wwPDB X-ray Structure Validation Summary Report (i)

Oct 16, 2021 – 10:42 PM EDT

PDB ID	:	1NEX
Title	:	Crystal Structure of ScSkp1-ScCdc4-CPD peptide complex
Authors	:	Orlicky, S.; Tang, X.; Willems, A.; Tyers, M.; Sicheri, F.
Deposited on	:	2002-12-12
Resolution	:	2.70 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:

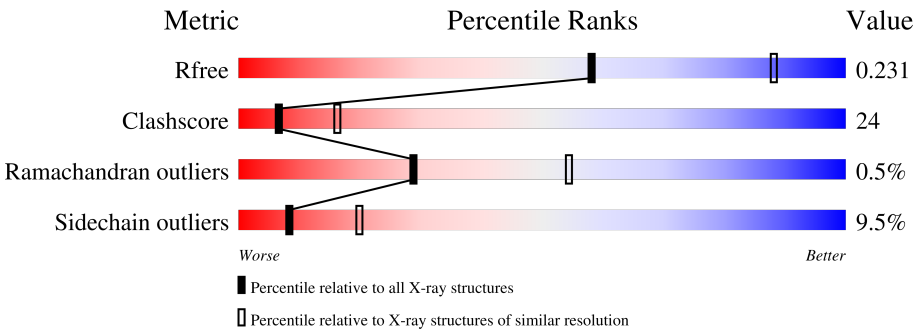
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 2.70 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}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)

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%

Mol	Chain	Length	Quality of chain
1	A	169	42% 28% 6% 24%
1	C	169	41% 30% 7% 23%
2	B	464	53% 37% 6% •
2	D	464	56% 34% 5% •
3	E	9	22% 11% 11% 56%
3	F	9	56% 22% 11% 11%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 9435 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 Centromere DNA-binding protein complex CBF3 subunit D.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	129	1047	666	182	195	1	3	0	0	0
1	C	130	1058	672	186	196	1	3	0	0	0

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	cloning artifact	UNP P52286
A	-1	ALA	-	cloning artifact	UNP P52286
A	0	HIS	-	cloning artifact	UNP P52286
A	1	MSE	MET	modified residue	UNP P52286
A	36	MSE	MET	modified residue	UNP P52286
A	?	-	HIS	deletion	UNP P52286
A	?	-	ASP	deletion	UNP P52286
A	?	-	SER	deletion	UNP P52286
A	?	-	ASN	deletion	UNP P52286
A	?	-	LEU	deletion	UNP P52286
A	?	-	GLN	deletion	UNP P52286
A	?	-	ASN	deletion	UNP P52286
A	?	-	ASN	deletion	UNP P52286
A	?	-	SER	deletion	UNP P52286
A	?	-	ASP	deletion	UNP P52286
A	?	-	SER	deletion	UNP P52286
A	?	-	GLU	deletion	UNP P52286
A	?	-	SER	deletion	UNP P52286
A	?	-	ASP	deletion	UNP P52286
A	?	-	SER	deletion	UNP P52286
A	?	-	ASP	deletion	UNP P52286
A	?	-	SER	deletion	UNP P52286
A	?	-	GLU	deletion	UNP P52286
A	?	-	THR	deletion	UNP P52286
A	?	-	ASN	deletion	UNP P52286

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	HIS	deletion	UNP P52286
A	?	-	LYS	deletion	UNP P52286
A	?	-	SER	deletion	UNP P52286
A	?	-	LYS	deletion	UNP P52286
A	?	-	ASP	deletion	UNP P52286
A	?	-	ASN	deletion	UNP P52286
A	?	-	ASN	deletion	UNP P52286
A	?	-	ASN	deletion	UNP P52286
A	77	MSE	MET	modified residue	UNP P52286
A	130	MSE	MET	modified residue	UNP P52286
A	157	MSE	MET	modified residue	UNP P52286
C	-2	GLY	-	cloning artifact	UNP P52286
C	-1	ALA	-	cloning artifact	UNP P52286
C	0	HIS	-	cloning artifact	UNP P52286
C	1	MSE	MET	modified residue	UNP P52286
C	36	MSE	MET	modified residue	UNP P52286
C	?	-	HIS	deletion	UNP P52286
C	?	-	ASP	deletion	UNP P52286
C	?	-	SER	deletion	UNP P52286
C	?	-	ASN	deletion	UNP P52286
C	?	-	LEU	deletion	UNP P52286
C	?	-	GLN	deletion	UNP P52286
C	?	-	ASN	deletion	UNP P52286
C	?	-	ASN	deletion	UNP P52286
C	?	-	SER	deletion	UNP P52286
C	?	-	ASP	deletion	UNP P52286
C	?	-	SER	deletion	UNP P52286
C	?	-	GLU	deletion	UNP P52286
C	?	-	SER	deletion	UNP P52286
C	?	-	ASP	deletion	UNP P52286
C	?	-	SER	deletion	UNP P52286
C	?	-	ASP	deletion	UNP P52286
C	?	-	SER	deletion	UNP P52286
C	?	-	GLU	deletion	UNP P52286
C	?	-	THR	deletion	UNP P52286
C	?	-	ASN	deletion	UNP P52286
C	?	-	HIS	deletion	UNP P52286
C	?	-	LYS	deletion	UNP P52286
C	?	-	SER	deletion	UNP P52286
C	?	-	LYS	deletion	UNP P52286
C	?	-	ASP	deletion	UNP P52286
C	?	-	ASN	deletion	UNP P52286

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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	ASN	deletion	UNP P52286
C	?	-	ASN	deletion	UNP P52286
C	77	MSE	MET	modified residue	UNP P52286
C	130	MSE	MET	modified residue	UNP P52286
C	157	MSE	MET	modified residue	UNP P52286

- Molecule 2 is a protein called CDC4 protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
2	B	444	3582	2296	618	656	6	6	0	0	0
			Total	C	N	O	S	Se			
2	D	444	3582	2296	618	656	6	6	0	0	0

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	261	GLY	-	cloning artifact	UNP P07834
B	262	ALA	-	cloning artifact	UNP P07834
B	381	MSE	MET	modified residue	UNP P07834
B	403	MSE	MET	modified residue	UNP P07834
B	530	MSE	MET	modified residue	UNP P07834
B	560	MSE	MET	modified residue	UNP P07834
B	590	MSE	MET	modified residue	UNP P07834
B	?	-	ASN	deletion	UNP P07834
B	?	-	ILE	deletion	UNP P07834
B	?	-	TRP	deletion	UNP P07834
B	?	-	ASN	deletion	UNP P07834
B	608	LEU	CYS	engineered mutation	UNP P07834
B	?	-	SER	deletion	UNP P07834
B	?	-	TYR	deletion	UNP P07834
B	?	-	ALA	deletion	UNP P07834
B	?	-	THR	deletion	UNP P07834
B	?	-	ASN	deletion	UNP P07834
B	?	-	SER	deletion	UNP P07834
B	?	-	ALA	deletion	UNP P07834
B	?	-	SER	deletion	UNP P07834
B	?	-	PRO	deletion	UNP P07834
B	?	-	CYS	deletion	UNP P07834
B	?	-	ALA	deletion	UNP P07834
B	?	-	LYS	deletion	UNP P07834
B	?	-	ILE	deletion	UNP P07834

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	GLY	deletion	UNP P07834
B	?	-	ALA	deletion	UNP P07834
B	625	MSE	MET	modified residue	UNP P07834
D	261	GLY	-	cloning artifact	UNP P07834
D	262	ALA	-	cloning artifact	UNP P07834
D	381	MSE	MET	modified residue	UNP P07834
D	403	MSE	MET	modified residue	UNP P07834
D	530	MSE	MET	modified residue	UNP P07834
D	560	MSE	MET	modified residue	UNP P07834
D	590	MSE	MET	modified residue	UNP P07834
D	?	-	ASN	deletion	UNP P07834
D	?	-	ILE	deletion	UNP P07834
D	?	-	TRP	deletion	UNP P07834
D	?	-	ASN	deletion	UNP P07834
D	608	LEU	CYS	engineered mutation	UNP P07834
D	?	-	SER	deletion	UNP P07834
D	?	-	TYR	deletion	UNP P07834
D	?	-	ALA	deletion	UNP P07834
D	?	-	THR	deletion	UNP P07834
D	?	-	ASN	deletion	UNP P07834
D	?	-	SER	deletion	UNP P07834
D	?	-	ALA	deletion	UNP P07834
D	?	-	SER	deletion	UNP P07834
D	?	-	PRO	deletion	UNP P07834
D	?	-	CYS	deletion	UNP P07834
D	?	-	ALA	deletion	UNP P07834
D	?	-	LYS	deletion	UNP P07834
D	?	-	ILE	deletion	UNP P07834
D	?	-	GLY	deletion	UNP P07834
D	?	-	ALA	deletion	UNP P07834
D	625	MSE	MET	modified residue	UNP P07834

- Molecule 3 is a protein called GLL(TPO)PPQSG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	E	4	33	20	4	8	1	0	0	0
			Total	C	N	O	P			
3	F	8	61	36	9	15	1	0	0	0

- Molecule 4 is water.

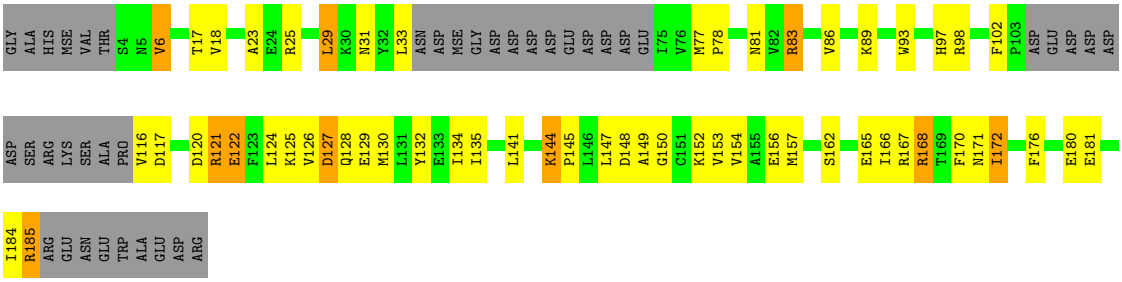
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	9	9	9	0	0
			Total	O		
4	B	25	25	25	0	0
			Total	O		
4	C	9	9	9	0	0
			Total	O		
4	D	27	27	27	0	0
			Total	O		
4	E	2	2	2	0	0

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.

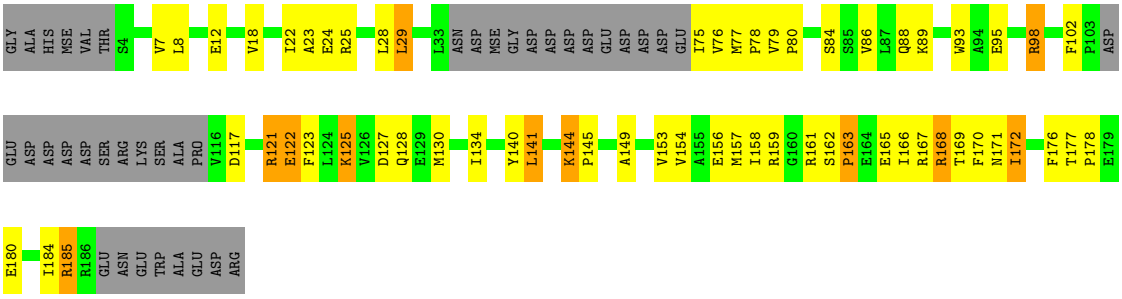
- Molecule 1: Centromere DNA-binding protein complex CBF3 subunit D

Chain A: 42% 28% 6% 24%



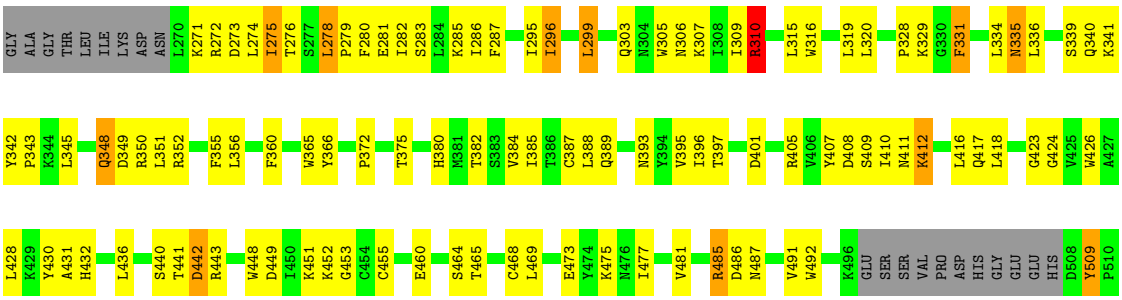
- Molecule 1: Centromere DNA-binding protein complex CBF3 subunit D

Chain C: 41% 30% 7% 23%



- Molecule 2: CDC4 protein

Chain B: 53% 37% 6% •



L511 V512 F513 H514 T515 P516 E517 E518 N519 P520 Y521 V525 L526 R527 R534 T535 V536 G540 V543 S547 Y548 D549 N550 T551 L552 I553 V554 W555 Q559 M560 K561 C562 L563 Y564 H569 I573 R582 K583 S587 A588 S589 M590 D591 T592 T593 I594 R595 D598

N605 G606 E607 L628 Q629 G630 L634 V635 G636 L637 L638 R639 L640 S641 D642 K643 F644 L645 A648 S653 I654 R655 G656 W657 N660 S663 H669 H670 T671 N672 L673 I676 F679 Y680 V681 S682 D683 N684 I685 L686 V687 S688 G689 S690 Q693 F694 N695 I696 Y697 N698

L699 L704 A707 N708 I709 L710 K711 D712 W717 S718 V719 N720 F721 K724 T725 L726 A729 K732 I740 F743 S744

- Molecule 2: CDC4 protein

Chain D: 56% 34% 5% •

GLY ALA GLY THR LEU ILE LYS ASP ASN L270 K271 R272 D273 L274 I275 T276 S277 L278 P279 F280 E281 I282 I286 F287 E293 D294 I295 I296 N297 S298 L299 Q303 M304 W305 N306 I309 R310 L315 W316 K317 F331 N335 L336 Q340 K344 L345 S346 D349 R350

F355 L356 I359 F360 I361 L362 W365 Y366 N367 P368 K369 F370 H380 M381 T382 I385 T386 C387 L388 Q389 F390 E391 D392 N393 T397 G398 A399 D400 D401 K402 M403 I404 R405 D408 S409 I410 N411 K412 L416 Q417 L418 G423 G424 V425 W426 A427 L428 K429 Y430 L436 V437

S438 G439 S440 T441 D442 R443 D449 I450 K451 K452 E460 S464 T465 C468 L469 V481 T482 R485 D486 N487 T488 L489 H490 V491 W492 K493 L494 P495 K496 GLU SER SER VAL PRO ASP HIS GLY GLU GLU HIS D508 Y509 P510 L511 H514 T515 P516 N519 P520 Y521 V525

L526 R527 G528 R534 T535 V536 V543 V544 S545 D549 N550 T551 L552 I553 V554 Q559 M560 K561 Y564 I565 L566 S567 G568 H569 I573 K583 S587 M590 D591 T592 T593 I594 R595 I596 W597 D598 L599 E600 N605 G606 E607 L608 M625 Y626 T627 L628 Q629 G630 L634 V635

G636 L637 L640 S641 D642 K643 F644 L645 A648 S653 I654 R655 G656 W657 D658 Y662 H669 H670 T671 N672 V681 I685 L686 V687 S688 G689 S690 Q693 F694 N695 L699 L704 A707 N708 I709 L710 K711 D712 A713 D714 Q715 I716 W717 F721 K724 T725 L726

A729 K732 S744

- Molecule 3: GLL(TPO)PPQSG

Chain E: 22% 11% 11% 56%

GLY LEU L3 T4 P5 P6 GLN SER GLY

- Molecule 3: GLL(TPO)PPQSG

Chain F: 56% 22% 11% 11%

GLY L2 L3 T4 P5 P6 Q7 S8 G9

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	107.67Å 107.67Å 168.30Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.99 – 2.70 19.99 – 2.70	Depositor EDS
% Data completeness (in resolution range)	95.7 (19.99-2.70) 98.2 (19.99-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.33 (at 2.71Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.239 , 0.273 0.233 , 0.231	Depositor DCC
R_{free} test set	9884 reflections (8.51%)	wwPDB-VP
Wilson B-factor (Å^2)	41.6	Xtriage
Anisotropy	0.034	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 18.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.23$	Xtriage
Estimated twinning fraction	0.244 for -h,-k,l 0.085 for h,-h-k,-l 0.078 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	9435	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.70% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.46	0/1061	0.65	0/1428
1	C	0.46	0/1072	0.63	0/1442
2	B	0.45	0/3657	0.69	3/4939 (0.1%)
2	D	0.45	0/3657	0.70	3/4939 (0.1%)
3	E	0.47	0/22	0.81	0/28
3	F	0.47	0/50	0.73	0/64
All	All	0.45	0/9519	0.68	6/12840 (0.0%)

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	310	ARG	NE-CZ-NH1	7.12	123.86	120.30
2	B	310	ARG	NE-CZ-NH1	6.22	123.41	120.30
2	D	275	ILE	CG1-CB-CG2	5.58	123.67	111.40
2	B	310	ARG	NE-CZ-NH2	-5.58	117.51	120.30
2	B	645	LEU	N-CA-C	-5.36	96.53	111.00

There are no chirality outliers.

There are no planarity outliers.

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	1047	0	1055	60	0
1	C	1058	0	1068	65	0
2	B	3582	0	3581	181	0
2	D	3582	0	3581	157	0
3	E	33	0	29	5	0
3	F	61	0	56	6	0
4	A	9	0	0	3	0
4	B	25	0	0	5	0
4	C	9	0	0	1	0
4	D	27	0	0	1	0
4	E	2	0	0	0	0
All	All	9435	0	9370	442	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 24.

The worst 5 of 442 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:167:ARG:HG2	1:A:172:ILE:HG22	1.30	1.12
2:D:491:VAL:HB	2:D:560:MSE:HE1	1.34	1.07
2:D:275:ILE:HG21	2:D:305:TRP:NE1	1.72	1.04
2:D:270:LEU:HD23	2:D:271:LYS:H	1.24	1.03
1:C:171:ASN:HD22	2:D:271:LYS:HD2	1.19	1.02

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	123/169 (73%)	114 (93%)	9 (7%)	0	100 100
1	C	124/169 (73%)	115 (93%)	8 (6%)	1 (1%)	19 43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	440/464 (95%)	406 (92%)	31 (7%)	3 (1%)	22	46
2	D	440/464 (95%)	423 (96%)	15 (3%)	2 (0%)	29	54
3	E	1/9 (11%)	1 (100%)	0	0	100	100
3	F	5/9 (56%)	3 (60%)	2 (40%)	0	100	100
All	All	1133/1284 (88%)	1062 (94%)	65 (6%)	6 (0%)	29	54

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	605	ASN
2	D	605	ASN
2	B	673	LEU
2	B	331	PHE
1	C	24	GLU

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	117/147 (80%)	103 (88%)	14 (12%)	5	11
1	C	118/147 (80%)	105 (89%)	13 (11%)	6	14
2	B	400/410 (98%)	367 (92%)	33 (8%)	11	25
2	D	400/410 (98%)	361 (90%)	39 (10%)	8	18
3	E	3/6 (50%)	3 (100%)	0	100	100
3	F	6/6 (100%)	6 (100%)	0	100	100
All	All	1044/1126 (93%)	945 (90%)	99 (10%)	8	20

5 of 99 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	168	ARG
2	D	349	ASP

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Mol	Chain	Res	Type
1	C	185	ARG
2	D	295	ILE
2	D	442	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	457	HIS
2	D	693	GLN
2	D	463	ASN
2	D	569	HIS
2	B	569	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	TPO	F	4	3	8,10,11	1.94	2 (25%)	10,14,16	0.85	0
3	TPO	E	4	3	8,10,11	2.21	3 (37%)	10,14,16	0.77	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	TPO	F	4	3	-	2/9/11/13	-
3	TPO	E	4	3	-	2/9/11/13	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	4	TPO	P-OG1	3.99	1.66	1.59
3	E	4	TPO	O-C	3.49	1.33	1.19
3	F	4	TPO	O-C	3.38	1.33	1.19
3	F	4	TPO	P-OG1	3.27	1.65	1.59
3	E	4	TPO	P-O1P	2.25	1.57	1.50

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	4	TPO	O-C-CA-CB
3	E	4	TPO	CG2-CB-OG1-P
3	F	4	TPO	O-C-CA-CB
3	F	4	TPO	CG2-CB-OG1-P

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	4	TPO	1	0
3	E	4	TPO	3	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 (i)

6.1 Protein, DNA and RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.