	3:C:99:THR:HB	2.16	0.45
2:B:190:ARG:NH1	2:B:199:GLN:HG2	2.31	0.45
3:C:77:LYS:HE3	3:C:246:GLN:CD	2.41	0.45
3:C:132:LEU:HD21	3:C:157:CYS:HB2	1.99	0.45
3:C:112:ARG:HG3	3:C:112:ARG:HH11	1.81	0.45
1:A:191:ASN:HB2	1:A:194:ARG:HH11	1.81	0.45
1:A:135:GLN:O	1:A:212:SER:HB2	2.16	0.45
1:A:133:LEU:HB3	3:C:54:TRP:CZ2	2.51	0.45
1:A:88:PHE:C	1:A:90:GLY:H	2.25	0.45
2:B:79:GLN:HG3	2:B:116:ALA:HB1	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:ASN:ND2	1:A:104:ASN:OD1	2.50	0.45
3:C:139:ASN:OD1	3:C:141:LEU:HD12	2.17	0.45
1:A:138:ARG:HH11	1:A:204:TRP:NE1	2.15	0.44
2:B:79:GLN:O	2:B:79:GLN:HG2	2.16	0.44
2:B:105:ASP:CG	2:B:201:PRO:HB3	2.43	0.44
3:C:20:TYR:O	3:C:24:ARG:HG2	2.17	0.44
2:B:86:ILE:CG2	2:B:109:LEU:HD13	2.47	0.44
2:B:122:ARG:HG2	2:B:122:ARG:NH1	2.29	0.44
1:A:137:TYR:OH	1:A:141:LEU:HD21	2.18	0.44
1:A:215:LEU:HB2	1:A:220:ASP:OD1	2.17	0.44
2:B:211:SER:O	2:B:212:GLU:C	2.60	0.44
1:A:177:LEU:HD22	1:A:181:TYR:CD2	2.52	0.44
3:C:132:LEU:HD23	3:C:133:PHE:N	2.32	0.44
1:A:77:ARG:NE	1:A:77:ARG:CA	2.81	0.44
1:A:70:GLU:OE1	3:C:174:PRO:HG3	2.18	0.44
1:A:144:THR:CG2	1:A:199:GLN:HE21	2.30	0.44
2:B:186:PHE:O	2:B:187:ILE:HD13	2.18	0.44
3:C:182:ARG:NE	3:C:196:TYR:HB2	2.32	0.44
1:A:253:GLU:CD	1:A:253:GLU:H	2.26	0.43
2:B:156:GLN:HE22	2:B:208:ARG:HH12	1.66	0.43
2:B:222:TYR:N	2:B:222:TYR:CD1	2.86	0.43
1:A:149:GLY:O	1:A:150:ALA:O	2.35	0.43
2:B:179:VAL:HG12	2:B:180:VAL:N	2.32	0.43
1:A:151:THR:HA	1:A:192:THR:OG1	2.18	0.43
3:C:85:PHE:CD1	3:C:85:PHE:C	2.96	0.43
1:A:148:THR:HB	1:A:244:SER:HB2	2.00	0.43
2:B:147:LEU:CD2	2:B:209:VAL:HA	2.47	0.43
3:C:86:PHE:CD1	3:C:98:ILE:HA	2.53	0.43
1:A:195:THR:CG2	1:A:196:GLY:H	2.18	0.43
1:A:219:GLY:C	1:A:221:LYS:H	2.26	0.43
2:B:139:PRO:HA	2:B:143:GLN:OE1	2.18	0.43
3:C:73:GLY:HA2	3:C:149:LEU:HB2	2.00	0.43
3:C:149:LEU:HD13	3:C:205:TYR:CB	2.47	0.43
3:C:55:THR:CB	3:C:231:LEU:HD23	2.49	0.43
2:B:86:ILE:HG23	2:B:109:LEU:HB3	1.99	0.43
3:C:234:PHE:O	3:C:235:ALA:CB	2.67	0.43
1:A:113:LEU:HD22	1:A:131:PHE:HB3	2.01	0.43
3:C:144:VAL:HG23	3:C:147:ILE:CD1	2.42	0.43
3:C:221:ARG:HH21	3:C:221:ARG:HG3	1.84	0.43
3:C:183:VAL:O	3:C:197:THR:HG22	2.19	0.43
3:C:183:VAL:HG22	3:C:184:ASN:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:ARG:NE	3:C:39:ASP:HB3	2.33	0.43
1:A:200:ILE:HG13	3:C:27:MET:HG3	2.00	0.43
3:C:182:ARG:HD2	3:C:196:TYR:O	2.18	0.43
1:A:130:PHE:C	1:A:132:ASN:H	2.27	0.42
2:B:138:ASN:N	2:B:139:PRO:HD3	2.34	0.42
3:C:127:HIS:HB3	3:C:210:LEU:HD11	2.00	0.42
3:C:149:LEU:HD13	3:C:205:TYR:HB3	2.01	0.42
1:A:223:ASP:OD2	2:B:190:ARG:NH1	2.51	0.42
2:B:205:LEU:HD23	2:B:205:LEU:C	2.44	0.42
2:B:216:GLY:HA3	3:C:215:ASN:C	2.44	0.42
3:C:211:THR:O	3:C:212:SER:HB3	2.18	0.42
2:B:90:ARG:N	2:B:90:ARG:HD2	2.35	0.42
1:A:106:GLU:CD	1:A:106:GLU:C	2.87	0.42
1:A:162:VAL:HG11	1:A:225:THR:O	2.19	0.42
3:C:140:GLU:CD	3:C:197:THR:H	2.27	0.42
1:A:254:GLN:OE1	3:C:35:ASP:HB3	2.19	0.42
1:A:268:ALA:O	1:A:270:LEU:HG	2.20	0.42
2:B:168:PRO:O	2:B:182:ILE:HD13	2.19	0.42
1:A:95:LEU:HA	1:A:127:LEU:HD12	2.01	0.42
3:C:245:THR:O	3:C:246:GLN:C	2.63	0.42
1:A:76:SER:C	1:A:77:ARG:HE	2.28	0.42
1:A:91:ARG:O	1:A:93:HIS:ND1	2.52	0.42
1:A:98:PHE:HZ	1:A:231:ILE:HD12	1.85	0.42
1:A:110:PRO:HD2	1:A:170:TRP:CE2	2.55	0.42
1:A:169:PRO:O	1:A:171:VAL:HG23	2.19	0.42
2:B:144:GLN:HB3	3:C:124:THR:CG2	2.50	0.42
3:C:31:LEU:C	3:C:33:GLN:N	2.78	0.42
2:B:100:GLU:OE1	2:B:103:LYS:HD3	2.20	0.41
2:B:210:TRP:NE1	3:C:225:TYR:OH	2.49	0.41
1:A:134:PHE:N	1:A:134:PHE:HD1	2.18	0.41
2:B:144:GLN:O	2:B:213:LEU:HD12	2.20	0.41
3:C:21:GLU:CD	3:C:21:GLU:N	2.78	0.41
1:A:83:MET:HB2	3:C:50:HIS:CE1	2.55	0.41
1:A:137:TYR:CG	1:A:138:ARG:N	2.88	0.41
1:A:130:PHE:C	1:A:130:PHE:CD1	2.98	0.41
2:B:85:LEU:HA	2:B:228:LEU:HD23	2.02	0.41
2:B:95:HIS:ND1	2:B:99:HIS:CD2	2.88	0.41
3:C:63:GLN:NE2	3:C:221:ARG:HD3	2.35	0.41
2:B:176:ILE:HG22	2:B:177:ASN:N	2.35	0.41
2:B:219:THR:HG22	2:B:220:SER:N	2.35	0.41
3:C:77:LYS:HE2	3:C:79:ILE:CD1	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:160:MET:SD	3:C:169:LEU:HB2	2.60	0.41
3:C:182:ARG:HD2	3:C:196:TYR:C	2.45	0.41
2:B:143:GLN:HG2	2:B:215:ILE:HG21	2.01	0.41
3:C:3:ARG:HG2	3:C:3:ARG:O	2.21	0.41
1:A:191:ASN:HB3	1:A:194:ARG:CD	2.50	0.41
1:A:233:ILE:HD12	1:A:233:ILE:O	2.20	0.41
1:A:243:LEU:HD22	1:A:245:PHE:HE1	1.85	0.41
1:A:259:PHE:CD2	1:A:260:PRO:HD2	2.45	0.41
2:B:175:ASN:HB2	3:C:123:PRO:O	2.21	0.41
3:C:85:PHE:O	3:C:86:PHE:HB3	2.20	0.41
3:C:133:PHE:CD1	3:C:204:VAL:HG22	2.56	0.41
3:C:119:PHE:O	3:C:168:THR:HA	2.21	0.41
3:C:175:TRP:O	3:C:176:ILE:HD13	2.21	0.41
1:A:93:HIS:HB2	1:A:127:LEU:CD2	2.50	0.40
3:C:122:PHE:N	3:C:123:PRO:HD3	2.35	0.40
1:A:85:ILE:H	1:A:85:ILE:HG13	1.73	0.40
1:A:143:LEU:HD12	1:A:248:TYR:O	2.21	0.40
3:C:40:PRO:O	3:C:41:SER:C	2.65	0.40
3:C:122:PHE:CE2	3:C:223:ASN:ND2	2.89	0.40
2:B:93:THR:OG1	2:B:221:ALA:HB1	2.21	0.40
3:C:31:LEU:C	3:C:33:GLN:H	2.29	0.40
3:C:59:THR:HG21	3:C:100:ALA:HB2	2.03	0.40
3:C:123:PRO:HB3	3:C:220:VAL:HG11	2.02	0.40
1:A:103:ASN:O	1:A:105:LYS:HG2	2.22	0.40
2:B:152:VAL:HG22	2:B:167:TYR:CD2	2.56	0.40
3:C:244:THR:C	3:C:246:GLN:H	2.29	0.40
1:A:89:MET:HB2	1:A:251:VAL:CG1	2.51	0.40
1:A:144:THR:HB	1:A:199:GLN:HG2	2.03	0.40
2:B:100:GLU:OE1	2:B:103:LYS:HB2	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	A	223/225 (99%)	182 (82%)	31 (14%)	10 (4%)	2	17
2	B	202/204 (99%)	160 (79%)	36 (18%)	6 (3%)	3	25
3	C	244/246 (99%)	198 (81%)	36 (15%)	10 (4%)	2	19
All	All	669/675 (99%)	540 (81%)	103 (15%)	26 (4%)	2	20

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	150	ALA
2	B	106	VAL
3	C	97	CYS
3	C	125	LYS
1	A	217	GLY
1	A	218	LEU
1	A	259	PHE
2	B	242	LEU
3	C	213	PRO
1	A	125	SER
1	A	131	PHE
1	A	170	TRP
2	B	212	GLU
3	C	10	THR
1	A	85	ILE
3	C	86	PHE
3	C	217	ALA
3	C	245	THR
2	B	238	GLY
1	A	79	THR
2	B	45	PHE
3	C	239	HIS
2	B	107	VAL
3	C	123	PRO
1	A	124	PRO
3	C	235	ALA

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	198/198 (100%)	191 (96%)	7 (4%)	32	57
2	B	177/177 (100%)	171 (97%)	6 (3%)	32	57
3	C	217/217 (100%)	214 (99%)	3 (1%)	59	71
All	All	592/592 (100%)	576 (97%)	16 (3%)	39	62

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	106	GLU
1	A	124	PRO
1	A	134	PHE
1	A	152	ASP
1	A	179	ILE
1	A	189	ARG
1	A	243	LEU
2	B	82	LYS
2	B	92	LEU
2	B	104	LEU
2	B	107	VAL
2	B	210	TRP
2	B	222	TYR
3	C	17	LEU
3	C	123	PRO
3	C	141	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	ASN
1	A	118	ASN
1	A	197	ASN
1	A	265	ASN
1	A	267	ASN
2	B	95	HIS
2	B	99	HIS
2	B	112	ASN
2	B	134	GLN
2	B	136	GLN
2	B	199	GLN

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Mol	Chain	Res	Type
2	B	237	HIS
3	C	63	GLN
3	C	74	GLN
3	C	75	GLN
3	C	90	ASN
3	C	95	GLN
3	C	208	ASN
3	C	230	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	$\# Z > 2$
5	SO4	A	303	-	4,4,4	0.32	0	6,6,6	0.09	0
5	SO4	B	301	-	4,4,4	0.33	0	6,6,6	0.07	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	A	225/225 (100%)	0.78	28 (12%) 8 6	155, 181, 222, 268	0
2	B	204/204 (100%)	0.64	18 (8%) 15 10	153, 174, 202, 269	0
3	C	246/246 (100%)	0.71	28 (11%) 10 7	152, 176, 199, 261	0
All	All	675/675 (100%)	0.71	74 (10%) 10 7	152, 177, 211, 269	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	113	GLY	6.2
2	B	41	GLY	6.2
1	A	174	GLU	4.8
3	C	146	GLY	4.7
1	A	59	VAL	4.4
3	C	175	TRP	4.3
1	A	217	GLY	4.1
1	A	61	ALA	4.1
1	A	154	ASP	4.1
2	B	235	GLU	3.9
3	C	189	GLU	3.8
3	C	45	GLY	3.8
3	C	128	SER	3.7
3	C	191	HIS	3.7
2	B	157	SER	3.6
3	C	164	GLY	3.6
1	A	64	VAL	3.5
3	C	163	ALA	3.4
3	C	44	GLY	3.4
1	A	189	ARG	3.1
2	B	163	SER	3.1
2	B	90	ARG	3.1
1	A	162	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	66	GLU	2.9
3	C	230	ASN	2.8
3	C	49	THR	2.8
3	C	143	ASP	2.8
1	A	75	GLU	2.8
1	A	272	THR	2.8
3	C	246	GLN	2.7
3	C	112	ARG	2.7
1	A	264	LEU	2.7
1	A	58	PRO	2.7
1	A	50	GLY	2.6
2	B	92	LEU	2.6
1	A	224	SER	2.6
2	B	42	ALA	2.6
2	B	50	GLN	2.6
1	A	238	HIS	2.6
2	B	161	ILE	2.6
2	B	53	VAL	2.6
3	C	171	PHE	2.5
3	C	186	TYR	2.5
3	C	209	ARG	2.5
1	A	212	SER	2.5
3	C	47	LYS	2.5
2	B	181	ARG	2.5
2	B	156	GLN	2.4
3	C	159	VAL	2.4
3	C	188	LYS	2.4
1	A	214	ALA	2.4
2	B	74	GLY	2.4
2	B	203	TRP	2.4
1	A	69	PRO	2.3
1	A	140	PRO	2.3
2	B	244	THR	2.3
1	A	62	LYS	2.3
3	C	233	CYS	2.3
1	A	132	ASN	2.3
2	B	158	TYR	2.3
1	A	194	ARG	2.3
3	C	114	ASP	2.1
3	C	151	GLN	2.1
3	C	98	ILE	2.1
1	A	234	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
3	C	56	SER	2.1
3	C	195	GLU	2.1
1	A	193	ARG	2.1
1	A	227	GLY	2.1
2	B	134	GLN	2.1
1	A	53	THR	2.0
1	A	208	LEU	2.0
3	C	58	PRO	2.0
2	B	94	THR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	CL	A	301	1/1	0.65	0.24	163,163,163,163	1
5	SO4	B	301	5/5	0.78	0.15	300,300,300,300	0
4	CL	A	302	1/1	0.84	0.13	141,141,141,141	1
5	SO4	A	303	5/5	0.91	0.10	300,300,300,300	0

6.5 Other polymers [i](#)

There are no such residues in this entry.