Full wwPDB X-ray Structure Validation Report ⓘ

Jun 13, 2024 – 11:14 AM EDT

PDB ID	:	1P22
Title	:	Structure of a beta-TrCP1-Skp1-beta-catenin complex: destruction motif binding and lysine specificity on the SCFbeta-TrCP1 ubiquitin ligase
Authors	:	Wu, G.; Xu, G.; Schulman, B.A.; Jeffrey, P.D.; Harper, J.W.; Pavletich, N.P.
Deposited on	:	2003-04-14
Resolution	:	2.95 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:

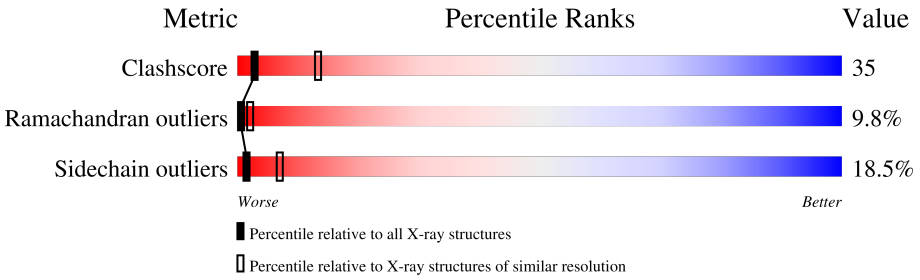
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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))
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	435	39% 38% 13% • 8%
2	B	145	37% 34% 17% • 10%
3	C	26	8% 23% 12% 58%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4340 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 F-box/WD-repeat protein 1A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	402	3221	2023	587	589	22	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	135	SER	-	CLONING ARTIFACT	UNP Q9Y297
A	136	PRO	-	CLONING ARTIFACT	UNP Q9Y297
A	137	ALA	-	CLONING ARTIFACT	UNP Q9Y297
A	138	ILE	-	CLONING ARTIFACT	UNP Q9Y297

- Molecule 2 is a protein called Skp1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	131	1040	664	169	202	5	0	0	0

- Molecule 3 is a protein called Beta-catenin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	C	11	79	42	13	22	2	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	33	SEP	SER	MODIFIED RESIDUE	UNP P35222
C	37	SEP	SER	MODIFIED RESIDUE	UNP P35222

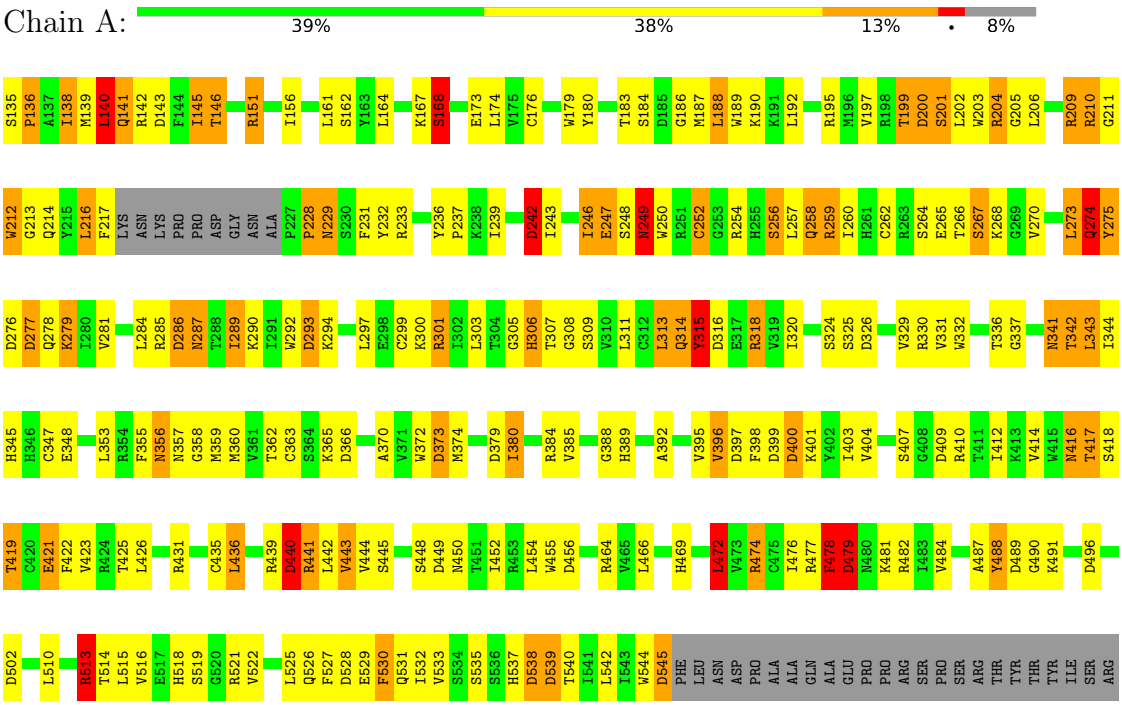
3 Residue-property plots (i)

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. 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. 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.

Note EDS was not executed.

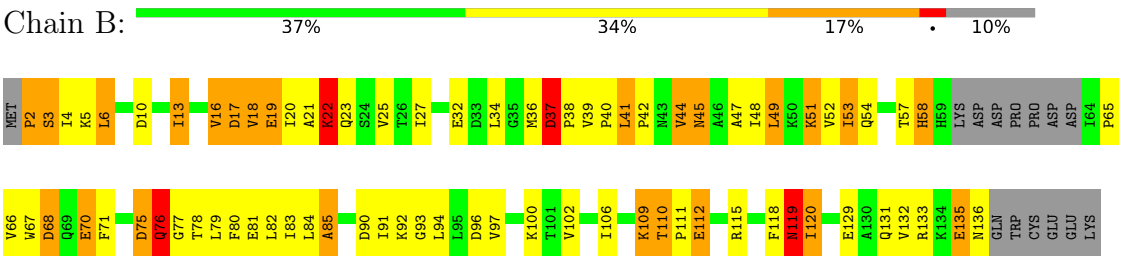
• Molecule 1: F-box/WD-repeat protein 1A

Chain A:



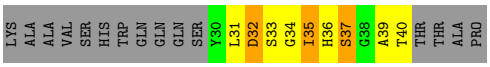
• Molecule 2: Skp1

Chain B:



• Molecule 3: Beta-catenin

Chain C:


LYS
ALA
ALA
VAL
SER
HIS
TRP
GLN
GLN
GLN
SER
Y30
L31
D32
S33
G34
I35
H36
S37
G38
A39
T40
THR
THR
ALA
PRO

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α, β, γ	82.60Å 82.60Å 111.50Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.95	Depositor
% Data completeness (in resolution range)	99.3 (20.00-2.95)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
Refinement program	REFMAC 5.1	Depositor
R, R_{free}	0.230 , 0.286	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4340	wwPDB-VP
Average B, all atoms (Å^2)	18.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.63	0/3283	1.02	20/4443 (0.5%)
2	B	0.61	0/1055	0.98	5/1426 (0.4%)
3	C	0.79	0/57	1.79	2/73 (2.7%)
All	All	0.63	0/4395	1.03	27/5942 (0.5%)

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
1	A	0	3
2	B	0	1
All	All	0	4

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	409	ASP	CB-CG-OD2	8.01	125.51	118.30
1	A	472	LEU	CA-CB-CG	7.97	133.63	115.30
1	A	140	LEU	CA-CB-CG	7.70	133.01	115.30
1	A	478	PHE	CB-CA-C	-7.12	96.17	110.40
1	A	528	ASP	CB-CG-OD2	6.90	124.51	118.30
1	A	200	ASP	CB-CG-OD2	6.65	124.29	118.30
2	B	2	PRO	N-CA-CB	6.44	111.03	103.30
1	A	373	ASP	CB-CG-OD2	6.36	124.03	118.30
2	B	75	ASP	CB-CG-OD2	6.27	123.94	118.30
1	A	136	PRO	N-CA-CB	6.15	110.68	103.30
1	A	286	ASP	CB-CG-OD2	6.15	123.83	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	37	ASP	CB-CG-OD2	6.15	123.83	118.30
1	A	489	ASP	CB-CG-OD2	5.93	123.64	118.30
3	C	31	LEU	CA-CB-CG	-5.90	101.73	115.30
1	A	142	ARG	NE-CZ-NH1	5.89	123.25	120.30
1	A	188	LEU	CA-CB-CG	-5.78	102.00	115.30
1	A	440	ASP	CB-CG-OD2	5.78	123.50	118.30
3	C	32	ASP	CB-CG-OD2	5.61	123.35	118.30
1	A	496	ASP	CB-CG-OD2	5.58	123.32	118.30
2	B	85	ALA	N-CA-C	-5.57	95.97	111.00
1	A	456	ASP	CB-CG-OD2	5.54	123.29	118.30
1	A	277	ASP	CB-CG-OD2	5.54	123.29	118.30
1	A	242	ASP	CB-CG-OD2	5.40	123.16	118.30
1	A	313	LEU	CA-CB-CG	5.30	127.48	115.30
2	B	10	ASP	CB-CG-OD2	5.19	122.97	118.30
1	A	400	ASP	CB-CG-OD2	5.14	122.93	118.30
1	A	539	ASP	CB-CG-OD2	5.14	122.92	118.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	274	GLN	Peptide
1	A	397	ASP	Peptide
1	A	436	LEU	Peptide
2	B	44	VAL	Peptide

5.2 Too-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 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	3221	0	3203	246	0
2	B	1040	0	1055	70	0
3	C	79	0	60	7	0
All	All	4340	0	4318	306	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 35.

All (306) 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:136:PRO:HA	2:B:78:THR:HG21	1.19	1.10
2:B:118:PHE:HB2	2:B:120:ILE:HD11	1.30	1.08
1:A:259:ARG:HG3	1:A:259:ARG:HH11	1.16	1.05
1:A:201:SER:HA	1:A:204:ARG:HD2	1.41	1.00
1:A:341:ASN:HD22	1:A:342:THR:H	1.10	0.98
1:A:513:ARG:NH1	1:A:513:ARG:HB3	1.78	0.97
1:A:341:ASN:HD22	1:A:342:THR:N	1.63	0.96
2:B:118:PHE:HB2	2:B:120:ILE:CD1	1.96	0.96
1:A:139:MET:HG3	1:A:141:GLN:N	1.82	0.95
1:A:145:ILE:HD11	1:A:179:TRP:HA	1.50	0.94
1:A:259:ARG:HH11	1:A:259:ARG:CG	1.81	0.93
1:A:151:ARG:HH11	1:A:151:ARG:CG	1.81	0.92
1:A:314:GLN:HE21	1:A:355:PHE:HB3	1.35	0.91
2:B:37:ASP:HB2	2:B:38:PRO:CD	2.01	0.91
1:A:443:VAL:HG13	1:A:455:TRP:HB2	1.49	0.91
1:A:374:MET:HG2	1:A:380:ILE:HG12	1.52	0.90
2:B:37:ASP:HB2	2:B:38:PRO:HD3	1.54	0.89
2:B:37:ASP:CB	2:B:38:PRO:HD3	2.02	0.89
2:B:118:PHE:CB	2:B:120:ILE:HD11	2.03	0.88
1:A:267:SER:HB2	1:A:285:ARG:HB3	1.55	0.88
1:A:478:PHE:O	1:A:479:ASP:HB3	1.76	0.86
1:A:136:PRO:HA	2:B:78:THR:CG2	2.02	0.86
1:A:444:VAL:HB	1:A:478:PHE:HE2	1.41	0.86
1:A:274:GLN:NE2	1:A:315:TYR:H	1.74	0.85
1:A:161:LEU:HD13	1:A:183:THR:HG22	1.58	0.85
1:A:151:ARG:HH11	1:A:151:ARG:HG3	1.39	0.84
1:A:201:SER:HB2	1:A:529:GLU:OE2	1.78	0.83
1:A:513:ARG:HB3	1:A:513:ARG:HH11	1.41	0.80
1:A:452:ILE:HG12	1:A:476:ILE:CD1	2.13	0.78
2:B:16:VAL:HG23	2:B:17:ASP:O	1.86	0.76
1:A:143:ASP:CG	1:A:146:THR:HG22	2.05	0.76
1:A:444:VAL:HB	1:A:478:PHE:CE2	2.22	0.74
1:A:143:ASP:CG	1:A:146:THR:CG2	2.55	0.74
1:A:359:MET:SD	1:A:398:PHE:HZ	2.10	0.74
2:B:18:VAL:O	2:B:19:GLU:HB2	1.86	0.74
2:B:37:ASP:CB	2:B:38:PRO:CD	2.64	0.74
1:A:201:SER:HA	1:A:204:ARG:CD	2.18	0.73
1:A:384:ARG:HG2	1:A:385:VAL:H	1.53	0.73
1:A:284:LEU:HD11	1:A:290:LYS:HE2	1.70	0.73
2:B:6:LEU:HD13	2:B:49:LEU:HD11	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:ASP:OD1	1:A:146:THR:HG22	1.89	0.72
1:A:395:VAL:HG11	1:A:436:LEU:H	1.55	0.72
1:A:139:MET:C	1:A:141:GLN:H	1.92	0.71
1:A:362:THR:CG2	1:A:372:TRP:HE1	2.04	0.71
1:A:416:ASN:HD22	1:A:418:SER:H	1.36	0.71
2:B:40:PRO:O	2:B:42:PRO:HD3	1.91	0.71
1:A:490:GLY:HA2	1:A:522:VAL:HG23	1.73	0.70
1:A:213:GLY:HA2	1:A:216:LEU:CD2	2.21	0.70
2:B:65:PRO:CB	2:B:68:ASP:HB2	2.21	0.69
1:A:254:ARG:HD3	1:A:545:ASP:O	1.91	0.69
1:A:259:ARG:CG	1:A:259:ARG:NH1	2.49	0.69
1:A:307:THR:HB	1:A:326:ASP:HB3	1.75	0.69
1:A:448:SER:HA	1:A:472:LEU:HD22	1.74	0.68
1:A:139:MET:HB3	1:A:141:GLN:HB2	1.73	0.68
1:A:362:THR:HG21	1:A:372:TRP:HE1	1.59	0.68
1:A:135:SER:CB	2:B:47:ALA:HB1	2.24	0.68
1:A:174:LEU:HD21	2:B:133:ARG:HG3	1.76	0.68
1:A:316:ASP:HB2	1:A:355:PHE:HE2	1.58	0.68
1:A:216:LEU:HB3	1:A:217:PHE:CD1	2.29	0.67
1:A:404:VAL:HG23	1:A:436:LEU:HD12	1.75	0.67
1:A:174:LEU:HD13	2:B:132:VAL:CG1	2.24	0.67
1:A:210:ARG:NH1	1:A:210:ARG:HB2	2.08	0.67
2:B:66:VAL:HG23	2:B:67:TRP:H	1.59	0.67
1:A:259:ARG:HG3	1:A:259:ARG:NH1	1.97	0.66
1:A:491:LYS:HG2	1:A:516:VAL:HG13	1.77	0.66
3:C:32:ASP:HB2	3:C:35:ILE:HG22	1.78	0.65
2:B:65:PRO:HB3	2:B:68:ASP:HB2	1.79	0.65
1:A:431:ARG:HB3	1:A:448:SER:HB2	1.78	0.65
1:A:233:ARG:HD2	2:B:135:GLU:HB2	1.79	0.64
1:A:341:ASN:ND2	1:A:342:THR:N	2.43	0.64
1:A:538:ASP:O	1:A:540:THR:N	2.30	0.64
1:A:478:PHE:O	1:A:527:PHE:CZ	2.51	0.64
2:B:21:ALA:O	2:B:23:GLN:N	2.30	0.64
1:A:286:ASP:O	1:A:287:ASN:HB2	1.99	0.63
1:A:314:GLN:HE21	1:A:355:PHE:CB	2.11	0.63
1:A:139:MET:HG3	1:A:141:GLN:H	1.62	0.63
1:A:250:TRP:HH2	1:A:532:ILE:HG13	1.63	0.63
1:A:256:SER:O	1:A:258:GLN:N	2.32	0.63
1:A:275:TYR:HE2	1:A:294:LYS:HZ1	1.48	0.62
1:A:275:TYR:CG	1:A:533:VAL:HG21	2.34	0.62
2:B:45:ASN:HB3	2:B:48:ILE:HB	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:ARG:HG3	1:A:151:ARG:NH1	2.10	0.62
1:A:140:LEU:C	2:B:76:GLN:HG3	2.20	0.61
1:A:436:LEU:CD2	1:A:445:SER:HB3	2.30	0.61
1:A:452:ILE:HG12	1:A:476:ILE:HD12	1.81	0.61
2:B:37:ASP:HB3	2:B:38:PRO:HD3	1.81	0.61
1:A:249:ASN:HD22	1:A:250:TRP:N	1.99	0.61
1:A:392:ALA:O	1:A:407:SER:CB	2.49	0.61
1:A:294:LYS:HD3	1:A:294:LYS:O	2.01	0.61
1:A:395:VAL:HG21	1:A:435:CYS:HA	1.84	0.60
1:A:488:TYR:CD1	1:A:521:ARG:HG2	2.37	0.60
1:A:140:LEU:HD23	1:A:140:LEU:O	2.02	0.60
1:A:527:PHE:HB2	1:A:531:GLN:O	2.01	0.60
1:A:205:GLY:HA3	1:A:530:PHE:HZ	1.67	0.59
1:A:267:SER:HB2	1:A:285:ARG:CB	2.31	0.59
1:A:140:LEU:HA	2:B:76:GLN:HG3	1.84	0.59
1:A:213:GLY:HA2	1:A:216:LEU:HD23	1.84	0.59
1:A:145:ILE:HG13	1:A:179:TRP:CE2	2.37	0.59
1:A:305:GLY:O	1:A:330:ARG:NH2	2.35	0.59
2:B:66:VAL:HG23	2:B:67:TRP:N	2.18	0.59
1:A:161:LEU:CD1	1:A:183:THR:HG22	2.31	0.59
1:A:167:LYS:O	1:A:168:SER:HB2	2.02	0.59
1:A:359:MET:SD	1:A:398:PHE:CZ	2.94	0.59
2:B:53:ILE:O	2:B:57:THR:HG23	2.02	0.59
1:A:301:ARG:HG3	1:A:303:LEU:HD23	1.85	0.58
1:A:274:GLN:HE22	1:A:315:TYR:HB2	1.67	0.58
2:B:2:PRO:O	2:B:3:SER:HB2	2.03	0.58
1:A:161:LEU:O	1:A:164:LEU:HG	2.02	0.58
1:A:362:THR:CG2	1:A:370:ALA:HB3	2.33	0.58
1:A:329:VAL:HG23	1:A:343:LEU:HD23	1.85	0.58
1:A:435:CYS:O	1:A:445:SER:HA	2.04	0.57
1:A:174:LEU:HD13	2:B:132:VAL:HG11	1.85	0.57
1:A:247:GLU:OE1	1:A:482:ARG:NH1	2.38	0.57
1:A:307:THR:HB	1:A:326:ASP:CB	2.34	0.57
1:A:513:ARG:HH11	1:A:513:ARG:CB	2.15	0.57
1:A:275:TYR:CD2	1:A:276:ASP:N	2.72	0.57
1:A:279:LYS:HG3	1:A:315:TYR:OH	2.04	0.57
1:A:329:VAL:HG22	1:A:343:LEU:HB2	1.87	0.57
1:A:145:ILE:HD11	1:A:179:TRP:CG	2.40	0.57
1:A:252:CYS:O	1:A:513:ARG:NH1	2.38	0.57
1:A:442:LEU:HD23	1:A:478:PHE:CE1	2.40	0.57
1:A:151:ARG:HH11	1:A:151:ARG:HG2	1.66	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:LEU:HD22	1:A:337:GLY:HA3	1.87	0.56
1:A:403:ILE:HG13	1:A:417:THR:HG23	1.88	0.56
1:A:363:CYS:SG	1:A:396:VAL:HB	2.45	0.56
1:A:359:MET:CG	1:A:398:PHE:HZ	2.19	0.56
1:A:143:ASP:OD2	1:A:146:THR:CG2	2.53	0.56
1:A:192:LEU:O	1:A:192:LEU:HG	2.04	0.56
1:A:314:GLN:NE2	1:A:355:PHE:HB3	2.15	0.56
1:A:478:PHE:O	1:A:527:PHE:HZ	1.87	0.56
1:A:228:PRO:HG2	1:A:231:PHE:H	1.71	0.55
2:B:79:LEU:HA	2:B:82:LEU:HD12	1.88	0.55
1:A:431:ARG:HB2	1:A:449:ASP:HB3	1.88	0.55
1:A:301:ARG:HG2	1:A:303:LEU:HD21	1.88	0.55
3:C:32:ASP:HB2	3:C:35:ILE:CG2	2.36	0.55
1:A:138:ILE:O	1:A:141:GLN:HB2	2.06	0.55
1:A:140:LEU:CA	2:B:76:GLN:HG3	2.37	0.55
1:A:202:LEU:HD21	1:A:243:ILE:HG23	1.89	0.55
1:A:431:ARG:NH1	3:C:37:SEP:O3P	2.40	0.55
1:A:210:ARG:HB2	1:A:210:ARG:HH11	1.71	0.55
1:A:203:TRP:CZ3	1:A:239:ILE:HG21	2.42	0.55
1:A:365:LYS:HD3	3:C:36:HIS:CE1	2.42	0.54
1:A:145:ILE:CD1	1:A:179:TRP:HA	2.33	0.54
1:A:275:TYR:HD1	1:A:526:GLN:HG3	1.72	0.54
1:A:276:ASP:HB2	1:A:315:TYR:OH	2.07	0.54
2:B:65:PRO:HB2	2:B:68:ASP:HB2	1.89	0.54
1:A:293:ASP:O	1:A:297:LEU:HA	2.06	0.54
1:A:139:MET:C	1:A:141:GLN:N	2.60	0.54
1:A:186:GLY:O	1:A:187:MET:C	2.46	0.54
1:A:389:HIS:CG	1:A:407:SER:HG	2.27	0.53
2:B:18:VAL:O	2:B:19:GLU:CB	2.56	0.53
1:A:199:THR:O	1:A:204:ARG:NH1	2.39	0.53
1:A:306:HIS:CE1	1:A:324:SER:HB2	2.43	0.53
1:A:303:LEU:HD22	1:A:337:GLY:CA	2.38	0.53
1:A:414:VAL:O	1:A:423:VAL:HG22	2.08	0.53
2:B:109:LYS:HB3	2:B:110:THR:HG23	1.90	0.53
1:A:285:ARG:HA	1:A:309:SER:HB3	1.91	0.52
1:A:274:GLN:NE2	1:A:315:TYR:HB2	2.23	0.52
1:A:284:LEU:CD1	1:A:290:LYS:HE2	2.40	0.52
2:B:133:ARG:O	2:B:136:ASN:HB2	2.09	0.52
2:B:19:GLU:HA	2:B:22:LYS:HB2	1.91	0.52
1:A:135:SER:O	2:B:78:THR:HG22	2.10	0.51
1:A:162:SER:O	1:A:195:ARG:NH1	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:TRP:C	1:A:214:GLN:H	2.11	0.51
2:B:6:LEU:HB3	2:B:39:VAL:HB	1.92	0.51
2:B:66:VAL:CG2	2:B:67:TRP:H	2.23	0.51
1:A:476:ILE:O	1:A:477:ARG:HG2	2.09	0.51
1:A:292:TRP:CZ3	1:A:299:CYS:HB2	2.45	0.51
1:A:347:CYS:O	1:A:348:GLU:HG3	2.10	0.51
1:A:469:HIS:ND1	1:A:487:ALA:HB2	2.26	0.51
1:A:286:ASP:O	1:A:287:ASN:CB	2.58	0.50
1:A:270:VAL:O	1:A:535:SER:HB3	2.11	0.50
2:B:36:MET:O	2:B:37:ASP:O	2.30	0.50
1:A:139:MET:CG	1:A:140:LEU:N	2.75	0.50
1:A:189:TRP:O	1:A:190:LYS:C	2.50	0.50
1:A:197:VAL:HG13	1:A:204:ARG:HA	1.94	0.50
2:B:115:ARG:O	2:B:119:ASN:N	2.44	0.50
1:A:515:LEU:HB3	1:A:544:TRP:CZ3	2.46	0.50
2:B:40:PRO:C	2:B:42:PRO:HD3	2.32	0.50
2:B:102:VAL:O	2:B:106:ILE:HG13	2.11	0.50
1:A:474:ARG:O	1:A:474:ARG:HD3	2.12	0.49
1:A:329:VAL:CG2	1:A:343:LEU:HD23	2.41	0.49
1:A:442:LEU:HB3	1:A:478:PHE:CE1	2.48	0.49
1:A:348:GLU:HB3	1:A:365:LYS:HB3	1.93	0.49
1:A:250:TRP:CH2	1:A:532:ILE:HG13	2.45	0.49
1:A:443:VAL:O	1:A:455:TRP:HD1	1.95	0.49
1:A:513:ARG:HB3	1:A:513:ARG:CZ	2.40	0.49
1:A:353:LEU:HD13	1:A:360:MET:HE1	1.94	0.49
2:B:40:PRO:O	2:B:42:PRO:CD	2.61	0.49
2:B:17:ASP:HB2	2:B:20:ILE:HD12	1.95	0.48
2:B:51:LYS:HG3	2:B:71:PHE:CE2	2.48	0.48
1:A:258:GLN:HB3	1:A:297:LEU:HD11	1.94	0.48
1:A:362:THR:HG22	1:A:370:ALA:HB3	1.94	0.48
1:A:416:ASN:ND2	1:A:418:SER:H	2.06	0.48
1:A:466:LEU:CD2	1:A:510:LEU:HD13	2.44	0.48
1:A:316:ASP:HB2	1:A:355:PHE:CE2	2.44	0.48
1:A:201:SER:CB	1:A:529:GLU:OE2	2.55	0.48
1:A:248:SER:O	1:A:250:TRP:N	2.47	0.48
1:A:190:LYS:HA	1:A:232:TYR:CD2	2.49	0.48
1:A:518:HIS:CE1	1:A:542:LEU:HD12	2.49	0.47
1:A:135:SER:CB	2:B:47:ALA:CB	2.92	0.47
1:A:176:CYS:SG	1:A:179:TRP:CD1	3.07	0.47
2:B:78:THR:HA	2:B:81:GLU:HB2	1.95	0.47
1:A:436:LEU:HA	1:A:444:VAL:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:469:HIS:CE1	1:A:487:ALA:HB2	2.49	0.47
1:A:212:TRP:C	1:A:214:GLN:N	2.68	0.47
1:A:276:ASP:HB3	1:A:279:LYS:O	2.15	0.47
1:A:301:ARG:CG	1:A:303:LEU:CD2	2.93	0.47
1:A:355:PHE:O	1:A:359:MET:O	2.33	0.47
1:A:173:GLU:O	1:A:180:TYR:HD2	1.97	0.47
1:A:289:ILE:HD11	1:A:332:TRP:CE2	2.50	0.46
1:A:301:ARG:HH11	1:A:301:ARG:HB2	1.80	0.46
1:A:392:ALA:O	1:A:407:SER:HB3	2.14	0.46
1:A:484:VAL:HG12	1:A:525:LEU:CD2	2.45	0.46
1:A:143:ASP:OD2	1:A:146:THR:HG21	2.15	0.46
1:A:320:ILE:N	1:A:332:TRP:O	2.48	0.46
1:A:139:MET:CG	1:A:141:GLN:H	2.27	0.46
1:A:401:LYS:C	1:A:417:THR:OG1	2.54	0.46
1:A:139:MET:CB	1:A:141:GLN:H	2.29	0.46
1:A:301:ARG:HG2	1:A:303:LEU:CD2	2.46	0.46
1:A:449:ASP:O	1:A:450:ASN:HB2	2.15	0.46
2:B:70:GLU:H	2:B:70:GLU:HG3	1.42	0.46
1:A:324:SER:HB3	1:A:326:ASP:OD1	2.16	0.46
1:A:359:MET:HG3	1:A:398:PHE:CZ	2.51	0.46
2:B:93:GLY:O	2:B:96:ASP:N	2.49	0.46
1:A:357:ASN:HB3	1:A:358:GLY:H	1.60	0.46
1:A:526:GLN:NE2	1:A:527:PHE:O	2.49	0.46
2:B:21:ALA:C	2:B:23:GLN:H	2.19	0.45
1:A:140:LEU:O	2:B:76:GLN:HG3	2.16	0.45
1:A:260:ILE:O	1:A:540:THR:HA	2.16	0.45
1:A:362:THR:HG22	1:A:372:TRP:HE1	1.81	0.45
1:A:419:THR:HB	1:A:421:GLU:HG2	1.98	0.45
1:A:389:HIS:ND1	1:A:407:SER:OG	2.47	0.45
1:A:145:ILE:HG13	1:A:179:TRP:NE1	2.31	0.45
1:A:209:ARG:O	1:A:210:ARG:C	2.55	0.45
1:A:355:PHE:O	1:A:356:ASN:O	2.35	0.45
1:A:249:ASN:HD22	1:A:249:ASN:C	2.19	0.45
1:A:439:ARG:HH21	1:A:479:ASP:HA	1.82	0.45
2:B:110:THR:HA	2:B:111:PRO:HD3	1.89	0.44
2:B:4:ILE:HG13	2:B:5:LYS:N	2.33	0.44
1:A:140:LEU:O	1:A:141:GLN:C	2.55	0.44
1:A:216:LEU:HB3	1:A:217:PHE:HD1	1.77	0.44
1:A:301:ARG:HB2	1:A:301:ARG:NH1	2.33	0.44
1:A:145:ILE:CG1	1:A:179:TRP:CE2	3.00	0.44
1:A:206:LEU:HD22	1:A:242:ASP:OD2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:119:ASN:C	2:B:120:ILE:HG13	2.37	0.44
1:A:331:VAL:HB	1:A:341:ASN:H	1.83	0.43
3:C:32:ASP:CB	3:C:34:GLY:H	2.31	0.43
1:A:306:HIS:CD2	1:A:330:ARG:HE	2.36	0.43
1:A:452:ILE:HB	1:A:466:LEU:HB2	2.00	0.43
1:A:533:VAL:HG23	1:A:533:VAL:O	2.19	0.43
1:A:275:TYR:OH	1:A:531:GLN:OE1	2.26	0.43
1:A:311:LEU:HD22	3:C:34:GLY:CA	2.49	0.43
2:B:51:LYS:O	2:B:71:PHE:HZ	2.01	0.43
2:B:97:VAL:HA	2:B:100:LYS:HD2	2.00	0.43
1:A:410:ARG:HG2	1:A:431:ARG:C	2.39	0.43
1:A:440:ASP:HB2	1:A:441:ARG:H	1.60	0.43
2:B:112:GLU:OE2	2:B:112:GLU:N	2.51	0.43
1:A:275:TYR:HE2	1:A:294:LYS:NZ	2.15	0.42
1:A:454:LEU:HD13	1:A:464:ARG:HG3	2.01	0.42
1:A:139:MET:HG3	1:A:140:LEU:N	2.33	0.42
1:A:151:ARG:CG	1:A:151:ARG:NH1	2.54	0.42
1:A:329:VAL:CG2	1:A:343:LEU:HB2	2.48	0.42
2:B:80:PHE:O	2:B:83:ILE:HB	2.20	0.42
1:A:441:ARG:CZ	1:A:441:ARG:HB3	2.49	0.42
1:A:228:PRO:O	1:A:229:ASN:HB3	2.20	0.42
2:B:51:LYS:O	2:B:71:PHE:CZ	2.73	0.42
1:A:236:TYR:N	1:A:237:PRO:HD2	2.35	0.42
1:A:260:ILE:HD11	1:A:297:LEU:HD22	2.01	0.42
1:A:308:GLY:HA3	1:A:325:SER:HB2	2.02	0.42
1:A:412:ILE:HB	1:A:426:LEU:HB2	2.00	0.42
1:A:276:ASP:HB3	1:A:279:LYS:H	1.85	0.42
2:B:34:LEU:HB3	2:B:36:MET:HG3	2.00	0.42
2:B:13:ILE:HD12	2:B:13:ILE:H	1.85	0.42
1:A:139:MET:HG3	1:A:141:GLN:CA	2.48	0.41
1:A:294:LYS:O	1:A:294:LYS:CD	2.67	0.41
1:A:301:ARG:CG	1:A:303:LEU:HD23	2.50	0.41
1:A:249:ASN:HD21	1:A:254:ARG:HD2	1.85	0.41
1:A:412:ILE:CG2	1:A:436:LEU:HD11	2.50	0.41
2:B:53:ILE:H	2:B:53:ILE:HG12	1.72	0.41
2:B:58:HIS:O	2:B:58:HIS:CG	2.73	0.41
1:A:173:GLU:OE2	1:A:233:ARG:NH1	2.52	0.41
1:A:246:ILE:HG22	1:A:247:GLU:N	2.35	0.41
1:A:246:ILE:O	1:A:248:SER:N	2.54	0.41
1:A:286:ASP:OD1	1:A:286:ASP:C	2.59	0.41
1:A:366:ASP:C	1:A:366:ASP:OD1	2.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:412:ILE:HG23	1:A:436:LEU:HD11	2.02	0.41
2:B:41:LEU:HB3	2:B:44:VAL:HG22	2.02	0.41
2:B:66:VAL:CG2	2:B:67:TRP:N	2.83	0.41
1:A:281:VAL:HB	1:A:315:TYR:HE1	1.85	0.41
2:B:49:LEU:HD23	2:B:49:LEU:HA	1.93	0.41
1:A:248:SER:C	1:A:250:TRP:H	2.24	0.41
1:A:320:ILE:HB	1:A:332:TRP:HB2	2.03	0.41
1:A:359:MET:CG	1:A:398:PHE:CZ	3.01	0.41
2:B:118:PHE:O	2:B:119:ASN:HB2	2.20	0.41
1:A:273:LEU:HD11	1:A:533:VAL:HG23	2.03	0.41
1:A:404:VAL:CG2	1:A:436:LEU:HD12	2.49	0.41
1:A:348:GLU:HB2	1:A:366:ASP:HB3	2.02	0.40
1:A:466:LEU:HD21	1:A:510:LEU:HD13	2.03	0.40
1:A:466:LEU:HD23	1:A:466:LEU:HA	1.93	0.40
2:B:27:ILE:HD13	2:B:39:VAL:HG11	2.03	0.40
1:A:139:MET:SD	1:A:140:LEU:HB3	2.61	0.40
1:A:484:VAL:HG12	1:A:525:LEU:HD21	2.03	0.40
2:B:75:ASP:O	2:B:76:GLN:C	2.59	0.40
1:A:374:MET:HA	1:A:380:ILE:HA	2.03	0.40
1:A:474:ARG:NE	3:C:32:ASP:OD2	2.55	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	398/435 (92%)	306 (77%)	56 (14%)	36 (9%)	1	3
2	B	127/145 (88%)	87 (68%)	25 (20%)	15 (12%)	0	1
3	C	7/26 (27%)	5 (71%)	1 (14%)	1 (14%)	0	1
All	All	532/606 (88%)	398 (75%)	82 (15%)	52 (10%)	0	2

All (52) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	257	LEU
1	A	265	GLU
1	A	266	THR
1	A	315	TYR
1	A	345	HIS
1	A	356	ASN
1	A	478	PHE
1	A	479	ASP
1	A	537	HIS
2	B	3	SER
2	B	37	ASP
2	B	41	LEU
2	B	45	ASN
2	B	85	ALA
2	B	109	LYS
1	A	168	SER
1	A	201	SER
1	A	210	ARG
1	A	211	GLY
1	A	212	TRP
1	A	229	ASN
1	A	318	ARG
1	A	344	ILE
1	A	440	ASP
1	A	513	ARG
1	A	539	ASP
2	B	22	LYS
2	B	58	HIS
2	B	76	GLN
2	B	110	THR
2	B	119	ASN
1	A	200	ASP
1	A	249	ASN
1	A	287	ASN
1	A	388	GLY
1	A	538	ASP
2	B	19	GLU
1	A	138	ILE
1	A	141	GLN
1	A	247	GLU
1	A	268	LYS
2	B	90	ASP

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Mol	Chain	Res	Type
3	C	39	ALA
1	A	228	PRO
1	A	246	ILE
1	A	256	SER
1	A	258	GLN
1	A	336	THR
1	A	380	ILE
1	A	400	ASP
2	B	120	ILE
2	B	77	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	353/384 (92%)	292 (83%)	61 (17%)	2 8
2	B	118/133 (89%)	93 (79%)	25 (21%)	1 4
3	C	5/18 (28%)	3 (60%)	2 (40%)	0 0
All	All	476/535 (89%)	388 (82%)	88 (18%)	1 7

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	140	LEU
1	A	145	ILE
1	A	146	THR
1	A	151	ARG
1	A	156	ILE
1	A	168	SER
1	A	184	SER
1	A	188	LEU
1	A	199	THR
1	A	204	ARG
1	A	209	ARG
1	A	216	LEU

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Mol	Chain	Res	Type
1	A	242	ASP
1	A	249	ASN
1	A	252	CYS
1	A	259	ARG
1	A	262	CYS
1	A	264	SER
1	A	267	SER
1	A	273	LEU
1	A	274	GLN
1	A	275	TYR
1	A	277	ASP
1	A	278	GLN
1	A	279	LYS
1	A	289	ILE
1	A	293	ASP
1	A	300	LYS
1	A	301	ARG
1	A	306	HIS
1	A	313	LEU
1	A	314	GLN
1	A	315	TYR
1	A	318	ARG
1	A	341	ASN
1	A	342	THR
1	A	343	LEU
1	A	373	ASP
1	A	379	ASP
1	A	396	VAL
1	A	399	ASP
1	A	416	ASN
1	A	417	THR
1	A	419	THR
1	A	421	GLU
1	A	422	PHE
1	A	425	THR
1	A	440	ASP
1	A	441	ARG
1	A	443	VAL
1	A	472	LEU
1	A	474	ARG
1	A	479	ASP
1	A	481	LYS

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Mol	Chain	Res	Type
1	A	488	TYR
1	A	502	ASP
1	A	513	ARG
1	A	514	THR
1	A	519	SER
1	A	530	PHE
1	A	545	ASP
2	B	6	LEU
2	B	13	ILE
2	B	16	VAL
2	B	17	ASP
2	B	18	VAL
2	B	22	LYS
2	B	25	VAL
2	B	32	GLU
2	B	49	LEU
2	B	51	LYS
2	B	52	VAL
2	B	53	ILE
2	B	54	GLN
2	B	68	ASP
2	B	70	GLU
2	B	76	GLN
2	B	84	LEU
2	B	91	ILE
2	B	92	LYS
2	B	94	LEU
2	B	112	GLU
2	B	119	ASN
2	B	129	GLU
2	B	131	GLN
2	B	135	GLU
3	C	35	ILE
3	C	40	THR

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

Mol	Chain	Res	Type
1	A	249	ASN
1	A	274	GLN
1	A	287	ASN
1	A	306	HIS

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Mol	Chain	Res	Type
1	A	314	GLN
1	A	341	ASN
1	A	416	ASN
1	A	526	GLN
2	B	54	GLN
2	B	119	ASN
3	C	36	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	SEP	C	33	3	8,9,10	1.70	1 (12%)	8,12,14	1.96	4 (50%)
3	SEP	C	37	3	8,9,10	1.47	1 (12%)	8,12,14	1.55	1 (12%)

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	SEP	C	33	3	-	1/5/8/10	-
3	SEP	C	37	3	-	5/5/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	33	SEP	P-O1P	3.28	1.61	1.50
3	C	37	SEP	P-O1P	2.91	1.59	1.50

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	37	SEP	O2P-P-OG	3.47	115.97	106.73
3	C	33	SEP	OG-CB-CA	-2.91	105.32	108.14
3	C	33	SEP	OG-P-O1P	-2.72	98.85	106.47
3	C	33	SEP	P-OG-CB	-2.65	111.01	118.30
3	C	33	SEP	O3P-P-OG	2.12	112.36	106.73

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	37	SEP	CB-OG-P-O1P
3	C	37	SEP	CB-OG-P-O2P
3	C	37	SEP	CB-OG-P-O3P
3	C	33	SEP	CB-OG-P-O1P
3	C	37	SEP	N-CA-CB-OG
3	C	37	SEP	CA-CB-OG-P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	37	SEP	1	0

5.5 Carbohydrates (i)

There are no monosaccharides 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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.