WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2014 – 03:45 AM GMT

PDB ID : 3DMJ
Title : CRYSTAL STRUCTURE OF HIV-1 V106A and Y181C MUTANT REVERSE
TRANSCRIPTASE IN COMPLEX WITH GW564511.
Authors : Ren, J.; Chamberlain, P.P.; Stammers, D.K.
Deposited on : 2008-07-01
Resolution : 2.60 Å(reported)

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1 Overall quality at a glance ⓘ

The reported resolution of this entry is 2.60 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	Percentile Ranks	Value
Rfree		0.280
Clashscore		21
Ramachandran outliers		1.5%
Sidechain outliers		3.0%
RSRZ outliers		2.0%

Worse *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
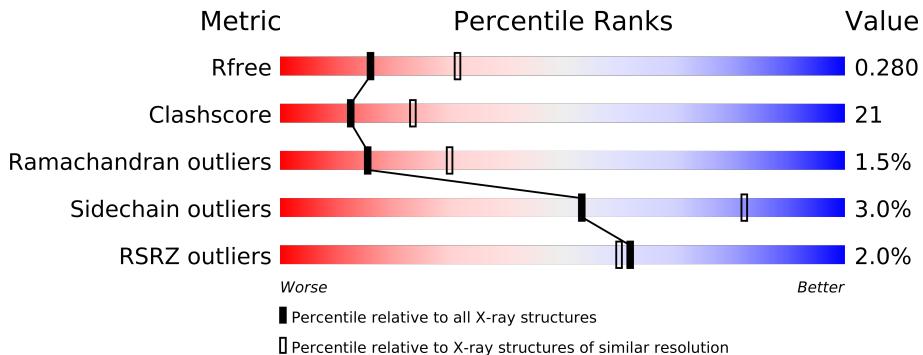
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1718 (2.60-2.60)
Clashscore	79885	2154 (2.60-2.60)
Ramachandran outliers	78287	2113 (2.60-2.60)
Sidechain outliers	78261	2113 (2.60-2.60)
RSRZ outliers	66119	1718 (2.60-2.60)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	560	
2	B	440	
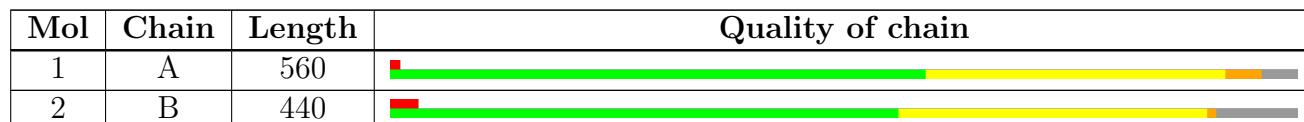
2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 7765 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Reverse transcriptase/ribonucleaseH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	532	Total 4347	C 2814	N 723	O 801	S 9	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	106	ALA	VAL	ENGINEERED	UNP P04585
A	181	CYS	TYR	ENGINEERED	UNP P04585

- Molecule 2 is a protein called p51 RT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	401	Total 3309	C 2151	N 552	O 598	S 8	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	106	ALA	VAL	ENGINEERED	UNP P04585
B	181	CYS	TYR	ENGINEERED	UNP P04585

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).
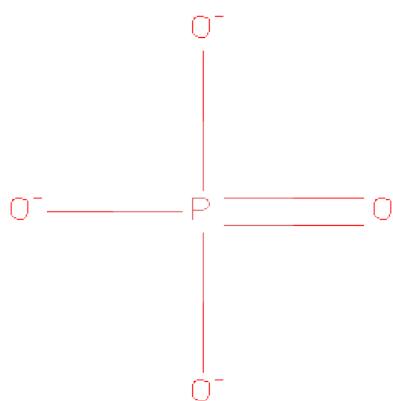
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 5	O 4	P 1	0	0
3	B	1	Total 5	O 4	P 1	0	0

- Molecule 4 is N-{4-[AMINO(DIHYDROXY)-LAMBDA 4 -SULFANYL]-2-METHYLPHEN YL}-2-(4-CHLORO-2-{[3-FLUORO-5-(TRIFLUOROMETHYL)PHENYL]CARBONYL}P HENOXY)ACETAMIDE (three-letter code: GWE) (formula: $C_{23}H_{19}ClF_4N_2O_5S$).
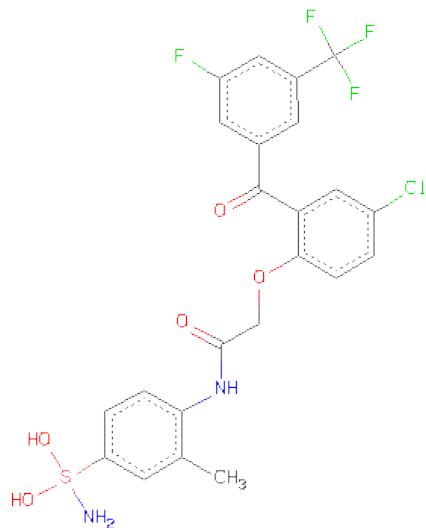
Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
4	A	1	Total 36	C 23	Cl 1	F 4	N 2	O 5	S 1	0	0

• Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	32	Total 32	O 32	0	0
5	B	31	Total 31	O 31	0	0

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: Reverse transcriptase/ribonucleaseH

Chain A:

- Molecule 2: p51 RT

Chain B:

G359 A360 H361 T362 N363 D364 V365 K366 Q367 L368 T369 E370 Q373 K374 I375 T376 T377 E378 S379 I380 V381 I382 W383 G384 K385 T386 P387 K388 F389 I393 Q394 W398 W402 F416 P420 V423 K424 L425 W426 L429 E430 K431 E432 P433 I434 V435 G436 A437 GLU THR PHE
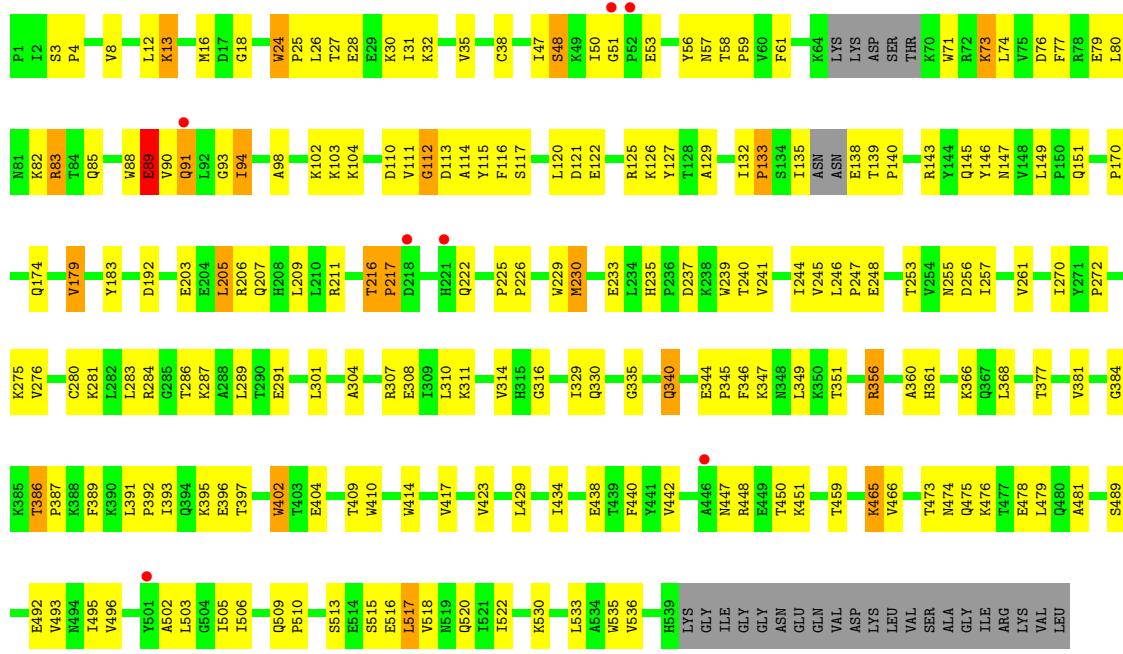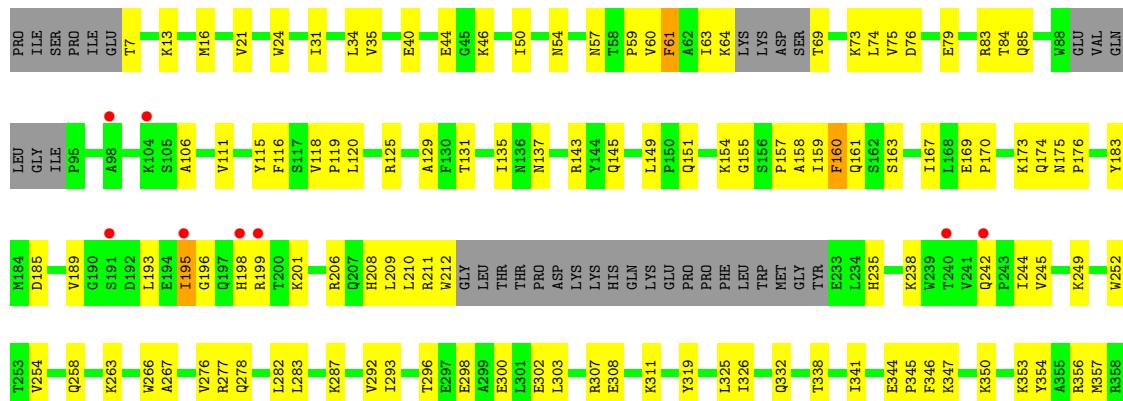
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	137.19Å 108.99Å 71.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.78 – 2.60 29.78 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.78-2.60) 99.9 (29.78-2.60)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.68 (at 2.61Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.197 , 0.284 0.199 , 0.280	Depositor DCC
R_{free} test set	1679 reflections (5.22%)	DCC
Wilson B-factor (Å^2)	55.5	Xtriage
Anisotropy	0.285	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 45.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$< |L| > = 0.50, < L^2 > = 0.34$	Xtriage
Outliers	1 of 33834 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7765	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.35% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GWE, CSD, PO4

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	0.39	0/4453	0.64	0/6051
2	B	0.39	0/3401	0.63	0/4618
All	All	0.39	0/7854	0.63	0/10669

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	183	TYR	Sidechain

5.2 Close contacts (i)

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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4347	0	4390	189	0
2	B	3309	0	3340	148	0
3	A	5	0	0	0	0
3	B	5	0	0	1	0
4	A	36	0	17	0	0
5	A	32	0	0	1	0
5	B	31	0	0	3	0
All	All	7765	0	7747	326	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 21.

All (326) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:353:LYS:HE3	2:B:430:GLU:HB3	1.31	1.12
2:B:235:HIS:HB2	2:B:238:LYS:HD2	1.47	0.94
1:A:448:ARG:NH2	1:A:475:GLN:H	1.67	0.93
1:A:115:TYR:HB2	1:A:151:GLN:HE21	1.37	0.89
1:A:217:PRO:HB2	1:A:222:GLN:HE21	1.42	0.84
2:B:7:THR:HG22	2:B:119:PRO:HG2	1.62	0.82
2:B:79:GLU:O	2:B:83:ARG:HG3	1.78	0.82
1:A:79:GLU:O	1:A:83:ARG:HD2	1.80	0.81
2:B:115:TYR:HB3	2:B:149:LEU:HB2	1.63	0.81
1:A:270:ILE:HG22	1:A:314:VAL:HG11	1.62	0.80
1:A:115:TYR:HB2	1:A:151:GLN:NE2	1.98	0.79
2:B:59:PRO:HG2	2:B:76:ASP:HB3	1.63	0.79
2:B:332:GLN:NE2	2:B:424:LYS:HE2	1.98	0.79
1:A:112:GLY:C	1:A:114:ALA:H	1.85	0.78
2:B:161:GLN:HA	2:B:161:GLN:NE2	2.02	0.73
2:B:195:ILE:HG13	2:B:196:GLY:H	1.54	0.72
1:A:518:VAL:O	1:A:522:ILE:HG13	1.90	0.72
2:B:63:ILE:HD13	2:B:74:LEU:HD22	1.72	0.72
2:B:73:LYS:HB3	2:B:73:LYS:NZ	2.05	0.71
1:A:393:ILE:HB	1:A:423:VAL:HG13	1.69	0.71
2:B:278:GLN:HG3	2:B:298:GLU:HB3	1.73	0.71
1:A:244:ILE:HB	1:A:310:LEU:HD13	1.73	0.71
1:A:206:ARG:HG2	1:A:216:THR:HG21	1.72	0.71
1:A:112:GLY:O	1:A:114:ALA:N	2.24	0.71
1:A:492:GLU:HG2	1:A:530:LYS:HB2	1.71	0.71
1:A:393:ILE:HB	1:A:423:VAL:CG1	2.19	0.70
1:A:217:PRO:HB2	1:A:222:GLN:NE2	2.06	0.70
2:B:195:ILE:HB	2:B:199:ARG:HH12	1.56	0.70
2:B:46:LYS:HD3	2:B:116:PHE:HD2	1.56	0.69

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:448:ARG:NE	1:A:474:ASN:H	1.89	0.69
1:A:465:LYS:HG3	1:A:466:VAL:N	2.06	0.69
1:A:24:TRP:HD1	1:A:25:PRO:HD2	1.57	0.68
1:A:73:LYS:HB2	1:A:73:LYS:NZ	2.08	0.68
2:B:158:ALA:O	2:B:161:GLN:HB2	1.93	0.68
1:A:89:GLU:O	1:A:91:GLN:N	2.27	0.67
1:A:366:LYS:NZ	2:B:394:GLN:NE2	2.41	0.67
2:B:155:GLY:O	2:B:159:ILE:HG12	1.95	0.67
2:B:195:ILE:HB	2:B:199:ARG:NH1	2.10	0.66
2:B:151:GLN:HG3	5:B:1004:HOH:O	1.96	0.66
1:A:239:TRP:CZ2	1:A:316:GLY:HA3	2.30	0.66
1:A:114:ALA:HA	1:A:117:SER:OG	1.96	0.66
2:B:54:ASN:O	2:B:143:ARG:NH2	2.29	0.65
1:A:448:ARG:HE	1:A:473:THR:HB	1.62	0.64
2:B:175:ASN:ND2	2:B:201:LYS:NZ	2.44	0.64
2:B:308:GLU:OE1	2:B:311:LYS:HD2	1.98	0.64
1:A:272:PRO:HA	5:A:1038:HOH:O	1.98	0.64
2:B:175:ASN:HD22	2:B:201:LYS:NZ	1.96	0.63
1:A:409:THR:O	2:B:364:ASP:HB2	1.99	0.63
1:A:31:ILE:O	1:A:35:VAL:HG23	1.98	0.63
1:A:395:LYS:HD3	1:A:414:TRP:CZ2	2.34	0.63
1:A:103:LYS:HE3	1:A:179:VAL:HG11	1.81	0.63
1:A:88:TRP:CE3	1:A:88:TRP:HA	2.34	0.62
1:A:366:LYS:HZ1	2:B:394:GLN:HE21	1.48	0.62
1:A:392:PRO:O	1:A:423:VAL:HG12	2.00	0.62
2:B:356:ARG:HH11	2:B:356:ARG:HG3	1.65	0.61
1:A:112:GLY:C	1:A:114:ALA:N	2.54	0.61
2:B:420:PRO:HB2	2:B:423:VAL:HG23	1.81	0.61
2:B:13:LYS:HB2	2:B:16:MET:HG3	1.83	0.61
2:B:356:ARG:HB2	2:B:367:GLN:HG2	1.82	0.61
2:B:376:THR:O	2:B:380:ILE:HG13	2.01	0.61
1:A:206:ARG:HH11	1:A:216:THR:CG2	2.13	0.60
1:A:448:ARG:HH21	1:A:475:GLN:H	1.44	0.60
2:B:111:VAL:HG22	2:B:185:ASP:O	2.00	0.60
2:B:249:LYS:HB2	2:B:252:TRP:CE2	2.36	0.60
2:B:369:THR:HG22	2:B:398:TRP:CH2	2.37	0.60
1:A:50:ILE:CG2	1:A:145:GLN:HG2	2.31	0.60
1:A:28:GLU:HA	1:A:135:ILE:HD11	1.84	0.60
1:A:340:GLN:HB3	1:A:351:THR:HG22	1.83	0.60
1:A:82:LYS:HB2	1:A:82:LYS:NZ	2.17	0.60
2:B:157:PRO:HD3	5:B:1016:HOH:O	2.00	0.59
1:A:442:VAL:HG22	1:A:496:VAL:O	2.03	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:479:LEU:HB2	1:A:517:LEU:HD13	1.83	0.59
1:A:126:LYS:HE2	1:A:127:TYR:CZ	2.38	0.59
2:B:254:VAL:O	2:B:258:GLN:HG3	2.01	0.59
2:B:167:ILE:HG22	2:B:212:TRP:CZ2	2.37	0.59
1:A:30:LYS:HE2	1:A:71:TRP:CZ3	2.38	0.58
1:A:116:PHE:HE2	1:A:146:TYR:HE1	1.52	0.58
1:A:50:ILE:HG21	1:A:145:GLN:HG2	1.85	0.58
1:A:344:GLU:HB2	1:A:347:LYS:HD2	1.84	0.58
1:A:206:ARG:HH11	1:A:216:THR:HG23	1.69	0.58
1:A:28:GLU:O	1:A:32:LYS:HB2	2.04	0.58
1:A:447:ASN:HB3	1:A:450:THR:OG1	2.04	0.58
2:B:263:LYS:HD3	2:B:429:LEU:HD21	1.86	0.58
1:A:27:THR:O	1:A:31:ILE:HG13	2.03	0.58
2:B:106:ALA:HA	2:B:189:VAL:O	2.03	0.58
1:A:335:GLY:HA3	1:A:356:ARG:HD3	1.85	0.58
2:B:173:LYS:O	2:B:176:PRO:HD3	2.03	0.57
2:B:175:ASN:HD22	2:B:201:LYS:HZ2	1.53	0.57
1:A:26:LEU:HD12	1:A:133:PRO:HG2	1.85	0.57
2:B:57:ASN:HA	2:B:129:ALA:O	2.05	0.57
2:B:235:HIS:CB	2:B:238:LYS:HD2	2.27	0.57
1:A:366:LYS:HZ1	2:B:394:GLN:NE2	2.02	0.57
1:A:24:TRP:CD1	1:A:25:PRO:HD2	2.39	0.56
1:A:502:ALA:HA	1:A:505:ILE:HD12	1.88	0.56
2:B:169:GLU:HB2	2:B:170:PRO:HD3	1.87	0.56
2:B:235:HIS:HB2	2:B:238:LYS:CD	2.27	0.56
2:B:361:HIS:HB3	5:B:1013:HOH:O	2.06	0.56
2:B:120:LEU:HD23	2:B:125:ARG:HG2	1.87	0.56
1:A:503:LEU:HD13	1:A:535:TRP:CG	2.41	0.56
1:A:402:TRP:CZ2	2:B:362:THR:HA	2.40	0.56
1:A:448:ARG:CZ	1:A:474:ASN:H	2.19	0.56
1:A:335:GLY:HA3	1:A:356:ARG:CD	2.35	0.56
1:A:206:ARG:HH12	1:A:222:GLN:NE2	2.03	0.56
1:A:434:ILE:HD13	1:A:530:LYS:HB3	1.88	0.55
1:A:16:MET:HE2	1:A:83:ARG:HG3	1.89	0.55
2:B:161:GLN:HA	2:B:161:GLN:HE21	1.68	0.55
1:A:31:ILE:HD12	1:A:135:ILE:HD13	1.88	0.55
1:A:138:GLU:HG2	1:A:139:THR:N	2.21	0.55
1:A:38:CYS:SG	1:A:132:ILE:HD11	2.47	0.54
2:B:31:ILE:O	2:B:35:VAL:HG23	2.07	0.54
2:B:353:LYS:CE	2:B:430:GLU:HB3	2.21	0.54
1:A:384:GLY:HA3	2:B:135:ILE:HD12	1.89	0.54
1:A:53:GLU:CD	1:A:53:GLU:H	2.10	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:366:LYS:HZ2	2:B:394:GLN:HE22	1.55	0.54
1:A:346:PHE:N	1:A:346:PHE:CD2	2.75	0.54
2:B:425:LEU:O	2:B:429:LEU:HD13	2.07	0.54
1:A:366:LYS:HZ2	2:B:394:GLN:NE2	2.06	0.53
2:B:376:THR:CG2	2:B:386:THR:HG22	2.38	0.53
1:A:402:TRP:CH2	2:B:362:THR:HA	2.42	0.53
2:B:356:ARG:NH1	2:B:357:MET:O	2.41	0.53
2:B:57:ASN:HD22	2:B:143:ARG:NH1	2.06	0.53
2:B:195:ILE:CB	2:B:199:ARG:HH12	2.20	0.53
2:B:73:LYS:HB3	2:B:73:LYS:HZ3	1.73	0.53
2:B:57:ASN:HD22	2:B:143:ARG:HH11	1.57	0.53
2:B:60:VAL:HG23	2:B:75:VAL:HG22	1.89	0.53
2:B:350:LYS:HE3	2:B:378:GLU:OE1	2.09	0.53
1:A:74:LEU:C	1:A:74:LEU:HD23	2.28	0.53
1:A:308:GLU:HA	1:A:311:LYS:CE	2.39	0.53
2:B:21:VAL:HB	2:B:59:PRO:HD3	1.91	0.52
2:B:159:ILE:C	2:B:161:GLN:H	2.13	0.52
2:B:245:VAL:HG23	2:B:431:LYS:HB2	1.90	0.52
1:A:73:LYS:HB2	1:A:73:LYS:HZ2	1.74	0.52
2:B:356:ARG:HG3	2:B:356:ARG:NH1	2.22	0.52
2:B:433:PRO:HB3	2:B:436:GLY:O	2.10	0.52
1:A:473:THR:OG1	1:A:476:LYS:HG3	2.10	0.52
1:A:479:LEU:CB	1:A:517:LEU:HD13	2.40	0.52
1:A:255:ASN:HD22	1:A:289:LEU:HB3	1.74	0.52
2:B:208:HIS:O	2:B:211:ARG:HG2	2.10	0.52
2:B:206:ARG:O	2:B:210:LEU:N	2.41	0.52
2:B:359:GLY:H	3:B:1300:PO4:P	2.31	0.52
2:B:34:LEU:CD2	2:B:73:LYS:HG3	2.40	0.52
2:B:73:LYS:HZ2	2:B:73:LYS:HB3	1.74	0.51
1:A:58:THR:HG23	1:A:59:PRO:HD2	1.91	0.51
2:B:277:ARG:HB3	2:B:277:ARG:CZ	2.39	0.51
1:A:115:TYR:O	1:A:149:LEU:HB2	2.10	0.51
2:B:278:GLN:NE2	2:B:278:GLN:HA	2.25	0.51
2:B:46:LYS:HD3	2:B:116:PHE:CD2	2.43	0.51
2:B:366:LYS:O	2:B:370:GLU:HG3	2.11	0.51
2:B:369:THR:O	2:B:373:GLN:HG3	2.10	0.51
1:A:356:ARG:HG2	1:A:356:ARG:HH11	1.76	0.51
1:A:139:THR:HB	1:A:140:PRO:CD	2.40	0.51
2:B:266:TRP:HZ3	2:B:426:TRP:CD1	2.29	0.51
1:A:206:ARG:HH22	1:A:222:GLN:NE2	2.09	0.51
1:A:51:GLY:HA3	1:A:53:GLU:OE1	2.10	0.51
2:B:245:VAL:CG2	2:B:431:LYS:HB2	2.40	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:516:GLU:O	1:A:520:GLN:HG3	2.11	0.51
1:A:257:ILE:O	1:A:261:VAL:HG23	2.11	0.51
1:A:206:ARG:CG	1:A:216:THR:HG21	2.41	0.50
2:B:211:ARG:HG3	2:B:212:TRP:CD1	2.46	0.50
1:A:116:PHE:CE2	1:A:146:TYR:HE1	2.28	0.50
1:A:308:GLU:HA	1:A:311:LYS:HE2	1.93	0.50
1:A:206:ARG:NH1	1:A:216:THR:HG23	2.26	0.50
2:B:244:ILE:HG13	2:B:426:TRP:CZ2	2.45	0.50
1:A:270:ILE:HG22	1:A:314:VAL:CG1	2.39	0.50
2:B:292:VAL:O	2:B:293:ILE:HD13	2.12	0.50
1:A:225:PRO:HA	1:A:226:PRO:C	2.32	0.50
1:A:377:THR:O	1:A:381:VAL:HG23	2.12	0.50
1:A:38:CYS:O	1:A:47:ILE:HD11	2.12	0.50
2:B:34:LEU:HD22	2:B:73:LYS:HG3	1.94	0.50
1:A:183:TYR:CD1	1:A:229:TRP:HH2	2.29	0.50
1:A:58:THR:HG23	1:A:76:ASP:O	2.12	0.50
1:A:205:LEU:HD22	1:A:209:LEU:HG	1.93	0.50
2:B:115:TYR:HB3	2:B:149:LEU:CB	2.40	0.49
2:B:354:TYR:OH	2:B:357:MET:HG2	2.12	0.49
2:B:365:VAL:O	2:B:369:THR:HG23	2.11	0.49
1:A:104:LYS:HD2	1:A:192:ASP:O	2.12	0.49
1:A:515:SER:HB3	1:A:518:VAL:HG23	1.94	0.49
1:A:122:GLU:CD	1:A:122:GLU:H	2.16	0.49
2:B:332:GLN:HG3	2:B:338:THR:HG23	1.94	0.49
1:A:88:TRP:HE3	1:A:88:TRP:HA	1.74	0.49
2:B:266:TRP:CZ3	2:B:426:TRP:CG	3.00	0.49
1:A:489:SER:HB2	1:A:493:VAL:HB	1.93	0.49
1:A:448:ARG:NE	1:A:473:THR:HB	2.27	0.49
2:B:356:ARG:CB	2:B:367:GLN:HG2	2.42	0.49
1:A:417:VAL:O	1:A:417:VAL:HG13	2.12	0.49
1:A:248:GLU:OE2	1:A:248:GLU:HA	2.12	0.49
1:A:83:ARG:HH11	1:A:83:ARG:HG2	1.77	0.49
1:A:402:TRP:CD1	1:A:402:TRP:C	2.85	0.49
1:A:57:ASN:HA	1:A:129:ALA:O	2.13	0.48
1:A:438:GLU:HG2	1:A:459:THR:HB	1.94	0.48
1:A:239:TRP:CE2	1:A:316:GLY:HA3	2.48	0.48
1:A:233:GLU:HB2	1:A:240:THR:OG1	2.12	0.48
1:A:448:ARG:HH11	1:A:448:ARG:HG3	1.79	0.48
1:A:73:LYS:HB2	1:A:73:LYS:HZ3	1.79	0.48
1:A:335:GLY:O	1:A:356:ARG:HA	2.12	0.48
2:B:64:LYS:HD2	2:B:69:THR:HG22	1.95	0.48
2:B:326:ILE:O	2:B:341:ILE:HA	2.12	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:151:GLN:HB3	2:B:185:ASP:OD1	2.14	0.48
2:B:436:GLY:O	2:B:437:ALA:HB2	2.12	0.48
1:A:253:THR:HG23	1:A:256:ASP:OD2	2.14	0.48
1:A:30:LYS:HE2	1:A:71:TRP:CH2	2.48	0.48
2:B:319:TYR:HE2	2:B:325:LEU:HD13	1.79	0.48
1:A:448:ARG:HE	1:A:473:THR:CB	2.25	0.48
1:A:515:SER:HB3	1:A:518:VAL:CG2	2.44	0.48
1:A:170:PRO:O	1:A:174:GLN:HG3	2.14	0.48
2:B:235:HIS:O	2:B:238:LYS:HG2	2.14	0.47
1:A:536:VAL:HG12	2:B:258:GLN:HB3	1.96	0.47
1:A:48:SER:O	1:A:50:ILE:HG23	2.14	0.47
1:A:211:ARG:HG2	1:A:211:ARG:HH11	1.79	0.47
2:B:332:GLN:HE22	2:B:424:LYS:HE2	1.79	0.47
2:B:325:LEU:HD22	2:B:385:LYS:HD2	1.95	0.47
1:A:98:ALA:HB2	1:A:349:LEU:O	2.14	0.47
2:B:345:PRO:O	2:B:346:PHE:HB2	2.15	0.47
1:A:478:GLU:O	1:A:481:ALA:HB3	2.15	0.47
2:B:170:PRO:O	2:B:174:GLN:HG3	2.15	0.47
2:B:160:PHE:CD1	2:B:160:PHE:O	2.68	0.47
1:A:110:ASP:O	1:A:217:PRO:HD3	2.15	0.46
2:B:282:LEU:HD21	2:B:296:THR:HG23	1.98	0.46
1:A:94:ILE:CD1	1:A:230:MET:HG2	2.45	0.46
2:B:319:TYR:OH	2:B:385:LYS:HE3	2.16	0.46
1:A:237:ASP:N	1:A:237:ASP:OD2	2.47	0.46
1:A:360:ALA:O	1:A:513:SER:HB2	2.16	0.46
1:A:393:ILE:CB	1:A:423:VAL:HG13	2.42	0.46
1:A:203:GLU:HG3	1:A:207:GLN:HE21	1.81	0.46
1:A:111:VAL:O	1:A:114:ALA:HB3	2.16	0.46
1:A:396:GLU:HG3	1:A:397:THR:N	2.29	0.46
1:A:356:ARG:HG2	1:A:356:ARG:NH1	2.30	0.46
1:A:98:ALA:HB1	1:A:349:LEU:HB3	1.97	0.46
1:A:102:LYS:HE2	1:A:237:ASP:HA	1.98	0.46
1:A:125:ARG:HD3	1:A:147:ASN:HA	1.98	0.46
1:A:226:PRO:HB3	1:A:235:HIS:ND1	2.32	0.45
2:B:393:ILE:O	2:B:416:PHE:HB3	2.17	0.45
2:B:376:THR:HG23	2:B:386:THR:HG22	1.98	0.45
1:A:255:ASN:ND2	1:A:289:LEU:HD13	2.31	0.45
1:A:115:TYR:CB	1:A:151:GLN:NE2	2.75	0.45
1:A:58:THR:CG2	1:A:76:ASP:O	2.65	0.45
1:A:448:ARG:HE	1:A:473:THR:CA	2.29	0.45
2:B:199:ARG:HG3	2:B:199:ARG:HH11	1.82	0.45
2:B:344:GLU:HB2	2:B:347:LYS:HD2	1.97	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:175:ASN:HD21	2:B:201:LYS:CE	2.30	0.45
2:B:40:GLU:O	2:B:44:GLU:HG3	2.17	0.45
1:A:16:MET:HE2	1:A:83:ARG:CG	2.47	0.44
1:A:434:ILE:CD1	1:A:530:LYS:HB3	2.46	0.44
1:A:139:THR:HB	1:A:140:PRO:HD2	2.00	0.44
2:B:325:LEU:HD21	2:B:383:TRP:CE3	2.52	0.44
1:A:93:GLY:O	2:B:137:ASN:HB3	2.17	0.44
1:A:492:GLU:HA	1:A:530:LYS:O	2.18	0.44
1:A:301:LEU:O	1:A:304:ALA:HB3	2.18	0.44
2:B:266:TRP:HZ3	2:B:426:TRP:CG	2.36	0.44
2:B:201:LYS:HD3	2:B:201:LYS:HA	1.85	0.44
2:B:369:THR:HG22	2:B:398:TRP:CZ3	2.51	0.44
1:A:429:LEU:CD1	1:A:506:ILE:HA	2.48	0.44
2:B:195:ILE:O	2:B:198:HIS:HB3	2.17	0.44
2:B:161:GLN:CA	2:B:161:GLN:NE2	2.72	0.43
2:B:31:ILE:HD12	2:B:135:ILE:CD1	2.48	0.43
1:A:440:PHE:CD2	1:A:459:THR:HG22	2.53	0.43
1:A:3:SER:HA	1:A:4:PRO:HD3	1.80	0.43
1:A:56:TYR:O	1:A:143:ARG:NH2	2.52	0.43
1:A:276:VAL:O	1:A:280:CSD:HB3	2.17	0.43
1:A:346:PHE:N	1:A:346:PHE:HD2	2.16	0.43
1:A:329:ILE:HD12	1:A:391:LEU:CD2	2.48	0.43
2:B:118:VAL:HB	2:B:149:LEU:HG	2.00	0.43
2:B:116:PHE:H	2:B:116:PHE:HD1	1.67	0.43
1:A:58:THR:CG2	1:A:59:PRO:HD2	2.49	0.43
2:B:242:GLN:OE1	2:B:242:GLN:HA	2.18	0.43
1:A:110:ASP:HB3	1:A:217:PRO:HG3	2.00	0.43
2:B:61:PHE:CD2	2:B:61:PHE:N	2.85	0.43
1:A:287:LYS:HG2	1:A:291:GLU:OE2	2.19	0.43
2:B:167:ILE:HG22	2:B:212:TRP:CH2	2.53	0.43
2:B:374:LYS:O	2:B:378:GLU:HG3	2.19	0.43
1:A:440:PHE:CG	1:A:459:THR:HG22	2.54	0.43
2:B:57:ASN:ND2	2:B:131:THR:OG1	2.52	0.43
1:A:31:ILE:HD12	1:A:135:ILE:CD1	2.48	0.43
2:B:398:TRP:O	2:B:402:TRP:HD1	2.02	0.43
2:B:426:TRP:O	2:B:429:LEU:HB2	2.19	0.43
1:A:12:LEU:O	1:A:13:LYS:O	2.37	0.43
2:B:50:ILE:CG2	2:B:145:GLN:HG2	2.49	0.42
1:A:448:ARG:NH2	1:A:475:GLN:N	2.50	0.42
1:A:502:ALA:O	1:A:506:ILE:HG13	2.19	0.42
1:A:283:LEU:O	1:A:286:THR:HG23	2.19	0.42
2:B:338:THR:HG22	2:B:353:LYS:HG2	2.01	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:154:LYS:O	2:B:157:PRO:HD2	2.19	0.42
1:A:77:PHE:CD2	1:A:80:LEU:HD23	2.54	0.42
1:A:246:LEU:O	1:A:307:ARG:NH1	2.47	0.42
1:A:18:GLY:HA3	1:A:56:TYR:CD1	2.54	0.42
1:A:245:VAL:HG23	1:A:245:VAL:O	2.20	0.42
1:A:329:ILE:HD12	1:A:391:LEU:HD22	2.01	0.42
1:A:116:PHE:HE2	1:A:146:TYR:CE1	2.35	0.42
2:B:287:LYS:HD3	2:B:293:ILE:HD11	2.01	0.42
1:A:211:ARG:HG2	1:A:211:ARG:NH1	2.34	0.42
2:B:116:PHE:CD1	2:B:116:PHE:N	2.87	0.42
2:B:267:ALA:HB2	2:B:426:TRP:CZ3	2.55	0.42
1:A:8:VAL:O	1:A:121:ASP:HB2	2.20	0.42
1:A:59:PRO:HG2	1:A:76:ASP:HB3	2.01	0.41
2:B:63:ILE:HD13	2:B:74:LEU:CD2	2.45	0.41
2:B:116:PHE:HZ	2:B:151:GLN:HE21	1.67	0.41
1:A:495:ILE:HB	1:A:533:LEU:HD23	2.02	0.41
2:B:276:VAL:HA	2:B:302:GLU:OE2	2.20	0.41
1:A:281:LYS:O	1:A:284:ARG:HG3	2.20	0.41
1:A:206:ARG:HH22	1:A:222:GLN:CD	2.23	0.41
2:B:377:THR:O	2:B:381:VAL:HG23	2.20	0.41
1:A:120:LEU:HD23	1:A:125:ARG:HG2	2.02	0.41
1:A:246:LEU:HA	1:A:247:PRO:HD2	1.85	0.41
2:B:303:LEU:O	2:B:307:ARG:HG3	2.19	0.41
1:A:24:TRP:HE3	1:A:61:PHE:CZ	2.38	0.41
2:B:84:THR:HB	2:B:154:LYS:HE2	2.02	0.41
2:B:163:SER:O	2:B:167:ILE:HG12	2.20	0.41
1:A:509:GLN:N	1:A:510:PRO:CD	2.84	0.41
1:A:340:GLN:CB	1:A:351:THR:HG22	2.48	0.41
1:A:329:ILE:HG22	1:A:330:GLN:N	2.36	0.41
2:B:175:ASN:ND2	2:B:201:LYS:CE	2.83	0.41
1:A:389:PHE:HB2	1:A:414:TRP:HB3	2.03	0.41
1:A:442:VAL:HB	1:A:481:ALA:HB1	2.03	0.41
1:A:345:PRO:O	1:A:346:PHE:HB2	2.21	0.40
1:A:115:TYR:CB	1:A:151:GLN:HE21	2.21	0.40
2:B:60:VAL:HG22	2:B:61:PHE:N	2.36	0.40
1:A:94:ILE:HD11	1:A:230:MET:HG2	2.04	0.40
1:A:409:THR:O	1:A:410:TRP:HB2	2.21	0.40
2:B:206:ARG:O	2:B:209:LEU:N	2.54	0.40
1:A:386:THR:HA	1:A:387:PRO:HD3	1.72	0.40
1:A:451:LYS:HE2	1:A:451:LYS:HB3	1.84	0.40
1:A:26:LEU:HD12	1:A:133:PRO:CG	2.51	0.40
2:B:135:ILE:H	2:B:135:ILE:HG12	1.73	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:287:LYS:HD3	2:B:293:ILE:CD1	2.51	0.40
2:B:344:GLU:CB	2:B:347:LYS:HD2	2.51	0.40
2:B:387:PRO:HG2	2:B:389:PHE:CE1	2.57	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	525/560 (94%)	486 (93%)	28 (5%)	11 (2%)	11	19
2	B	393/440 (89%)	364 (93%)	26 (7%)	3 (1%)	27	53
All	All	918/1000 (92%)	850 (93%)	54 (6%)	14 (2%)	15	30

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	90	VAL
1	A	113	ASP
2	B	195	ILE
1	A	91	GLN
1	A	133	PRO
1	A	85	GLN
1	A	361	HIS
1	A	89	GLU
1	A	217	PRO
1	A	356	ARG
2	B	160	PHE
2	B	85	GLN
1	A	13	LYS
1	A	112	GLY

5.3.2 Protein sidechains (i)

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	475/498 (95%)	456 (96%)	19 (4%)	42	73
2	B	363/399 (91%)	357 (98%)	6 (2%)	73	92
All	All	838/897 (93%)	813 (97%)	25 (3%)	53	82

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	TRP
1	A	48	SER
1	A	73	LYS
1	A	83	ARG
1	A	89	GLU
1	A	94	ILE
1	A	179	VAL
1	A	205	LEU
1	A	216	THR
1	A	230	MET
1	A	241	VAL
1	A	275	LYS
1	A	340	GLN
1	A	368	LEU
1	A	386	THR
1	A	402	TRP
1	A	404	GLU
1	A	465	LYS
1	A	517	LEU
2	B	24	TRP
2	B	61	PHE
2	B	193	LEU
2	B	283	LEU
2	B	300	GLU
2	B	433	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	ASN
1	A	151	GLN
1	A	207	GLN
1	A	222	GLN
1	A	242	GLN
1	A	255	ASN
1	A	278	GLN
1	A	336	GLN
1	A	475	GLN
1	A	487	GLN
1	A	500	GLN
1	A	519	ASN
1	A	520	GLN
2	B	57	ASN
2	B	137	ASN
2	B	161	GLN
2	B	174	GLN
2	B	175	ASN
2	B	182	GLN
2	B	197	GLN
2	B	269	GLN
2	B	278	GLN
2	B	332	GLN
2	B	394	GLN
2	B	428	GLN

5.3.3   RNA ⓘ

There are no RNA chains in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	#$|Z| > 2$
1	CSD	A	280	1	7,7,8	7.01	2 (28%)	6,8,10	5.97	4 (66%)

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
1	CSD	A	280	1	-	0/3/6/8	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	280	CSD	O-C	18.21	1.23	1.11
1	A	280	CSD	CA-C	2.92	1.53	1.48

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	280	CSD	CA-CB-SG	10.91	126.39	110.82
1	A	280	CSD	C-CA-N	-6.29	107.55	113.83
1	A	280	CSD	OD2-SG-CB	5.58	119.87	97.42
1	A	280	CSD	OD2-SG-OD1	4.86	117.46	109.39

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

3 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	PO4	A	1301	-	4,4,4	0.88	0	6,6,6	0.31	0
4	GWE	A	999	-	37,38,38	2.55	10 (27%)	57,57,57	4.88	12 (21%)
3	PO4	B	1300	-	4,4,4	0.85	0	6,6,6	0.31	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	PO4	A	1301	-	-	0/0/0/0	0/0/0/0
4	GWE	A	999	-	-	0/29/29/29	0/3/3/3
3	PO4	B	1300	-	-	0/0/0/0	0/0/0/0

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	999	GWE	C17-C18	6.26	1.51	1.40
4	A	999	GWE	C2-C1	5.87	1.51	1.40
4	A	999	GWE	C3-C4	5.69	1.48	1.38
4	A	999	GWE	C5-C6	5.47	1.49	1.38
4	A	999	GWE	C21-C22	4.79	1.48	1.38
4	A	999	GWE	C19-C20	4.55	1.49	1.39
4	A	999	GWE	C19-C18	-3.01	1.34	1.39
4	A	999	GWE	C9-C10	2.95	1.42	1.37
4	A	999	GWE	C9-C8	2.44	1.43	1.39
4	A	999	GWE	C11-C10	2.02	1.41	1.37

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	999	GWE	C20-S1-N2	-35.29	109.07	109.75
4	A	999	GWE	O4-S1-C20	3.90	109.33	106.91
4	A	999	GWE	C2-C7-C8	2.99	124.83	119.65
4	A	999	GWE	C1-C2-C7	-2.66	118.90	122.73
4	A	999	GWE	O5-S1-C20	2.49	108.45	106.91
4	A	999	GWE	O2-C15-C16	-2.35	103.89	110.78
4	A	999	GWE	C11-C10-C9	-2.31	120.21	123.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	999	GWE	O1-C7-C8	-2.29	116.35	120.02
4	A	999	GWE	C22-C17-C18	-2.17	118.02	120.62
4	A	999	GWE	O4-S1-O5	-2.10	110.85	117.62
4	A	999	GWE	C15-O2-C1	2.06	122.30	117.55
4	A	999	GWE	F2-C14-C12	-2.01	108.33	112.97

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers (i)

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	532/560 (95%)	-0.31	7 (1%)	74	75	25, 56, 96, 137	0
2	B	401/440 (91%)	-0.19	12 (2%)	48	45	29, 53, 98, 123	0
All	All	933/1000 (93%)	-0.26	19 (2%)	62	60	25, 55, 98, 137	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	195	ILE	3.9
1	A	52	PRO	3.9
1	A	221	HIS	3.8
2	B	432	GLU	3.1
2	B	198	HIS	2.8
2	B	240	THR	2.7
2	B	434	ILE	2.6
2	B	98	ALA	2.5
2	B	191	SER	2.4
1	A	51	GLY	2.4
1	A	501	TYR	2.3
2	B	435	VAL	2.2
2	B	199	ARG	2.2
2	B	104	LYS	2.1
1	A	91	GLN	2.1
1	A	446	ALA	2.1
1	A	218	ASP	2.1
2	B	242	GLN	2.1
2	B	433	PRO	2.0

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

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	RSR	LLDF	B-factors(Å^2)	Q<0.9
1	CSD	A	280	8/9	0.13	-0.22	45,53,58,72	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	PO4	B	1300	5/5	0.24	0.77	123,126,136,137	0
4	GWE	A	999	36/36	0.14	-0.23	26,44,59,81	0
3	PO4	A	1301	5/5	0.13	-0.24	116,123,130,134	0

6.5 Other polymers ⓘ

There are no such residues in this entry.