



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:34 AM GMT

PDB ID : 2AX0
Title : Hepatitis C Virus NS5b RNA Polymerase in complex with a covalent inhibitor (5x)
Authors : Powers, J.P.; Piper, D.E.; Li, Y.; Mayorga, V.; Anzola, J.; Chen, J.M.; Jaen, J.C.; Lee, G.; Liu, J.; Peterson, M.G.; Tonn, G.R.; Ye, Q.; Walker, N.P.; Wang, Z.
Deposited on : 2005-09-02
Resolution : 2.00 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
<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

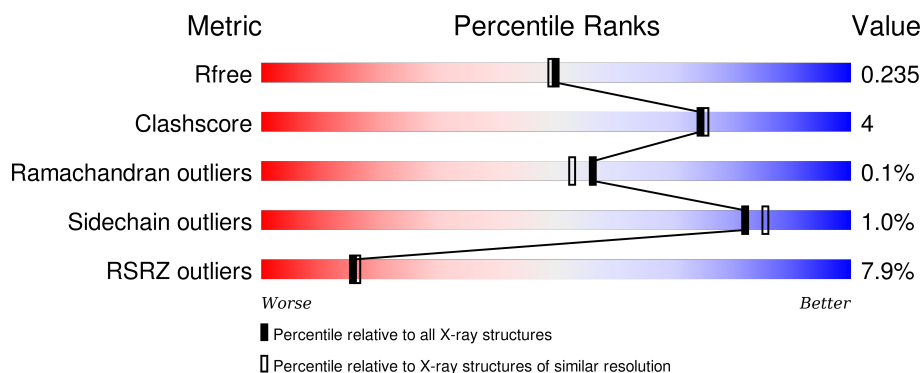
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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 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	A	580	<div> <div>8%</div> <div>84%</div> <div>10%</div> <div>• •</div> </div>
1	B	580	<div> <div>7%</div> <div>88%</div> <div>7%</div> <div>• •</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	5X	A	1001	-	-	-	X
3	5X	B	1002	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9595 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 Genome polyprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	554	Total	C	N	O	S	0	0	0
			4315	2722	764	798	31			
1	B	557	Total	C	N	O	S	0	0	0
			4329	2730	767	801	31			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	499	ALA	VAL	ENGINEERED	UNP P26663
A	506	ASN	SER	ENGINEERED	UNP P26663
A	514	ARG	GLN	ENGINEERED	UNP P26663
A	520	ILE	THR	ENGINEERED	UNP P26663
A	540	ALA	PRO	ENGINEERED	UNP P26663
A	543	GLY	SER	ENGINEERED	UNP P26663
A	549	SER	GLY	ENGINEERED	UNP P26663
A	552	THR	VAL	ENGINEERED	UNP P26663
A	563	GLY	SER	ENGINEERED	UNP P26663
A	564	VAL	LEU	ENGINEERED	UNP P26663
A	566	HIS	ARG	ENGINEERED	UNP P26663
A	571	HIS	-	EXPRESSION TAG	UNP P26663
A	572	HIS	-	EXPRESSION TAG	UNP P26663
A	573	HIS	-	EXPRESSION TAG	UNP P26663
A	574	HIS	-	EXPRESSION TAG	UNP P26663
A	575	HIS	-	EXPRESSION TAG	UNP P26663
A	576	HIS	-	EXPRESSION TAG	UNP P26663
A	577	HIS	-	EXPRESSION TAG	UNP P26663
A	578	HIS	-	EXPRESSION TAG	UNP P26663
A	579	HIS	-	EXPRESSION TAG	UNP P26663
A	580	HIS	-	EXPRESSION TAG	UNP P26663
B	499	ALA	VAL	ENGINEERED	UNP P26663
B	506	ASN	SER	ENGINEERED	UNP P26663
B	514	ARG	GLN	ENGINEERED	UNP P26663
B	520	ILE	THR	ENGINEERED	UNP P26663

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Chain	Residue	Modelled	Actual	Comment	Reference
B	540	ALA	PRO	ENGINEERED	UNP P26663
B	543	GLY	SER	ENGINEERED	UNP P26663
B	549	SER	GLY	ENGINEERED	UNP P26663
B	552	THR	VAL	ENGINEERED	UNP P26663
B	563	GLY	SER	ENGINEERED	UNP P26663
B	564	VAL	LEU	ENGINEERED	UNP P26663
B	566	HIS	ARG	ENGINEERED	UNP P26663
B	571	HIS	-	EXPRESSION TAG	UNP P26663
B	572	HIS	-	EXPRESSION TAG	UNP P26663
B	573	HIS	-	EXPRESSION TAG	UNP P26663
B	574	HIS	-	EXPRESSION TAG	UNP P26663
B	575	HIS	-	EXPRESSION TAG	UNP P26663
B	576	HIS	-	EXPRESSION TAG	UNP P26663
B	577	HIS	-	EXPRESSION TAG	UNP P26663
B	578	HIS	-	EXPRESSION TAG	UNP P26663
B	579	HIS	-	EXPRESSION TAG	UNP P26663
B	580	HIS	-	EXPRESSION TAG	UNP P26663

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



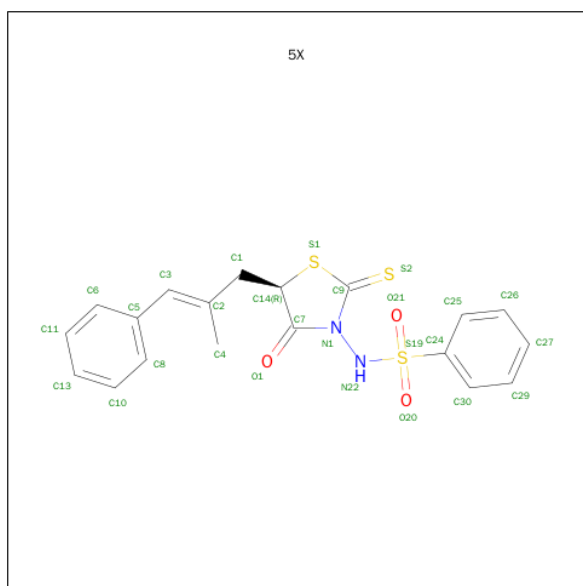
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

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

- Molecule 3 is 5R-(2E-METHYL-3-PHENYL-ALLYL)-3-(BENZENESULFONYLAMINO)-4-OXO-2-THIONOTHIAZOLIDINE (three-letter code: 5X) (formula: C₁₉H₁₈N₂O₃S₃).



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.

Chain A:

8% 84% 10%

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44 45 46 47 48 49 50 51 52 53 54 55 56 57 58 59 60 61 62 63 64 65 66 67 68 69 70 71 72 73 74 75 76 77 78 79 80 81 82 83 84 85 86 87 88 89 90 91 92 93 94 95 96 97 98 99 100 101 102 103 104 105 106 107 108 109 110 111 112 113 114 115 116 117 118 119 120 121 122 123 124 125 126 127 128 129 130 131 132 133 134 135 136 137 138 139 140 141 142 143 144 145 146 147 148 149 150 151 152 153 154 155 156 157 158 159 160 161 162 163 164 165 166 167 168 169 170 171 172 173 174 175 176 177 178 179 180 181 182 183 184 185 186 187 188 189 190 191 192 193 194 195 196 197 198 199 200 201 202 203 204 205 206 207 208 209 210 211 212 213 214 215 216 217 218 219 220 221 222 223 224 225 226 227 228 229 230 231 232 233 234 235 236 237 238 239 240 241 242 243 244 245 246 247 248 249 250 251 252 253 254 255 256 257 258 259 260 261 262 263 264 265 266 267 268 269 270 271 272 273 274 275 276 277 278 279 280 281 282 283 284 285 286 287 288 289 290 291 292 293 294 295 296 297 298 299 300 301 302 303 304 305 306 307 308 309 310 311 312 313 314 315 316 317 318 319 320 321 322 323 324 325 326 327 328 329 330 331 332 333 334 335 336 337 338 339 340 341 342 343 344 345 346 347 348 349 350 351 352 353 354 355 356 357 358 359 360 361 362 363 364 365 366 367 368 369 370 371 372 373 374 375 376 377 378 379 380 381 382 383 384 385 386 387 388 389 390 391 392 393 394 395 396 397 398 399 400

[illegible]

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	87.16Å 87.31Å 163.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.00 28.60 – 2.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.00) 92.3 (28.60-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.06 (at 2.00Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.212 , 0.238 0.208 , 0.235	Depositor DCC
R_{free} test set	7852 reflections (10.08%)	DCC
Wilson B-factor (Å ²)	29.3	Xtriage
Anisotropy	0.257	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 56.3	EDS
Estimated twinning fraction	0.013 for k,h,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 77901 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9595	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.10% 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

Bond lengths and bond angles in the following residue types are not validated in this section: 5X, SO4

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	0.31	0/4409	0.55	0/5980
1	B	0.33	0/4423	0.55	0/5999
All	All	0.32	0/8832	0.55	0/11979

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	A	4315	0	4335	40	0
1	B	4329	0	4348	27	0
2	A	15	0	0	0	0
2	B	20	0	0	0	0
3	A	27	0	17	3	0
3	B	27	0	17	2	0
4	A	415	0	0	5	0
4	B	447	0	0	0	0
All	All	9595	0	8717	69	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 4.

All (69) 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:B:1002:5X:H8	3:B:1002:5X:H41	1.62	0.81
3:A:1001:5X:H8	3:A:1001:5X:H41	1.67	0.76
1:A:83:LEU:HB2	1:A:173:MET:HA	1.67	0.76
1:B:336:LEU:HD22	1:B:356:PRO:HG3	1.73	0.71
1:A:197:PRO:HB2	4:A:1164:HOH:O	1.95	0.67
1:B:446:GLN:HE22	1:B:451:CYS:HB2	1.60	0.67
1:B:82:LEU:HD13	1:B:249:ALA:HB2	1.81	0.63
1:B:83:LEU:HB2	1:B:173:MET:HA	1.81	0.62
1:B:280:ARG:HD2	1:B:291:ASN:OD1	1.99	0.62
1:A:336:LEU:HD22	1:A:356:PRO:HG3	1.82	0.59
1:A:152:GLY:O	1:B:44:SER:HA	2.03	0.59
1:B:241:GLN:OE1	1:B:250:ARG:HG3	2.02	0.59
1:A:18:GLU:HB3	1:A:401:ARG:NH2	2.18	0.59
1:B:233:ILE:HD13	1:B:262:ILE:HA	1.88	0.54
1:A:160:ILE:HD12	1:A:282:SER:OG	2.07	0.54
1:B:150:GLU:C	1:B:152:GLY:H	2.11	0.53
1:B:346:TYR:O	1:B:347:SER:HB3	2.10	0.52
1:A:375:ASP:O	1:A:475:HIS:HE1	1.92	0.52
1:A:81:LYS:HE3	1:A:82:LEU:O	2.09	0.52
1:A:119:ILE:HD13	1:A:169:VAL:HG11	1.93	0.51
1:A:233:ILE:HD13	1:A:261:TYR:O	2.11	0.51
3:B:1002:5X:H43	3:B:1002:5X:S1	2.51	0.50
1:A:455:GLU:HB3	4:A:1225:HOH:O	2.10	0.50
1:A:445:CYS:SG	1:A:454:ILE:HD12	2.52	0.50
1:A:486:ALA:O	1:A:490:ARG:HG3	2.12	0.50
1:A:488:CYS:HB2	4:A:1357:HOH:O	2.11	0.49
1:B:119:ILE:HD13	1:B:169:VAL:HG11	1.95	0.48
1:A:462:ILE:O	1:A:466:LEU:HG	2.14	0.48
1:B:151:LYS:HG2	1:B:151:LYS:O	2.13	0.48
1:B:461:GLN:HG2	1:B:541:ALA:HB3	1.95	0.48
1:A:197:PRO:HB3	3:A:1001:5X:H13	1.97	0.46
1:A:308:LEU:HB2	1:A:311:CYS:SG	2.56	0.46
1:A:38:TYR:CZ	1:A:154:ARG:HG3	2.51	0.46
1:A:184:GLN:C	1:A:184:GLN:HE21	2.19	0.46
1:B:462:ILE:O	1:B:466:LEU:HG	2.17	0.45
1:B:150:GLU:OE2	1:B:152:GLY:HA3	2.16	0.45
1:A:7:THR:HG21	1:A:273:ASN:ND2	2.32	0.45
1:A:220:ASP:HB2	4:A:1390:HOH:O	2.17	0.45
1:A:268:ASN:HB3	1:A:274:CYS:SG	2.57	0.45
1:A:346:TYR:O	1:A:347:SER:HB3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1001:5X:S1	3:A:1001:5X:H43	2.58	0.44
1:B:115:ALA:O	1:B:119:ILE:HG13	2.17	0.44
1:A:466:LEU:HD22	1:A:551:PHE:HE1	1.83	0.43
1:A:183:PRO:HG3	1:A:289:CYS:SG	2.58	0.43
1:A:151:LYS:O	1:A:151:LYS:HG2	2.19	0.43
1:B:78:VAL:HG21	1:B:182:LEU:HD12	2.00	0.43
1:A:249:ALA:O	1:A:253:ILE:HG13	2.18	0.43
1:A:50:LYS:HD2	1:B:152:GLY:HA3	2.02	0.42
1:B:390:THR:HB	1:B:391:PRO:HD3	1.99	0.42
1:B:149:PRO:HG2	1:B:150:GLU:H	1.84	0.42
1:B:308:LEU:HB2	1:B:311:CYS:SG	2.60	0.42
1:B:38:TYR:CE1	1:B:154:ARG:HB3	2.54	0.42
1:A:506:ASN:HD21	1:A:510:ARG:HH11	1.68	0.42
1:B:361:GLU:OE1	1:B:372:VAL:HG23	2.20	0.42
1:B:93:PRO:HG3	1:B:561:TYR:HB2	2.02	0.41
1:A:485:VAL:O	1:A:489:LEU:HG	2.21	0.41
1:B:485:VAL:O	1:B:489:LEU:HG	2.20	0.41
1:B:150:GLU:C	1:B:152:GLY:N	2.74	0.41
1:A:398:GLU:OE2	1:A:408:TRP:HD1	2.02	0.41
1:A:219:TYR:HB3	1:A:320:LEU:HD23	2.02	0.41
1:B:455:GLU:HA	1:B:456:PRO:HD2	1.96	0.41
1:A:93:PRO:HG3	1:A:561:TYR:HB2	2.04	0.40
1:A:112:SER:O	1:A:116:VAL:HG23	2.22	0.40
1:A:86:GLU:H	1:A:86:GLU:CD	2.25	0.40
1:A:198:GLY:N	4:A:1164:HOH:O	2.54	0.40
1:A:118:HIS:O	1:A:122:VAL:HG23	2.22	0.40
1:A:319:ASP:CG	1:A:366:CYS:H	2.25	0.40
1:A:160:ILE:HA	1:A:282:SER:OG	2.22	0.40
1:A:155:LYS:HA	1:A:156:PRO:HD3	1.97	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	550/580 (95%)	541 (98%)	9 (2%)	0	100	100
1	B	553/580 (95%)	546 (99%)	6 (1%)	1 (0%)	52	48
All	All	1103/1160 (95%)	1087 (98%)	15 (1%)	1 (0%)	56	53

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	151	LYS

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	471/492 (96%)	466 (99%)	5 (1%)	80	83
1	B	471/492 (96%)	467 (99%)	4 (1%)	86	89
All	All	942/984 (96%)	933 (99%)	9 (1%)	82	85

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	81	LYS
1	A	154	ARG
1	A	184	GLN
1	A	366	CYS
1	A	445	CYS
1	B	150	GLU
1	B	184	GLN
1	B	366	CYS
1	B	461	GLN

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

Mol	Chain	Res	Type
1	A	28	ASN

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Mol	Chain	Res	Type
1	A	184	GLN
1	A	206	ASN
1	A	438	GLN
1	A	461	GLN
1	A	475	HIS
1	A	506	ASN
1	B	35	ASN
1	B	273	ASN
1	B	330	GLN
1	B	446	GLN

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 ⓘ

9 ligands are modelled in this entry.

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	$\# Z > 2$
3	5X	A	1001	1	26,29,29	1.76	3 (11%)	31,41,41	1.62	5 (16%)
2	SO4	A	1101	-	4,4,4	0.84	0	6,6,6	0.09	0
2	SO4	A	1102	-	4,4,4	0.93	0	6,6,6	0.10	0
2	SO4	A	1103	-	4,4,4	0.95	0	6,6,6	0.07	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	5X	B	1002	1	26,29,29	1.71	2 (7%)	31,41,41	1.46	4 (12%)
2	SO4	B	1104	-	4,4,4	0.91	0	6,6,6	0.12	0
2	SO4	B	1105	-	4,4,4	0.97	0	6,6,6	0.08	0
2	SO4	B	1106	-	4,4,4	0.93	0	6,6,6	0.08	0
2	SO4	B	1107	-	4,4,4	0.88	0	6,6,6	0.08	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	5X	A	1001	1	-	0/17/35/35	0/3/3/3
2	SO4	A	1101	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1102	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1103	-	-	0/0/0/0	0/0/0/0
3	5X	B	1002	1	-	0/17/35/35	0/3/3/3
2	SO4	B	1104	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1105	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1106	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1107	-	-	0/0/0/0	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1001	5X	C14-S1	-3.17	1.76	1.82
3	B	1002	5X	C14-S1	-2.56	1.77	1.82
3	A	1001	5X	C5-C3	2.10	1.51	1.46
3	A	1001	5X	S19-N22	5.12	1.76	1.65
3	B	1002	5X	S19-N22	5.31	1.76	1.65

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1001	5X	O1-C7-N1	-4.62	119.34	124.33
3	B	1002	5X	O1-C7-N1	-3.99	120.02	124.33
3	A	1001	5X	C7-C14-S1	-3.84	102.37	105.99
3	B	1002	5X	C7-C14-S1	-3.74	102.46	105.99
3	A	1001	5X	C6-C5-C3	-2.12	113.96	121.23
3	B	1002	5X	S1-C9-N1	2.20	112.69	110.58
3	A	1001	5X	S1-C9-N1	2.61	113.08	110.58
3	B	1002	5X	C1-C14-S1	3.24	116.23	112.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1001	5X	C1-C14-S1	3.25	116.24	112.97

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1001	5X	3	0
3	B	1002	5X	2	0

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	554/580 (95%)	0.56	48 (8%)	13 13	18, 28, 44, 49	0
1	B	557/580 (96%)	0.44	40 (7%)	18 20	17, 27, 43, 56	0
All	All	1111/1160 (95%)	0.50	88 (7%)	15 16	17, 27, 43, 56	0

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	149	PRO	7.1
1	B	150	GLU	6.9
1	B	402	HIS	6.1
1	B	152	GLY	5.0
1	A	106	LYS	4.9
1	B	151	LYS	4.9
1	B	102	GLY	4.9
1	A	498	ARG	4.8
1	A	402	HIS	4.7
1	A	535	LYS	4.3
1	A	128	GLU	4.2
1	B	425	LEU	4.2
1	A	412	ILE	4.0
1	A	110	ASN	4.0
1	B	246	ALA	3.8
1	B	101	PHE	3.8
1	A	376	ALA	3.8
1	B	543	GLY	3.8
1	B	76	SER	3.8
1	A	483	ASN	3.7
1	A	421	ALA	3.6
1	A	425	LEU	3.6
1	A	405	VAL	3.6
1	B	148	GLN	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	535	LYS	3.6
1	B	424	ILE	3.5
1	A	424	ILE	3.4
1	B	531	LYS	3.4
1	A	403	THR	3.3
1	B	421	ALA	3.2
1	B	16	ALA	3.1
1	A	260	LEU	3.1
1	A	247	PRO	3.1
1	A	426	MET	3.0
1	B	498	ARG	3.0
1	A	73	ALA	3.0
1	B	412	ILE	3.0
1	A	490	ARG	2.8
1	B	113	SER	2.8
1	B	405	VAL	2.8
1	A	401	ARG	2.8
1	A	261	TYR	2.7
1	A	404	PRO	2.7
1	A	377	SER	2.7
1	B	15	ALA	2.7
1	B	420	TRP	2.6
1	A	30	LEU	2.6
1	A	256	LEU	2.6
1	B	103	TYR	2.6
1	A	430	PHE	2.5
1	B	322	VAL	2.5
1	B	77	THR	2.5
1	B	501	ARG	2.5
1	A	501	ARG	2.5
1	B	14	CYS	2.4
1	A	487	SER	2.3
1	A	392	LEU	2.3
1	B	540	ALA	2.3
1	A	105	ALA	2.2
1	A	158	ARG	2.2
1	B	392	LEU	2.2
1	A	101	PHE	2.2
1	B	403	THR	2.2
1	B	532	THR	2.2
1	A	322	VAL	2.2
1	A	439	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	490	ARG	2.2
1	A	270	LYS	2.2
1	A	532	THR	2.1
1	B	430	PHE	2.1
1	A	174	ALA	2.1
1	A	120	HIS	2.1
1	A	81	LYS	2.1
1	A	525	LEU	2.1
1	A	15	ALA	2.1
1	B	247	PRO	2.1
1	A	179	VAL	2.1
1	A	531	LYS	2.1
1	B	541	ALA	2.1
1	B	18	GLU	2.1
1	A	244	ASP	2.1
1	A	8	GLY	2.1
1	A	9	ALA	2.1
1	B	441	LYS	2.1
1	B	418	THR	2.0
1	A	552	THR	2.0
1	A	104	GLY	2.0
1	B	539	ILE	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
3	5X	A	1001	27/27	0.82	0.19	2.54	34,41,48,53	0
3	5X	B	1002	27/27	0.83	0.18	2.15	34,40,48,52	0
2	SO4	A	1102	5/5	0.84	0.19	1.91	57,58,58,58	0
2	SO4	A	1103	5/5	0.94	0.28	0.81	50,50,51,51	0
2	SO4	B	1106	5/5	0.94	0.20	-0.10	64,64,64,64	0
2	SO4	A	1101	5/5	0.96	0.13	-0.20	48,48,48,48	0
2	SO4	B	1104	5/5	0.97	0.12	-0.46	36,36,36,37	0
2	SO4	B	1105	5/5	0.98	0.09	-1.37	32,32,32,32	0
2	SO4	B	1107	5/5	0.92	0.29	-	62,62,62,62	0

6.5 Other polymers [i](#)

There are no such residues in this entry.